

Annex I

Appendices to the Agenda of the Eighteenth General Assembly

1. Appendix A: Report of the Executive Committee

1.1. Executive Committee and Finance Committee meetings

The Executive Committee met in Seattle in August 1996 before and during the General Assembly, in Lisbon, Portugal, in August 1997 at the time of the Seventeenth European Crystallographic Meeting and in Arlington, USA, in July 1998 at the time of the American Crystallographic Association annual meeting. The Finance Committee met in March 1996, August 1996, March 1997, August 1997, March 1998 and July 1998, 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.* Section C and the *Journal of Applied Crystallography*, approval of appointments of Co-editors, electronic publishing, Special Issues, format of offprints, and other matters concerning the IUCr journals;
- (2) appointment of a Promotions Representative;
- (3) approval of the audited accounts for the previous year;
- (4) the General Fund estimates and the level of the unit contribution;
- (5) investment policy;
- (6) funding and uses of the Publications and Journals Development Fund and the Research and Education Fund;
- (7) sponsorship and financial support for meetings, including young scientists' support;
- (8) cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and the Fachinformationszentrum Karlsruhe;
- (9) progress with Volumes A, A1 (formerly H), B, C, D, E, F and G of *International Tables* and development of associated software, consideration of suggestions for new volumes;
- (10) the *IUCr Newsletter*, the Tenth Edition of the *World Directory of Crystallographers*;
- (11) fiftieth anniversary of the IUCr;
- (12) appointment of the Selection Committee for the fifth Ewald Prize;
- (13) discussion of the arrangements for the Glasgow General Assembly and Congress;
- (14) approval of the membership of the Programme Committee for the Glasgow Congress;
- (15) level of financial support for the Glasgow Congress;
- (16) importance of crystallography;
- (17) nominations for Officers of the IUCr and for Chairs and members of Commissions, and proposals from the National Committees for these positions.

Other items dealt with in this way were:

- (18) consideration of a proposal to establish an Inter-Union Bioinformatics Group;
- (19) the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* and other uses of CIF, patent 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;

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

(21) charges for visas;

(22) crystallography in Africa;

(23) use of financial support through ICSU;

(24) access to large-scale research facilities;

(25) review of the activities of Commissions;

(26) review of the activities of Regional Associates;

(27) review of the reports of IUCr Representatives on other bodies.

Items concerning the Chester office were:

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

(29) upgrading of office technology in the IUCr office in Chester, provision of Internet services, domain site name, formation of an IUCr web editorial board, and establishment of mirror sites.

1.2. Publications

The subscription prices (in Danish Kroner) 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 1996, 1997 and 1998 were:

	1996	1997	1998
<i>Acta Crystallographica Section A</i>	1,010	863	1,049
<i>Acta Crystallographica Section B</i>	1,078	1,045	943
<i>Acta Crystallographica Section C</i>	3,262	2,004	2,026
<i>Acta Crystallographica Section D</i>	1,246	821	1,500
<i>Journal of Applied Crystallography</i>	759	1,191	988
<i>Journal of Synchrotron Radiation</i>	326	405	1,431
Total	7,681	6,329	7,937

In addition, in 1996 *Acta Cryst.* Section A included a Supplement of 688 pages of abstracts communicated to the Seattle Congress.

The November 1998 issue (Part 6, Number 1) of *Acta Cryst.* Section A was a celebration of 50 years of *Acta Crystallographica* and the IUCr, edited by H. Schenk. It contained 269 pages of 26 invited papers presenting state-of-the-art research from sciences in which crystallography has played a major role. The first paper was 'Aspects of the History of the International Union of Crystallography' by D. W. J. Cruickshank. This issue of *Acta Cryst.* was also published as a book entitled *Crystallography Across the Sciences*.

The October 1997 issue (Part 5, Number 2) of *JAC* contained 320 pages of papers presented at the Tenth International Conference on Small-Angle Scattering, Campinas, Brazil, 21–26 July 1996. The November 1998 issue (Part 6, Number 1) of *Acta Cryst.* Section D contained 142 pages of 'Databases for Macromolecular Crystallographers', the Proceedings of the CCP4 Study Weekend, Reading, UK, January 1998. The May 1998 issue of *JSR* contained 1,054 pages of papers presented at the Sixth International Conference on

Synchrotron Radiation Instrumentation, SRI '97, Himeji, Japan, 4–8 August 1997.

Submission of papers to *Acta Cryst.* Section C in fully electronic CIF format is complete and automatic data validation software and CIF-access electronic-only publication have been introduced. The other journals are now produced in SGML format ready for on-line publication.

The IUCr home page on the web continues to expand and the main site in Chester, UK, is currently mirrored in France, Israel, 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). The number of requests per day is typically of the order of 10,000.

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 Tenth Edition of the *World Directory of Crystallographers*, edited by Y. Epelboin, was published in 1997. This is held as an electronic database in STAR file format and this also allows the automated typesetting of the *Directory*. The database may be accessed *via* the web.

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

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 G 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. Schenk in this triennium. A list of IUCr-sponsored meetings is given in Appendix J 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: Mr M. H. Dacombe (Executive Secretary), Mrs A. Cawley (Part-time Administrative Assistant to the Executive Secretary), Mrs M. J. Robinson (Part-time Secretary to the Executive Secretary), Mr P. R. Strickland (Managing Editor), Mrs S. E. King (Technical Editor), Mr B. McMahon (Research and Development Officer), Dr A. S. Berry (Assistant Technical Editor), Miss C. A. Moore (Editorial Systems Developer), Dr G. F. Holmes, Mrs L. E. Clark-Jones, Mrs J. K. Bradshaw, Mr S. Conway and Dr N. J. Ashcroft (Senior Editorial Assistants), Dr A. Weight, Dr S. Froggatt, Dr S. Glynn and Miss F. Reid (Editorial Assistants), Dr M. A. Hoyland, Dr D. Holden and Dr D. Hoare (Research and Development Assistants), Mrs L. Rathbone and Mrs C. Cook (Secretaries) and Miss A. J. Sharpe (Promotions Officer).

1.7. Acknowledgements

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the British Crystallographic Association, on behalf of the Royal Society, for the invitation to hold the Eighteenth General Assembly and International Congress of Crystallography in Glasgow. It particularly wishes to thank the Chair of the Programme Committee, Professor J. A. K. Howard, and the Chair of the Organizing Committee, Professor C. Gilmore.

The continuing support shown by UNESCO in the form of its annual subvention received by the IUCr through ICSU, 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 1996 and 1997 have already been published [*Acta Cryst.* (1997), A53, 814–852 and (1999), A55, 585–600]. The accounts for 1998 have been audited and will be published in due course in *Acta Crystallographica* Section A. The accounts for the three years 1996, 1997 and 1998 are summarised in Tables 1–15. All amounts are expressed in Swiss Francs. The notations used in this report for the various currencies of the IUCr's activities are CHF = Swiss Franc, GBP = Pound Sterling, USD = US Dollar, NLG = Netherlands Guilder, DKK = Danish Kroner.

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 increased by CHF 1,691,377 from CHF 5,224,690 to CHF 6,916,067, or 32%, 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 increased by CHF 1,266,115 from CHF 5,968,695 to CHF 7,234,810, or 21%, over the triennium.

Table 2 shows the distribution of the assets. The debtors includes, in part, the IUCr's funding of the Glasgow General Assembly and Congress paid in advance. The great majority of the other amounts under debtors and creditors have since been settled.

The total investments at 31 December 1998 are CHF 6,163,824 at market value, as shown in Table 2, of which 23% is held by Merrill Lynch, 60% by Foreign & Colonial and 17% 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 Seattle 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 1996, 1997 and 1998. The total number of membership units was 152 for each year, while the budget was based on 151 for each year. The yield from investments is less than the budgeted amount by CHF 223,035.

The administration expenses for the journals are calculated as 35% 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 1996, 1997 and 1998. 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 Seattle Congress in 1996, the cost of the 1998 meeting of the Programme Committee for the Glasgow Congress, the expenses of the non-publishing Commissions, financial support to meetings and schools, the expenses of the three IUCr50 symposia held in association with the meetings of the Regional Associates in 1998, and expenses incurred in connection with STAR/CIF and the IUCr/FIZ Agreement. The financial support for young scientists attending meetings and schools is charged to the Research and Education Fund, see Table 13. In Table 4, the unfavourable deviation from budget of

Table 1

Balance Sheet, Fund Accounts (Swiss Francs).

	31 December 1995	Fluctuations in rates of exchange	31 December 1998
General Fund	1,190,554	1,157,293	3,059,757
President's Fund	48,386	745	58,947
<i>Acta Crystallographica</i>	1,544,696	26,724	1,583,252
<i>Journal of Applied Crystallography</i>	342,556	6,659	152,033
<i>Journal of Synchrotron Radiation</i>	71,534	2,132	19,391
<i>Structure Reports</i>	85,979	–	–
<i>International Tables</i>	264,045	3,746	195,270
Book Fund	12,522	1,586	25,600
Publications and Journals			
Development Fund	579,275	12,673	457,847
Research and Education Fund	739,304	15,881	886,870
Ewald Fund	294,098	6,364	419,858
Newsletter Fund	51,741	1,084	57,242
Total accumulated balance	5,224,690	1,234,887	6,916,067

Table 2

Balance sheet, Assets (Swiss Francs).

	31 December 1995	31 December 1998
Current assets		
Stock	–	26,061
Cash at banks		
Current accounts	39,755	19,765
Deposit and savings accounts	325,404	421,499
Cash with Union officials	34,878	30,763
Debtors	194,071	293,490
Subscriptions due	35,978	60,000
	630,086	851,578
<i>Deduct</i> Creditors and accrued charges	–357,182	–229,748
Net current assets	272,904	621,830
Investments at market value	4,882,698	6,163,824
Fixed assets		
Tangible fixed assets	69,088	130,413
Total assets	5,224,690	6,916,067

CHF 334,417 is largely accounted for by a lower than predicted return on investments and an increase in administration costs, most of which are incurred in GBP. The increase in administration costs is attributable to the strong increase (25%) in the value of the GBP against the CHF that occurred during the triennium.

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. The total number of pages printed for AC, JAC and

international union of crystallography

Table 3
General Fund (Swiss Francs).

	1996	1997	1998
Income			
Subscriptions from Adhering Bodies	148,822	151,562	159,692
Yield from investments and bank accounts (including profit/loss on disposal of investments)	178,982	228,431	239,552
17th General Assembly refund	–	7,150	–
Grants from UNESCO/ICSU	22,359	23,200	16,072
Amount charged to other Funds:			
<i>Acta Crystallographica</i>	66,248	60,398	76,634
<i>Journal of Applied Crystallography</i>	7,703	15,508	13,136
<i>Journal of Synchrotron Radiation</i>	3,081	5,713	19,706
	<u>427,195</u>	<u>491,962</u>	<u>524,792</u>
Expenditure			
Administration	220,091	313,338	348,751
Subscriptions to ICSU/ICSU bodies	7,127	8,661	10,598
Executive Committee	75,374	38,219	33,201
Finance Committee	16,508	22,763	21,223
17th General Assembly and Congress expenses	63,028	–	–
18th General Assembly and Congress expenses	–	27,705	72,990
IUCr Representatives on other bodies	3,784	1,958	3,377
STAR/CIF	4,646	22,656	1,943
Expenses of Commissions	28,842	2,945	5,495
Sponsorship of meetings	40,169	10,525	5,475
President's secretarial	14,322	1,206	4,486
IUCr/FIZ Agreement	16,225	–4,569	–7,320
IUCr50 symposia	–	–	22,103
Bad debts – subscriptions	6,000	–6,000	2,000
Programming and development costs	–	12,721	25,600
	<u>496,116</u>	<u>452,128</u>	<u>549,922</u>
<i>Excess of income over expenditure</i>	<u>–68,921</u>	<u>39,834</u>	<u>–25,130</u>
Transfers to other Funds:			
President's Fund	–50,000	–	–20,000
Publications and Journals Development Fund	–100,000	–	–
Research and Education Fund	–	–50,000	–50,000
<i>Newsletter</i> Fund	–	–	–30,000
	<u>–150,000</u>	<u>–50,000</u>	<u>–100,000</u>
Fluctuations in rates of exchange	<u>755,294</u>	<u>707,003</u>	<u>–305,004</u>
Movement in market value	<u>266,072</u>	<u>412,142</u>	<u>387,913</u>
Accumulated balance at end of year	<u>1,992,999</u>	<u>3,101,978</u>	<u>3,059,757</u>

Table 4
General Fund. Comparison of budget and accounts for the years 1996–1998 inclusive (Swiss Francs).

	Budget	Accounts	Difference
Income			
Subscriptions from Adhering Bodies	453,000	460,076	7,076
Yield from investments and bank accounts (including profit/loss on disposal of investments)	870,000	646,965	–223,035
Grants from UNESCO/ICSU	60,000	61,631	1,631
	<u>1,383,000</u>	<u>1,168,672</u>	<u>–214,328</u>
Expenditure			
Administration (net)	541,500	674,388	132,888
Subscriptions to ICSU/ICSU bodies	24,300	26,386	2,086
Administrative meetings	258,000	216,407	–41,593
Scientific meetings	279,000	305,708	26,708
Transfers to other Funds	300,000	300,000	–
	<u>1,402,800</u>	<u>1,522,889</u>	<u>120,089</u>
Unfavourable variant from budget			–334,417
Estimated profit or deficit	<u>–19,800</u>		<u>–19,800</u>
<i>Deficit of income over expenditure</i>		<u>–354,217</u>	<u>–354,217</u>

JSR were 7,681, 6,329 and 7,937 in 1996, 1997 and 1998, respectively. The Finance Committee (FC) and the Executive Committee (EC) have monitored the financial development for all journals very closely. Taking account of the different costs involved in producing

each journal (those with a significant colour content are more expensive to produce), the prices were increased differentially during the triennium, with Section D of AC, JAC and JSR receiving the higher increases. The total number of subscriptions (including full

Table 5
President's Fund (Swiss Francs).

	1996	1997	1998
Income			
Donations, transfers and interest	2,476	2,210	2,216
Expenditure			
Grants	7,125	7,558	2,403
<i>Excess of income over expenditure</i>	-4,649	-5,348	-187
Transfers from other Funds:			
General Fund	-	-	20,000
Fluctuations in rates of exchange	654	301	-210
Accumulated balance at end of year	44,391	39,344	58,947

and reduced-rate) decreased by about 6% for AC and 10% for JAC over the triennium. JSR was launched in 1995, with an inaugural issue in October 1994; it was distributed free of charge in 1995. The numbers of subscribers were 253, 269 and 288 in 1996, 1997 and 1998. The proportion of reduced-rate subscribers to JSR is high (48%) compared to the other journals (typically 15%). For further details see the Triennial Report by the Chairs of the Commission on Journals (Appendix D to the Agenda).

2.5. Structure Reports

The *Structure Reports* accounts are shown in Table 9. This Fund was closed in 1996, when the final volumes were published, and the balance transferred to the Publications and Journals Development Fund.

2.6. International Tables

The *International Tables* accounts are shown in Table 10. The costs of printing and reprinting the various volumes are charged to the appropriate years. Sales of Volume C were low in 1998 when it became out of print (pending the publication of the Second, Revised Edition in 1999). For further details see the Triennial Report by the Chair of the Commission on *International Tables* (Appendix D to the Agenda).

2.7. Book Fund

Table 11 gives the accounts of the Book Fund. The accumulated balance of this fund increased during the triennium. The main activity concerned the publication and sale of the Tenth Edition of the *World Directory of Crystallographers*.

2.8. Publications and Journals Development Fund

Table 12 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, 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 12. During the triennium, the major expenses are related to the purchase of computer hardware and software, programming and development, an electronic publishing project aimed at producing all the journals in SGML format in preparation for on-line publishing, the appointment of a Promotions

Representative and Special Issue costs (see *Journals Funds* above). As the programming and development costs underpin much of the Union's activity, in 1997 the EC decided that these 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.

It is the EC's policy to support and encourage the IUCr's highly qualified staff by supplying them with the best equipment.

2.9. Research and Education Fund

Table 13 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 232,624 was given as young scientists' support during the triennium.

2.10. Ewald Fund

The accounts of the Ewald Fund are given in Table 14. The interest on the capital is intended to cover the costs of the Prize. It is calculated as 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 100,615 has been transferred to the fund during the triennium.

2.11. Newsletter Fund

Table 15 shows the accounts of the Newsletter Fund (NF). The fund was established in 1994 following the successful launch of the *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 66,950 in 1996, CHF 84,574 in 1997 and CHF 74,059 in 1998.

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 recognise 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

Table 6
Acta Crystallographica (Swiss Francs).

	1996	1997	1998
Income			
Subscriptions	1,910,033	2,229,054	2,535,290
Sale of back numbers and single issues	28,369	29,327	13,503
Airfreight charged to subscribers	53,691	52,914	51,687
Profit/loss on offprints	-12,039	-1,313	-27,515
Special issue income	-	-	20,852
Royalties, copyright fees	5,852	8,531	10,441
	<u>1,985,906</u>	<u>2,318,513</u>	<u>2,604,258</u>
Less Publisher's commission	-135,688	-158,087	-178,416
Yield from advertisements	683	1,459	37,946
Recharge to Publications and Journals	-	-	-
Development Fund for Special Issue	-	-	-
	<u>1,850,901</u>	<u>2,161,885</u>	<u>36,428</u>
			<u>2,500,216</u>
Expenditure			
Printing and binding	686,225	559,821	651,293
Distribution and postage	108,129	90,611	121,594
Airfreight costs	25,072	18,531	5,984
Annual index/other incidental costs	459	2,046	36,043
Special Issue costs	-	-	59,019
<i>Acta</i> Supplement	37,415	-	-
Editorial expenses	849,990	992,429	1,055,873
Programming and Development	-	168,747	153,609
Administration expenses	66,248	60,398	76,634
	<u>1,773,538</u>	<u>1,892,583</u>	<u>2,160,049</u>
<i>Excess of income over expenditure</i>		<u>77,363</u>	<u>340,167</u>
Transfers to other Funds:			
Publications and Journals			
Development	-175,000	-50,000	-150,000
<i>Journal of Synchrotron Radiation</i>	-	-	-100,000
Newsletter Fund	-75,000	-75,000	-50,000
	<u>-250,000</u>	<u>-125,000</u>	<u>-300,000</u>
Fluctuations in rates of exchange		<u>20,514</u>	<u>11,851</u>
Accumulated balance at end of year		<u>1,392,573</u>	<u>1,583,252</u>

Professor J. M. Cowley and Dr A. F. Moodie. The second Prize was presented during the Bordeaux Congress to Professor B. K. Vainshstein. 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 May 1999, it was announced that the fifth Ewald Prize had been awarded to Professor G. N. Ramachandran for his outstanding contributions to the field of crystallography: in the area of anomalous scattering and its use in the solution of the phase problem, in the analysis of the structure of fibres, collagen in particular, and, foremost, for his fundamental works on the macromolecular conformation and the validation of macromolecular structures by means of the 'Ramachandran plot', which even today remains the most useful validation tool.

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

4. Appendix D: Reports of Commissions of the Union

4.1. Commission on Journals

In the last triennium, a number of developments for the IUCr journals should be highlighted. In the triennium the 50th Anniversary of *Acta Crystallographica* and the IUCr occurred, as did the 30th Anniversary of the *Journal of Applied Crystallography*. A special 50th Anniversary Issue of *Acta Crystallographica* was published in

Section A in November 1998, comprising especially commissioned articles. The Guest Editor was H. Schenk whose excellent work and contribution is acknowledged here. This special issue was distributed to all subscribers of IUCr journals free of charge and is available for purchase at a very competitive price in book form. Authors' choice within the IUCr journals is broad, encompassing all aspects of crystallography and its cognate subjects across the sciences. The further expansion into the synchrotron field has been greatly facilitated by the *Journal of Synchrotron Radiation*, which has published the major proceedings from SRI '97 held in Himeji, Japan, and also the XAFS X Conference held in Chicago, USA, in 1998. The biological community expands apace and *Acta Cryst. Section D (Biological Crystallography)* is now published monthly. Publication of the very popular Daresbury CCP4 Conference Proceedings series commenced as a supplement to *Acta Cryst. Section D* in 1998. Chemical crystallography capability has also greatly expanded and to handle this all crystal structure data for publication in *Acta Cryst. Sections B and C* are now submitted electronically in the Crystallographic Information File (CIF) format. The *Journal of Applied Crystallography* has continued as a very successful publication and a new section on cryotechniques is proving popular.

The IUCr web coverage of the journals, including the services to authors and Co-editors for manuscript tracking, is extensive. A 50-year searchable index has been introduced and this is a powerful tool for accessing the vast archive of IUCr publications. Most recently, proofs have been made available electronically to authors. Prepara-

Table 7
Journal of Applied Crystallography (Swiss Francs).

	1996	1997	1998
Income			
Subscriptions	320,069	333,119	344,372
Sale of back numbers and single issues	2,805	3,589	3,366
Airfreight charged to subscribers	7,958	7,604	7,541
Profit/loss on offprints	-10,987	1,894	-22,542
Special issue income	-	21,885	-
Royalties, copyright fees	2,406	2,328	1,240
	<u>322,251</u>	<u>370,419</u>	<u>333,977</u>
Less Publisher's commission	-22,601	-23,570	-24,342
Yield from advertisements	-	-	3,207
Recharge to Publications and Journals	-	-	-
Development Fund for Special Issue	-	96,488	-
	<u>299,650</u>	<u>443,337</u>	<u>312,842</u>
Expenditure			
Printing and binding	88,512	82,601	116,019
Distribution and postage	14,262	15,181	31,133
Airfreight costs	3,157	2,193	1,050
Special Issue costs	-	118,373	-
Editorial expenses	106,352	199,622	187,165
Programming and Development	-	25,442	25,602
Administration expenses	7,703	15,508	13,136
	<u>219,986</u>	<u>458,920</u>	<u>374,105</u>
Excess of income over expenditure	<u>79,664</u>	<u>-15,583</u>	<u>-61,263</u>
Transfers to other Funds:			
Research and Education	-50,000	-50,000	-
<i>Journal of Synchrotron Radiation</i>	-	-50,000	-
Ewald Fund	-	-50,000	-
<i>Newsletter Fund</i>	-	-	-
	<u>-50,000</u>	<u>-150,000</u>	<u>-</u>
Fluctuations in rates of exchange	<u>5,565</u>	<u>1,636</u>	<u>-542</u>
Accumulated balance at end of year	<u>377,785</u>	<u>213,838</u>	<u>152,033</u>

tion for web access to the journals themselves is most advanced for *Acta Cryst.* Section D and release is imminent at the time of writing. The upcoming triennium includes an expansion of this electronic access for subscribers to the IUCr's journals.

There is a greater emphasis on the marketing of the journals to the crystallographic community, as well as to structural science communities in biology, chemistry, materials science and physics. Highlighting *via* mini-reviews of IUCr journal articles within the *IUCr Newsletter* has commenced. This opens a channel to 15,000 readers and is clearly an exciting promotional strategy. Details of each journal can be found in the accompanying reports below.

At the end of this triennium we say farewell to Section C Editor S. R. Hall who has steered Section C firmly and effectively into the electronic era, spearheading developments adopted now by various other structural chemistry and physics based journals. Also, A. M. Glazer has kept the *Journal of Applied Crystallography* at the forefront of experimental techniques, and launched various new sections in the journal. They are warmly wished an enjoyable and well earned respite from their heavy workloads.

4.1.1. *Acta Crystallographica* Section A (A. Authier, Editor). In the triennium 1996–1998, Section A has published 18 bimonthly issues and a Special Issue dedicated to the 50th Anniversary of *Acta Crystallographica* and the IUCr. The total number of pages was 2,922, corresponding to 227 Research Papers, 3 Lead Articles, 2 Topical Reviews, 26 papers in the Special Issue, and 32 Short Communications. The number of pages and papers published in 1997 was low, but picked up again in 1998. Many efforts have been devoted successfully

at every stage to reduce the processing and printing times. The average review time is down to about four months. Efforts will continue to be made to address this crucial issue.

A highlight of the year 1998 was the Special Issue celebrating the 50th Anniversary of *Acta Crystallographica* and the IUCr. Its Guest Editor was H. Schenk. The Special Issue starts with a paper about the history of the IUCr and spans all aspects of crystallography, symmetrical, structural, physical, chemical and biological, with papers devoted to the most important landmarks in the development of crystallography over the past 50 years. It has also been printed as a book, under the title *Crystallography Across the Sciences*. This Special Issue is undoubtedly a success and more are planned. More Lead Articles and Topical Reviews are also in the pipeline.

The format of Section A seems well adapted to its purpose and no suggestions to modify it have been received in the past, but any suggestion for modification and improvement will be welcome.

4.1.2. *Acta Crystallographica* Section B (F. H. Allen, Editor). In the triennium 1996–1998, Section B published 3,066 pages, comprising 335 full Research Papers, 16 Short Communications and 3 Topical Reviews (with more in the pipeline). The chemical balance of these papers is *ca* 45% dealing with inorganic materials, 15% dealing with metal-organics and 40% dealing with organics. Apart from papers reporting structural studies from this broad chemical spectrum, Section B continues to serve the needs of those working on charge-density studies, structural systematics from the inorganic and small-molecule databases, the modelling and prediction of crystal structures, powder diffraction methodologies, studies of phase transitions

Table 8
Journal of Synchrotron Radiation (Swiss Francs).

	1996	1997	1998
Income			
Subscriptions	77,945	93,282	115,323
Sale of back numbers and single issues	1,684	3,498	5,038
Airfreight charged to subscribers	2,393	2,695	5,233
Profit/loss on offprints	-1,427	-10,655	-25,730
Special issue income	-	-	108,040
Royalties, copyright fees	30	187	273
	80,625	89,007	208,177
<i>Less</i> Publisher's commission	-5,574	-6,775	-8,482
Yield from advertisements	6,055	2,356	19,667
Recharge to Publications and Journals			
Development Fund for Special Issue	-	-	84,588
	81,106	84,588	414,066
Expenditure			
Printing and binding	60,164	70,300	62,348
Distribution and postage	4,276	8,213	19,957
Airfreight costs	760	437	1,729
Special Issue costs	-	-	302,744
Editorial expenses	46,425	117,024	100,114
Programming and Development	-	25,442	25,602
Administration expenses	3,081	5,713	19,706
	114,706	227,129	532,200
<i>Excess of income over expenditure</i>	-33,600	-142,541	-118,134
Transfers from other Funds:			
<i>Acta Crystallographica</i>	-	54	100,000
<i>Journal of Applied Crystallography</i>	90,000	50,000	-
	90,000	50,000	100,000
Fluctuations in rates of exchange	1,913		-69
	1,913	288	-69
Accumulated balance at end of year	129,847	37,594	19,391

Table 9
Structure Reports (Swiss Francs).

	1996	1997	1998
Income			
Sales of copies	-	-	-
<i>Less</i> Publisher's commission	-	-	-
Expenditure			
Printing and binding	-	-	-
<i>Excess of income over expenditure</i>	-	-	-
Transfers to other Funds:			
Publication and Journals Development	-85,979		
Fluctuations in rates of exchange	-	-	-
Accumulated balance at end of year	-	-	-

etc. The quantity of review material carried by Section B has been lower than expected. However, the value of this material lies in its quality, and it is no easy matter to secure authoritative material of this kind. Following a slight downturn in papers at the beginning of the previous triennium, coincident with the launch of Section D and the loss of biologically oriented papers, Section B has now recovered its normal average output of 1,000+ pages per annum.

Technically, Section B has come a long way during the period. CIF submission has become mandatory for structural papers, many other papers are received in machine-readable form, and in-house typesetting at the Chester office has been introduced. This latter project caused the first two issues of 1998 to be smaller than usual (*ca* 10 papers each), but later issues in that year soon returned to the norm of more than 20 papers per issue.

In 1997, procedures were set in place to reduce publication times. A major component of the longer publication times has been the time taken by authors to revise manuscripts in light of referee comments. This time has now been reduced to a maximum of three months, with most authors revising in much shorter times than this. Now that the in-house typesetting is in place, we would expect to see shorter publication times from 1999 onwards.

Impact statistics show that Section B remains fourth of seventeen current crystallography journals, just behind three other IUCr publications. A 'citation half-life' of more than 10 years reflects the lasting value of Section B papers.

4.1.3. *Acta Crystallographica* Section C (S. R. Hall, Editor). A number of important changes have been made to the editorial and publication procedures of Section C during this triennium. Most have flowed from decisions made at the Commission meetings at the Seattle Congress in response to a rapid expansion in journal page numbers and significantly increased publication costs. The decisions spawned a number of initiatives, which are intended to make the publication of structural studies more efficient for authors and the journal.

In 1997, a new electronic publication mode, known as CIF-access, was introduced. This provides for the fast, minimum-text, publication of structure determinations. The CIF-access paper is not printed but its title, scheme and synopsis appear in the Contents page of the journal in the month that the submitted material is deposited in the IUCr CIF archive. A CIF-access submission is checked identically to a full paper except that the text entries remain the responsibility of the authors. In 1998 seventy six CIF-access papers were published.

In Seattle, the Section C board decided that specific quality standards were needed to promote consistent acceptance criteria for structural data, and to provide explicit author guidelines on the

Table 10
International Tables (Swiss Francs).

	1996		1997		1998	
Income						
Sales:						
Volume A	60,078		69,461		74,067	
Volume A Teaching Edition	3,562		5,556		3,899	
Volume B	53,349		33,918		32,791	
Volume C	46,016		77,726		16,562	
Volumes II, III and IV	55		–		59	
Less Publisher's commission	–42,394	120,666	–40,641	146,020	–33,185	94,193
Expenditure						
Printing/typesetting Volume A	11,646		16,426		26,318	
Printing/typesetting Volume A Teaching Edition	6,296		1,987		2,194	
Printing/typesetting Volume B	–5,379		47,209		3,508	
Printing/typesetting Volume C	7,779		32,288		18,693	
Editorial expenses	22,152		17,117		26,665	
Programming and Development	–	42,494	22,898	137,925	25,603	102,981
Excess of income over expenditure		78,172		8,095		–8,788
Transfers to other Funds:						
Research and Education	–60,000		–		–	
Publications and Journals Development	–90,000	–150,000	–	–	–	–
Fluctuations in rates of exchange		2,874		1,567		–695
Accumulated balance at end of year		195,091		204,753		195,270

Table 11
Book Fund (Swiss Francs).

	1996		1997		1998	
Income						
Sales:						
<i>Historical Atlas of Crystallography</i>	332		436		–	
<i>World Directory of Crystallographers</i> , 9th Edition	1,267		–		–	
<i>World Directory of Crystallographers</i> , 10th Edition	–		8,468		12,108	
Escher <i>Kaleidozyklen</i>	–		83		27	
<i>Structure Reports</i>	2,120		384		402	
Sundry publications	182		1,093		–	
Royalties						
IUCr/OUP Book Series	1,158	5,059	1,090	11,554	1,814	14,351
Expenditure						
<i>Historical Atlas of Crystallography</i>	–		–		105	
<i>World Directory of Crystallographers</i> , 9th Edition	1,419		–		–	
<i>World Directory of Crystallographers</i> , 10th Edition	–	1,419	8,059	8,059	9,274	9,379
Excess of income over expenditure		3,640		3,495		4,972
Transfers to other Funds:						
Ewald Fund	–615	–615	–	–	–	–
Fluctuations in rates of exchange		1,518		159		–91
Accumulated balance at end of year		17,065		20,719		25,600

submission requirements. These criteria were introduced into the 1997 Notes for Authors, and became the basis for CIF checking within the Chester office. They have remained essentially unchanged over the triennium and are largely responsible for the higher quality of papers currently being published by the journal.

Another change instituted in 1997 was the removal of the atomic coordinate/anisotropic displacement parameter tables from the printed paper, except in special cases. This reduction in printed structural data was possible because archived CIFs can now easily be accessed *via* the IUCr web site, and this approach is more efficient and reliable as a source of structural parameters than the printed

page. The recent availability of software, which can be linked to the web browser means that published structures may be easily downloaded, examined and manipulated, with a few mouse clicks. These and other web services are, as planned, providing new approaches to examining published structures, and are certain to influence the future publication directions of Section C.

The most recent change to Section C operations has been the introduction of a comprehensive suite of automatic validation and checking tests. These are used in the Chester office and as part of the, now mandatory, CHECKCIF facility. These tests are accessible *via* e-mail or the web. The algorithms used in this checking suite are

international union of crystallography

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

	1996	1997	1998
Income			
Investment income		20,313	33,986
			17,518
Expenditure			
Computer expenses:			
Purchase of computer equipment and software	17,722	2,485	36,272
Programming and Development	174,880	254,423	256,016
Programming and Development recharged to other Funds		-254,423	-256,016
Electronic Publishing Committee/Section Editors' meeting	1,573	1,344	985
Electronic Publishing Project	46,546	27,545	5,333
Promotions Representative	-	17,334	87,888
No. 6 Abbey Square	-	1,194	
Web input	-	3,676	1,863
Special Issue costs	-	96,488	231,132
Depreciation on leasehold property	12,637		
		253,358	150,066
			363,473
<i>Excess of income over expenditure</i>		-233,045	-116,080
			-345,955
Transfers from other Funds:			
<i>Acta Crystallographica</i>	175,000	50,000	150,000
<i>Structure Reports</i>	85,979	-	-
General Fund	100,000	-	-
		360,979	50,000
			150,000
Fluctuations in rates of exchange		9,288	5,016
			-1,631
Accumulated balance at end of year		716,497	655,433
			457,847

Table 13
Research and Education Fund (Swiss Francs).

	1996	1997	1998
Income			
Investment income		40,416	43,671
			47,549
Expenditure			
Young scientist support	64,409	91,816	76,399
Moscow ECM Funds	9	-	530
Visiting Professorship Programme	1,290	16,661	8,837
		65,708	108,477
			8,837
			85,766
<i>Excess of income over expenditure</i>		-25,292	-64,806
			-38,217
Transfers from other Funds:			
General Fund	-	50,000	50,000
<i>Journal of Applied Crystallography</i>	50,000	50,000	-
<i>International Tables</i>	60,000	-	-
		110,000	100,000
			-
			50,000
Fluctuations in rates of exchange		12,320	6,721
			-3,160
Accumulated balance at end of year		836,332	878,247
			886,870

based primarily on the criteria defined in the 1997 Notes for Authors, with the addition of 'alert level' messages to indicate the degree of departure from the expected standard. The requirement that authors pre-check their CIFs prior to submission using CHECKCIF has meant that less time and effort is wasted by authors and editorial staff on faulty submissions. In addition, authors now receive much more detailed information about the review expectations of the journal. If the author believes that any of the reported error alerts are inappropriate for a particular study, this can be explained in a supplied electronic form, known as the Validation Response Form (VRF). The VRF is, if need be, inserted into the CIF submitted for publication, and the explanations are assessed and handled by a special Co-editor prior to the normal review step. The automatic checks have effectively shifted the emphasis of data validation and checking from the editorial office to the author, and this is of long-term importance

to the efficiency of the journal, and to knowledge within the discipline.

The changes to Section C in this triennium represent the transition to faster, more efficient publication modes for delivering structural information, and ensure a consistently high standard of publication through explicit acceptance criteria. The magnitude and speed of these changes has certainly stimulated some authors and, not unexpectedly, been more difficult for others. As expected of an IUCr journal, these efforts are pioneering future approaches to structural publications. This has involved a considerable effort on the part of the Chester office staff and the members of the Section C board. Their large contributions are most gratefully acknowledged.

4.1.4. *Acta Crystallographica* Section D (J. P. Glusker, Editor). Section D, devoted to biological crystallography, started in 1993 as a publication that appeared every other month. Since January 1999, it

Table 14
Ewald Fund (Swiss Francs).

	1996	1997	1998
Income			
Investment income	15,335	19,580	23,850
Bequest	–	–	73
		<u>15,335</u>	<u>19,580</u>
			<u>23,923</u>
Expenditure			
Selection Committee and expenses	2,520	–	1,537
Ewald Prize	36,000	–	–
		<u>38,520</u>	<u>–</u>
			<u>1,537</u>
<i>Excess of income over expenditure</i>		<u>–23,185</u>	<u>19,580</u>
			<u>22,386</u>
Transfers from other Funds:			
<i>Journal of Applied Crystallography</i>	–	50,000	–
Book Fund	615	–	–
General Fund	50,000	–	–
		<u>50,615</u>	<u>–</u>
			<u>–</u>
Fluctuations in rates of exchange		<u>4,807</u>	<u>3,053</u>
			<u>–1,496</u>
Accumulated balance at end of year		<u>326,335</u>	<u>398,968</u>
			<u>419,858</u>

Table 15
Newsletter Fund (Swiss Francs).

	1996	1997	1998
Income			
Advertisements	65,521	82,248	121,456
Reimbursement of 18GAC circular	–	–	6,387
		<u>65,521</u>	<u>82,248</u>
			<u>127,843</u>
Expenditure			
Editorial honoraria	4,585	5,600	5,360
Editorial expenses	32,110	42,432	75,855
Printing and distribution	79,396	98,228	90,323
Advertising costs	16,380	20,562	30,364
		<u>132,471</u>	<u>166,822</u>
			<u>201,902</u>
<i>Excess of income over expenditure</i>		<u>–66,950</u>	<u>–84,574</u>
			<u>–74,059</u>
Transfers from other Funds:			
<i>Acta Crystallographica</i>	–	75,000	50,000
General Fund	75,000	–	30,000
		<u>75,000</u>	<u>80,000</u>
			<u>–</u>
Fluctuations in rates of exchange		<u>894</u>	<u>394</u>
			<u>–204</u>
Accumulated balance at end of year		<u>60,685</u>	<u>51,505</u>
			<u>57,242</u>

has appeared monthly. It contains Fast Communications, Topical Reviews, Research Papers, Short Communications, Crystallization Papers, Book Reviews and Letters. In addition, the Proceedings of the CCP4 Study Weekend, January 1998, entitled 'Databases for Macromolecular Crystallographers' was published as Part 1 of the November 1998 issue. Articles on results of crystallization experiments continue to provide important and useful information on macromolecules under study. In order to be published in Section D, deposition of all crystallographic data on biological structures (atomic coordinates and structure factors) at the Protein Databank is required. This deposition is generally as mmCIF files, so that data are available for re-refinement if needed. Publication of figures in colour is provided free of charge, but only when the colour adds to the scientific content of the article. In addition, all authors are asked to sign a form attesting to the fact that they have seen the final manuscript; this is done to obviate some problems that have occurred in the past. I thank J. R. Helliwell, the Editor-in Chief, and P. R. Strickland, the Managing Editor, for their continued support and advice through the last few years.

The subjects of research papers have included structures of a wide variety of proteins and nucleic acids. Of these, many interesting structures reported were those of a channel-forming integral membrane protein and an enzyme containing a transition-state structure in the active site. New structures, refinements of structures already known, structures of enzymes from different biological sources with somewhat different modes of action, structures as large as those of viruses, nucleosomes and ribosomes, were all reported in this journal. Details of intermolecular associations, including hydrogen bonding between water and aromatic groups, were also analysed.

The methods used to obtain such interesting structures were reported, with several articles that addressed the experimental problems encountered, how to overcome them, and discussion of the credence that should be given to the three-dimensional information that results. Subjects of articles included techniques for cryogenic data collection, methods of analysis of diffraction patterns, synchrotron data collection, X-ray structure analyses combined with electron microscopy, and the use of krypton and xenon as heavy atoms in

proteins. Problems with twinning and the assignment of space group were also discussed. Crystal structures of macromolecules and their complexes are now being reported at 1.2 to 1.4 Å resolution, so that anisotropic displacement parameters and ordering of side chains at low temperatures can be evaluated. Those articles involving crystallization research addressed heterogeneity effects, descriptions of imperfections in protein crystals, comparisons of crystal growth in magnetic fields and in space and on earth, and the use of isothermal microcalorimetry, dynamic light scattering, NMR and Raman spectroscopy to study nucleation, orientational disorder, the mode of breakdown of protein crystals on melting and the structural effects of flash freezing of a crystal. Macromolecular crystal growth kinetics and morphology and the formation of polymorphs were also analysed. Articles describing methods of phasing the diffraction data involved multiple wavelength anomalous scattering with a variety of scatterers in the crystal, the various methods of density modification, phase improvement, and error estimates in macromolecular structure determinations. Molecular replacement was the subject of many articles, and it was shown that similar proteins need not necessarily associate in the same way. Patterson and real-space methods of structure determination were also addressed. Triplet phases from three-beam diffraction have been used to initiate direct methods for high-resolution protein data. Refinements of many macromolecular structures provided a more detailed picture of the atomic arrangement and the molecular folding, and several articles addressed ways of determining the reliability of a protein structure determination. Pitfalls and cautionary tales on these methods will be helpful to others with problems solving their structures.

The focus on crystallographic databases that was provided by the CCP4 Proceedings comes at a time when there is particular interest in this subject as a result of the general use of the web. Those databases of protein and nucleic acid structures, currently in place, were described together with other available databases, including those of structural motifs, intermolecular contacts and protein sequence alignment techniques. The organizers, J. Murray-Rust, L. Potterton, B. Luisi, E. Dodson and S. Bailey, are to be thanked for a highly useful publication. 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.

Our sincere thanks to the many members of the crystallographic community who have served as reviewers of submitted papers. The staff at Chester have done an excellent job in shepherding the articles to the publishers, and they are also thanked. The Co-editors are also deserving of our thanks; they oversee the publication fate of a large proportion of the submitted manuscripts. Without their careful work the expansion of the journal to a monthly issue in 1999 would not have been possible.

4.1.5. *Journal of Applied Crystallography* (A. M. Glazer, Editor). An analysis of the contents of the *Journal of Applied Crystallography* over the last triennium is presented below:

	1996	1997	1998
Pages	759	320+871	988
Research Papers	81	62+92	102
Short Communications	5	15	15
Fast Communications	5	10	4
Computer Programs	10	7	8
Computer Program Abstracts	6	11	12
Laboratory Notes	9	9	7
Cryocrystallography Papers	5	1	6
CIF Applications	1	1	4
Teaching and Education	1	0	2
Lead Articles	1	1	0
Software Reviews	0	1	0

Note that in 1997 the first numbers under Pages and Research Papers refer to the Special Issue containing papers presented at the Small-Angle Scattering Conference held in Campinas, Brazil. Publication of this Special Issue resulted in a slowing down of the normal publication cycle, but this matter has now been addressed, so that new arrangements for the publication of Special Issues should not interfere seriously with the normal journal production.

Even excluding the Small-Angle Scattering issue, certain healthy trends are apparent. In particular, there has been a steady growth in the number of pages published, most obviously seen in the increase in normal Research Papers. This is clearly a good situation for a journal in the present climate where electronic publication may be seen as a possible threat to paper publishing. It is gratifying also to see that the new Cryocrystallography section has shown signs of becoming popular, especially in the most recent year. Similarly, the new Teaching and Education section is looking like it will be a valuable part of the journal in the future. It is also apparent that the *Journal of Applied Crystallography* remains the most significant of the IUCr journals carrying details about crystallographic software, although it has to be said that the Software Reviews section has been disappointing, and will need further consideration.

4.1.6. *Journal of Synchrotron Radiation* (S. S. Hasnain, J. R. Helliwell, H. Kamitsubo, Editors). It is now more than four years since the *Journal of Synchrotron Radiation* (*JSR*) was launched. In this time approximately 500 research articles in over 2,400 pages have been published, providing a focus for the whole of the synchrotron radiation community. The number of papers published in *JSR* over the triennium has steadily increased. For the journal, the main achievement of the triennium was the successful publication of the SRI '97 Proceedings, the largest ever undertaken by the IUCr journals team, comprising over 1,050 pages. The papers for that issue were refereed to the usual *JSR* standards, rather than at the meeting, and we believe that this effort is reflected in the improved quality of the Proceedings over those published previously. The SRI '97 Proceedings formed the May 1998 issue of *JSR*. Many of the lessons learnt with SRI '97 were applied to the Proceedings of the XAFS X Meeting, held in Chicago, USA, August 1998, which is to be published in May 1999. This was again fully refereed but was produced in camera-ready format.

We have entered into the citation ranking tables and are already ranked third out of thirty seven journals covering instruments and instrumentation with *Review of Scientific Instruments* placed fifth, *NIMS B* placed sixth and *NIMS A* placed eighth. The review and production times for the journal have been rapid. Centralised submission was introduced in 1997 and is being used to improve review times; our current strategy is to cut production times by increasing electronic publication of the journal. We are currently putting together a Synchrotron Radiation and Structural Biology Special Issue (July 1999 issue of *JSR*) to celebrate J. Walker's (now Sir John Walker) share in the 1997 Nobel Prize in Chemistry, which is indeed the first synchrotron-radiation-related Nobel prize. Overall, the high impact factor for the journal and its excellent review and publication turn-around times for authors are fine achievements, indeed making us the best journal for the synchrotron-radiation community's papers in synchrotron radiation instrumentation, methods and applications.

J. R. Helliwell, Chair
A. M. Glazer, Co-Chair

4.2. Commission on International Tables

During the Seattle Congress, the Commission held one Open Meeting and three closed meetings, in addition to numerous personal

contacts between volume editors, technical editors and authors. The Open Commission Meeting featured six lectures on the status of the *International Tables* volumes, either published or in preparation. Reports about this meeting are available on the web as part of the IUCr home page (see below), in the Newsletter of the British Crystallographic Association (No. 58, September 1996; No. 59, December 1996), and in the *IUCr Newsletter* (Vol. 5, No. 2, 1997). Another Open Commission Meeting will be held at the Glasgow Congress.

At their Seattle meeting, the Executive Committee approved two new *International Tables* volumes:

Volume F: *Macromolecular Crystallography*, editors M. G. Rossmann and E. A. Arnold;

Volume G: *Crystallographic Information*, editors B. McMahon and S. R. Hall.

A summary of the information on all volumes of *International Tables*, either published, in the process of revision, or being prepared or planned, has been collected in the form of a home page of the Commission. It is accessible from the main IUCr home page (<http://www.iucr.org/>) and the sub-pages (i) Activities of the Commissions, and subsequently (ii) Commission on *International Tables for Crystallography*. The home page is maintained by U. Shmueli in Tel Aviv and its updated versions are retrieved by B. McMahon at the IUCr office in Chester.

During ECM-17 at Lisbon, Portugal, August 1997, all Commission members present met with the IUCr's Managing Editor, P. R. Strickland, in order to discuss the future production and printing schedules of all *International Tables* volumes, in particular of those volumes ready for publication or for a new edition (Volumes A, B, C, E). Subsequent changes to this schedule were transmitted to all persons concerned.

In the spring of 1998, a new volume of *International Tables* was proposed by U. Müller, Kassel; the volume is tentatively called 'A2' and has the title: *Relations of Wyckoff Positions between Space Groups and their Maximal Subgroups*. The proposal is presently being considered by the Executive Committee.

Detailed reports of sales and stock figures for the individual volumes of *International Tables*, published up to 31 December 1998 and currently active, are given below:

Volume	II	III	IV	A	Brief A	B	C
Date of publication	1959	1962	1974	1983	1985	1993	1992
Dates of reprinting	1967	1968	1989	1984	1988	1996	1995
	1972	1983	–	1987	1989	–	–
	1985	1985	–	1989	1993	–	–
	1989	–	–	1992	1996	–	–
	–	–	–	1995	–	–	–
	–	–	–	1998	–	–	–
Number of copies sold							
up to end 1996	9,474	8,764	4,268	5,982	4,402	1,048	1,398
in 1996	20	19	21	1,179	89	509	715
in 1997	0	0	0	346	325	192	198
in 1998	0	0	0	354	218	177	68
up to end 1998	9,494	8,783	4,289	7,861	5,034	1,926	2,379
Stock at 31 December							
1998	0	0	0	284	45	497	0

4.2.1. Volume A. Space-Group Symmetry; Editor Th. Hahn. The Fourth, Revised Edition of Volume A, published in March 1995, has sold so well that a Corrected Reprint became necessary, which appeared in October 1996. It contains corrections of all errors and flaws known at that time. A further reprint became necessary and appeared in June 1998.

The Fourth, Revised Edition of the *Brief Teaching Edition of Volume A* appeared in October 1996. It is based on the Corrected

Reprint of the Fourth, Revised Edition of Volume A, mentioned above.

Preparations for the Fifth, Revised Edition of Volume A continued throughout the triennium. This edition will be completely 'computerized' in the following ways:

(i) The space-group tables in this volume (Sections 6 and 7) are being transferred to L^AT_EX files by M. Aroyo and his colleagues in Sofia, Bulgaria. These files will be the basis for the printing of the Fifth Edition. This work was completed by the end of 1998; checking of the data is in progress.

(ii) The remaining text sections will be re-keyed in Chester. The SGML conversion of these sections will be carried out in the second half of 1999.

The new edition will have a substantial number of corrections and small improvements. Three larger changes stand out:

(i) Systematic introduction of the new symbol 'e' for the 'double glide plane' throughout the volume; this symbol was first used in the Fourth Edition, but in a few places only.

(ii) Addition of a small new Section 9.4: *Some Further Properties of Lattices* by B. Gruber, Prague, Czech Republic.

(iii) Revision of some parts of Section 15 on normalizers, especially Table 15.3.2.

The scheduled publication date of the Fifth Edition is now the spring of 2000.

The Fifth Edition of Volume A will also be the basis of the Fifth Edition of the *Brief Teaching Edition of Volume A*.

4.2.2. Volume B. Reciprocal Space; Editor U. Shmueli. The First Edition of Volume B was published in 1993, a Corrected Reprint appeared in 1996 and the work on the Second Edition was at a fairly advanced stage during the Seattle Congress. The editorial work on the Second Edition was completed during the triennium 1996–1998. All the material received from the authors is in the hands of the Technical Editor in Chester.

As pointed out in previous annual reports, the publication of the Second Edition of Volume B (as well as other volumes of *International Tables*) was delayed by the recently undertaken translation of the *Tables* to Standard Generalized Mark-up Language (SGML) which will facilitate their access through a variety of electronic media.

We summarise here all the major revisions in the First Edition of Volume B, and the newly incorporated contributions to the Second.

Revised/corrected chapters and sections (for the Second Edition):

B.1.2. *The structure factor* (by P. Coppens)

B.1.3. *Fourier transforms in crystallography* (by G. Bricogne)

B.1.4. *Symmetry in reciprocal space* (by U. Shmueli; revised Appendix B by U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve)

B.2.1. *Statistical properties of the weighted reciprocal lattice* (by U. Shmueli and A. J. C. Wilson)

B.2.3. *Patterson and molecular-replacement techniques* (by M. G. Rossmann and E. Arnold)

B.2.5. *Electron diffraction and electron microscopy in structure determination – Foreword* (by J. M. Cowley)

B.2.5.2. *Space-group determination by convergent-beam electron diffraction* (by P. Goodman)

B.3.3. *Molecular modelling and graphics* (by R. Diamond)

B.4.1. *Thermal diffuse scattering of X-rays and neutrons* (by B. T. M. Willis)

B.5.1. *Dynamical theory of X-ray diffraction* (by A. Authier)

New contributions (to the Second edition):

B.1.5. *Crystallographic viewpoints in the classification of space group representations* (by M. I. Aroyo and H. Wondratschek)

B.2.5.6. *Direct methods in electron crystallography* (by D. L. Dorset)

B.4.5. *Polymer crystallography* (by D. L. Dorset and R. P. Millane)

B.4.6. *Reciprocal-space images of aperiodic crystals* (by W. Steurer and T. Haibach)

B.5.3. *Dynamical theory of neutron diffraction* (by M. Schlenker and J.-P. Guigay)

The scheduled publication date of the Second Edition of Volume B is January 2000.

4.2.3. Volume C. *Mathematical, Physical and Chemical Tables*; Editor E. Prince. At the time of the Seattle Congress the task of assembling material for a Second, Revised Edition of Volume C was largely complete. Although most of the text of the First Edition had been composed by the authors on one word-processing system or another, very few of the original computer files still existed in any machine-readable form, and, as a result, a large part had to be typeset manually for the Second Edition. The manual typesetting has been carried out with a computerized system used by commercial printers, and the entire contents now exist as machine-readable files. One by-product of this procedure was that numerous entries whose authors had initially said that they did not want to revise them actually were substantially revised at the galley proof stage. As of January 1999, the entire volume, except for some front and back matter, was in page proof, and the project was on schedule for publication in the spring of 1999.

The First Edition contained several chapters and sections that had been carried over from the earlier series of *International Tables*, and some of the data was from the 1930's. Only one of these chapters remains, and that was judged to be sufficiently authoritative not to require revision. The Second Edition contains two entirely new chapters, and many others have been substantially rewritten. The timely completion of the Second Edition could not have been achieved without the cooperation of the many authors and the staff in Chester, and the entire crystallographic community is in their debt.

4.2.4. Volume D. *Physical Properties of Crystals*; Editor A. Authier. The preparation of Volume D has progressed steadily during the triennium. The few manuscripts still missing are expected to be delivered during the first half of 1999. The manuscripts, which were already in the hands of the Editor, were updated by their authors during 1998, and the whole volume will be sent to the Technical Editor in July 1999, even if one or two manuscripts are still outstanding. Volume D will include two accompanying software packages on a CD ROM. The first, dealing with tensors and irreducible representations, calculates representations of finite three-dimensional point groups and the components of invariant tensors in arbitrary dimension, of arbitrary rank, and with arbitrary permutation symmetry of the indices under the action of a three-dimensional crystallographic point group. The second, dealing with phase transitions, will give tables for equitranslational phase transitions, and for tensor properties at any group-subgroup phase transition: spontaneous tensor components, up to rank four, that appear in the distorted phase and non-zero tensor components that are the same in both phases.

Two meetings took place, the first in Nijmegen, The Netherlands, in February 1997 and the second in Prague, Czech Republic, in January 1998, in order to define and coordinate the contents of the two software packages. Alpha versions have been produced and tested. A beta version of the CD ROM including the two packages and a presentation page prepared by the IUCr Research and Development Officer should be ready for distribution in the spring of 1999.

4.2.5. Volume E. *Subperiodic Groups*; Editors V. Kopsky and D. B. Litvin. A final draft of Volume E was prepared with the following content:

Part 1: Subperiodic Group Tables: Frieze Groups, Rod Groups, and Layer Groups

Section 1: Symbols and Terms used in Part 1

Section 2: Guide to the Use of the Subperiodic Group Tables

Section 3: The 7 Frieze Groups

Section 4: The 75 Rod Groups

Section 5: The 80 Layer Groups

Part 2: Scanning of Space Groups

Section 6: Symbols and Terms used in Part 2

Section 7: Guide to the Use of the Scanning Tables

Section 8: The Scanning Tables

The scheduled publication date of Volume E is April 2000.

4.2.6. Volume F. *Macromolecular Crystallography*; Editors M. G. Rossmann and E. A. Arnold. Our goal in preparing Volume F of *International Tables* is to produce a comprehensive, yet concise, reference work for macromolecular crystallography. This first *International Tables* volume devoted to macromolecular crystallography is intended to complement the existing volumes as well as other reference materials pertinent to modern structural biology. The emergence of Volume F recognizes the increasing size and vitality of the field of macromolecular crystallography. It is hoped that this volume will be particularly useful for at least 10 to 12 years. Volume F will cover the theory and practice of macromolecular crystallography with an estimated total of 700 pages. In addition, there will be surveys of the principles of macromolecular structure and of commonly used macromolecular crystallographic program systems. Approximately 100 authors have accepted invitations to write 95 articles in a total of 27 chapters. Two advisors and an international Advisory Board consisting of 27 members have assisted in the planning of the volume. A web site at the IUCr Offices at Chester (address: <http://www.iucr.org/~commit/itf/>) has been set up to facilitate inter-author communication during the preparation of the volume. The volume will include numerous figures in colour and a CD ROM version will be produced to provide electronic access to the volume and accompanying materials.

As of January 1999, manuscripts have been received for approximately three-quarters of the projected articles in the volume. The papers are reviewed for scientific content and overall consistency of style and expression; completed manuscripts following revisions are sent to the IUCr offices in Chester. The overall quality of the contributions received is very high. We anticipate that most articles will have been completed by the time of the Glasgow Congress and hope that Volume F will be completed and published in 2000.

4.2.7. Volume G. *Crystallographic Information*; Editors B. McMahon and S. R. Hall. Volume G was approved by the Executive Committee at the Seattle Congress as a reference handbook for crystallographic information, and specifically in its early editions as a documentation of the Crystallographic Information File (CIF) project. Chapters in the volume will document the file structure and formal grammar of CIF, the techniques and software libraries available for creating, editing and reading CIFs, and, most substantially, the definitions of public data names maintained by the IUCr. Much of the time since the Seattle Congress has been taken up with approving and maintaining dictionaries of definitions appropriate to small-molecule single-crystal structure determination, to powder diffraction studies, and to the determination and description of biological macromolecular structures. Now that these procedural developments have taken place, manuscripts are being collected from participants in the CIF project with a view to publication of Volume G in the latter part of 2000.

4.2.8. Volume A1. *Maximal Subgroups of Space and Plane Groups*; Editor H. Wondratschek. The publication of Volume A1,

for some time named 'Volume H', was approved by the Executive Committee in August 1995. It provides complete tables and diagrams of the maximal subgroups for each space and plane group; for the Contents see the Report for 1995 in *Acta Cryst.* (1996), **A52**, 962.

Meanwhile, the data for the subgroup tables are complete and have been checked in several runs by hand, by the mathematical program system GAP, and by *ad hoc* programs. The homogenization of the data on isomorphic and on non-isomorphic subgroups that originate from different sources is in progress. Many transformations from unconventional to standard settings have been changed in order to make the tables more user-friendly for the comparison of symmetry-related crystal structures. There are still problems to be settled, in particular for those space groups that are presented twice in Volume A because of different settings. The user's guide and the theoretical part are in preparation. In addition to the tables, the subgroup relations will be presented in the form of diagrams, separate for *translationengleiche* and *klassengleiche* subgroups. These diagrams have been completed.

Th. Hahn, Chair

4.3. Commission on Aperiodic Crystals

Members of the Commission had opportunities to meet during various international conferences, the most important event being in Alpe d'Huez, France, during the Aperiodic '97 Conference, which took place in August 1997. In the past three years, the Commission focused its work along three main directions: the establishment of standards for the publication of aperiodic structures; the organization of international conferences and micro-symposia on the same topic; and, finally, the coordination of conference activities between different communities working in related fields of aperiodic structures.

The checklist for the publication of incommensurately modulated crystals appeared in *Acta Cryst.* [(1997), **A53**, 95–100]. This document, established by the Commission, was published following broad consultations with specialists in the field of incommensurate crystal structures. It contains numerous recommendations and suggestions to authors for the publication of refined structures described in the superspace-group approach. This document can be consulted on the IUCr web site.

Work on the CIF dictionary of modulated structures is progressing. A version close to the final draft is already available on the web. The feedback of specialists working in the field of modulated structures will be required. Moreover, a preliminary database containing more than fifty modulated structures is currently being tested.

The Aperiodic '97 conference took place in Alpe d'Huez in August 1997. The members of the Commission participated actively in the preparation of the conference in the role of the International Advisory Board. During the conference, specialists from many different areas related to aperiodic crystal structures presented the current state of research in their respective fields of interest. The Proceedings of the conferences (edited by de Boissieu, Verger-Gaugry & Currat) have recently been published by World Scientific, Singapore (1998). The next Aperiodic conference will take place in Nijmegen, The Netherlands, in 2000.

Commission members contributed actively to the organization of many sessions devoted to aperiodic crystals in various international conferences, in particular ECM-17, ECM-18 and the Glasgow Congress.

The coordination between the organizers of the International Conference on Quasicrystals and the Commission was also successful and resulted in a better calendar of future conferences.

During the Prague ECM, a Special Interest Group (SIG) on Aperiodic Crystals was officially established as one of the first four in the European Crystallographic Association (ECA). Many Commission members participated actively in the foundation of the group and are presently members of the steering committee. A web site dedicated to this particular SIG provides useful information on the topic of aperiodic crystals. This site is maintained and constantly updated with new information.

G. C. Chapuis, Chair

4.4. Commission on Biological Macromolecules

In 1997/1998, the Commission was engaged in discussions about publications and the associated release of the atomic parameters of the published molecular structures.

In several editorials of relevant journals and in a poll by *Nature Structural Biology*, the polarization of the scientific community in this matter was clearly expressed – should there be (1) immediate release of atomic parameters with publication date or (2) a certain delay time of about one year? This issue was considered in a Letter to the Editor of *Acta Crystallographica Section D* by E. N. Baker and W. Saenger [*Acta Cryst.* (1999), **D55**, 2–3]. This Letter will be taken as the basis for a meeting of the Commission to be held during the Glasgow Congress. Following this discussion, a recommendation will be formulated for consideration by the IUCr.

W. H. E. Saenger, Chair

4.5. Commission on Charge, Spin and Momentum Densities

The Commission promotes the study of electron-density distributions in both real and momentum space by bringing together physicists, chemists and crystallographers in conferences, workshops and schools, and by initiating and executing projects. The web page (<http://www.tuwien.ac.at/theochem/iucr/csm.html>) is linked to the IUCr home page and contains updated information on the activities of the Commission.

4.5.1. Projects. Multipole Refinement (C. Lecomte). During the past decades, several programs have been written to carry out multipole refinements of the electron density distribution. Comparison of the results showed qualitative differences and thus made limitations apparent. This has led to the initiation of a new project for a critical assessment of the multipole refinement method. Theoretical structure factors (at $T = 0$) were used as a benchmark to test various schemes in order to determine whether or not the different refinement methods were able to recover the original data. These tests have been tried with or without the addition of statistical errors or temperature broadening to the theoretical structure factors. The first report has been given at the Oxford Gordon Research Conference (see below) with a poster by Pillet, Souhassou, Lecomte, Schwarz, Blaha, Rerat & Lichanot.

The XD Program (T. Koritsanszky). The development of the program *XD* by an international team under the leadership of T. Koritsanszky has been accomplished successfully and versions of this program were sent to several groups for critical tests.

Maximum Entropy Method (MEM) (M. Sakata). Since 1991, the MEM has received the full attention of the community served by the Commission. Some highly controversial results have been reported at several conferences since. There was inconclusive and rather diffuse discussion about the MEM project mainly concerning the basis used in MEM. No subject led to more heated discussions than this. The need for high-quality data became apparent for successful applications of MEM. Presently it is planned to supply a few data sets, both

theoretical and experimental, in order to test MEM. They will probably be for Si, Al₂O₃ and MgCu₂ and will be made available on the web page. The first conclusion is that reliable results in precise electron-density studies may be obtained if not flat prior probabilities are used.

Fermiology (A. Bansil). This project focuses on the determination of the fermiology *via* high-resolution synchrotron-based Compton scattering. The first step consists of standardising procedures for evaluating high-resolution Compton data. The ability of Compton scattering to contribute to the fermiology of metallic systems is evaluated. Synchrotron-based instruments are to be combined with quantum-mechanical calculations based on density functional theory. The experimental results obtained by different groups showed substantial differences, whereas on the theoretical side, quite different methodologies – FLAPW and KKR – yield highly similar results.

Density Matrices (W. Weyrich). A unified quantum-mechanical description of the electronic structure from experimental charge and momentum densities is attempted. The aim of the project is to investigate to what extent the combination of accurate experimental density data from both position and momentum space can enable a direct access to wavefunctions and density matrices for systems of increasing complexity. In addition to unifying position and momentum space, density matrices reveal the nature and range of chemical bonding. The possibility of obtaining information on the non-diagonal elements of the density matrix from coherent Compton scattering experiments adds to the value of the field.

4.5.2. Meetings, workshops and schools. Since bringing scientists from different disciplines together is one of the main objectives of the Commission, meetings play a major role in its activities. Several were organized either under the close guidance of the Commission, such as the triennial Sagamore conferences, or in some other form of co-operation, such as the Gordon Conference, or in an intermediate form of interaction.

The First European Charge Density Meeting. This meeting was organized by C. Lecomte and held at the Abbaye de Premontres (14–16 November 1996). Sessions included materials science, maximum entropy, high-resolution synchrotron data, electrostatics, modelling of charge density and transferability, extension of experimental work to large systems and theoretical calculations. This meeting started a new series to be held every three years.

XD User Group Meeting. This ‘Computing School on Practical Aspects of Charge Density Determination’ was held 15–18 September 1997 at FU-Berlin, Germany, and was organized by T. Koritsanzsky and P. Luger. The meeting covered not only important aspects of experimental charge density determination but also theoretical considerations. It included practical aspects of data collection at low temperatures, data reduction and model refinements with emphasis on the interpretation of the results and detection of ambiguities in the procedure. Hands-on tutorials based on the *XD* program package were given.

Sagamore XII Conference. The Sagamore Conference was held in Waskesiu (in Prince Albert Park, near Saskatoon, Saskatchewan, Canada), 27 July–1 August 1997, and was organized by B. Robertson on behalf of the Commission. This meeting was more physics oriented and showed that the field of interest is still an excellent focal point for scientists of different disciplines. Progress was noted in all parts of the field: the theoreticians discussed beyond local density methods; experimentalists, coming from neutron sources and from synchrotron facilities, brought new results on magnetisation densities; and computational scientists hotly discussed maximum-entropy methods.

Good progress was made with the interpretation of the experimental results.

The Gordon Conference. The Gordon Conference on Electron Distributions and Chemical Bonding was chaired by K. Schwarz and C. Lecomte. The meeting was organized at Queen’s College in Oxford, UK, 30 August–4 September 1998. About 72 crystallographers, theoretical chemists and physicists discussed experimental determination, quantum-chemical calculation, and the interpretation and the use of electron-density distributions. Area detectors, the use of the maximum-entropy method and the contribution of electron diffraction raised much interest and heated discussions. The field ranged from biomolecules to inorganic materials science applications. By electing two members of the Commission as organizers of the next conference, the participants made sure that the Gordon Conference fits nicely into the activities of the Commission.

Future meetings. The Second European Charge Density Meeting will be held in Sitges, Barcelona, Spain, 30 September–2 October 1999 and will be chaired by E. Espinosa. The next Sagamore Conference will be organized by L. Dobrzynski and will be held in Poland, 1–5 September 2000. The next Gordon Conference will be organized by C. Lecomte and J. Spence in summer 2001, provided approval is obtained by the Gordon authorities. A satellite meeting to ECM-19 on Crystallographic Computing for Electron Density Analysis, chaired by N. K. Hansen, will be held in Nancy, France, 24–25 August 2000 (<http://www.lc3b.u-nancy.fr/ecm19/>).

Commission meetings. The Commission met in Seattle during the Congress in its new composition to discuss the next Sagamore Conference. Other meetings were held at the Sagamore Conference in Canada, where it was decided to have the next Sagamore meeting in Poland. The fields of Multipole Refinements and Maximum Entropy, Magnetisation Densities, and Encounter of Theory and Experiment in Charge Density Studies were identified for micro-symposia at the Glasgow Congress (all honoured). At the Gordon Conference a proposal was made for new candidates and the next Chair. At all meetings the projects were discussed.

A Special Interest Group on charge, spin and momentum densities of the European Crystallographic Association was approved at ECM-18, Prague, Czech Republic, thanks to D. Feil and other promoters. The Chair is P. Becker.

K. Schwarz, Chair

4.6. Commission on Crystal Growth and Characterization of Materials

During the triennium, the activities of the Commission were again directed to the organization of international schools on crystal growth and characterization for young scientists. An attempt to prepare a School on Epitaxial Growth in Trieste, Italy, in 1997, together with the International Centre of Theoretical Physics as co-organizer and sponsor, failed because of budget problems. In 1998, the Commission helped to organize the following two Schools.

(1) The Tenth International Summer School on Crystal Growth (ISSCG-10), Rimini, Italy, 1–6 June 1998. This school was organized by Chairs R. Fornari (MASPEC, Parma, Italy) and C. Paorici (former Commission Chair, University of Parma, Italy) in connection with the Twelfth International Congress of Crystal Growth (ICCG-12), which was held 26–31 July 1998 in Jerusalem, Israel. The Commission was engaged in the lecturing programme with three former and two past Commission members as speakers. The school was sponsored and financially supported by the IUCr and other national and international institutions. It was attended by about 60 participants, mostly

PhD students, from 19 countries. The lectures are collected in the book *Theoretical and Technological Aspects of Crystal Growth*, published by Trans. Tech. Publ. Ltd, Zürich (*Materials Science Forum*, 276–277, 1998).

(2) The First International School on Crystal Growth Technology (ISCGT-1), Beatenberg, Switzerland, 5–16 September 1998, was organized by H. J. Scheel (Lausanne, Switzerland) and T. Fukuda (Sendai, Japan). Three Commission members were engaged in the International Advisory and Programme Committee and contributed to the programme as lecturers. ISCGT-1 was sponsored and financially supported by the IUCr and other national and international institutions. It was attended by about 55 participants from 13 countries. The lecture notes of the 55 one-hour presentations and their extended abstracts are assembled in a voluminous book. The publication of the proceedings of this school is in progress.

Four Commission members attended the Twelfth International Congress of Crystal Growth (ICCG-12) in Jerusalem, Israel, 26–31 July 1998. They met during the congress and discussed two main topics: (1) candidates for the Commission Chair and Commission members for the triennium 1999–2001, and (2) an International School on Crystal Growth (ISCG) in Brazil. The latter point was discussed with R. Caram, University of Campinas, Brazil. It was decided to hold the ISCG 18–24 July 1999 in Campinas, Brazil, with R. Caram as Chair and H. Klapper as Co-chair. The preparation of this School was the main activity of the Commission in 1999. The School is sponsored and supported by the IUCr by support for two lecturers under the Visiting Professorship Programme.

During the Twelfth International Congress on Crystal Growth, 26–31 July 1998, in Jerusalem, Israel, the Commission Chair attended the business meetings of the International Organization of Crystal Growth (IOCG). It was again agreed to continue the cooperation of the IUCr and the IOCG in fields of common interest, in particular in the promotion of international schools for young scientists. The essential agenda of the IOCG business meetings and their results are presented in the report on the IOCG (Appendix K to the Agenda).

The Commission recommended IUCr sponsorship for the following international schools and conferences: Tenth International Summer School on Crystal Growth (ISSCG-10), Rimini, Italy, 1–6 June 1998, and the Twelfth International Congress on Crystal Growth (ICCG-12), Jerusalem, Israel, 26–31 July 1998. In addition, the Commission contributed to the programme of the Glasgow Congress, by establishing two microsymbiosia on crystal growth.

H. Klapper, Chair

4.7. Commission on Crystallographic Computing

In the triennium, the Commission has been engaged in the following activities, presented in chronological order.

1. At the Seattle Congress, the Commission sponsored an Open Session entitled ‘General Advances and Application of Crystallographic Computing’. The session was organized by G. J. Kruger and P. E. Bourne and chaired by D. Viterbo.

2. The seventh IUCr-sponsored computing school took place in 1996 following the Seattle Congress. The school was organized by Commission members P. E. Bourne and K. Watenpaugh and took place in Bellingham, USA. The School attracted 106 attendees from 16 countries. Of these, 38 were either speakers or tutors. The School covered the latest developments in macromolecular crystallographic computing for all aspects of the experiment and subsequent structure analysis.

3. School Proceedings, provided to attendees in draft form and after the school revised by the speakers, were made available on the

Commission’s web site in March 1997. For the period March 1997 through the end of that year, there were 27,090 hits on the web page. Recently, there were still several downloads per day of individual papers.

4. The 1996 School Proceedings are in the final stages of being published. It has taken hundreds of hours of additional author volunteer effort and support from the San Diego Supercomputer Center (SDSC) to get them into a format acceptable to Oxford University Press. The cost of the Proceedings is being off-set by unspent funds raised for running the School.

5. An Open Session of the Commission has been organized for the Glasgow Congress, entitled ‘Improved Accuracy through Software’. Invited speakers are J. Albertsson, H. Berman, C. M. Gramaccioli, B. McMahon and P. S. White. The session was organized by all members of the Commission and will be chaired by P. E. Bourne.

6. The 1999 Computing School ‘Frontiers in Computational Crystallography’ will be held in Hixton, near Cambridge, UK, following the Glasgow Congress. G. Bricogne and D. Watkin are organizing the School.

Enhancements to the Commission’s web site to include reports, Proceedings of the 1996 School and forthcoming events have been made throughout this period. Little progress has been made on the charge of providing high-quality standard data sets that would be used by software developers to validate their work. Available information was to include experimental data derived from powders and single crystals of inorganic and organic compounds, including proteins at various resolutions. Results derived from using these data by different software programs would also be available. Users would be able to obtain all data and results from the Commission’s web site and from CD ROM. It is hoped that the incoming Commission will take up this charge.

P. E. Bourne, Chair

4.8. Commission on Crystallographic Nomenclature

The Commission met in Seattle shortly before the Congress opened; all its other work throughout the triennium was accomplished either electronically or by ‘snail-mail’, with the following exception. Several members of the Sub-committee on the Nomenclature of *n*-Dimensional Crystallography met in person in July 1997 in Nijmegen, The Netherlands, in December 1997 in Paris, France, and in August 1997 in Geneva, Switzerland. Membership of the Commission is entirely *ex officio*, by virtue of a primary IUCr responsibility closely related to crystallographic nomenclature. Six new members joined the Commission following appointment either as Editor of an individual Volume of *International Tables for Crystallography*, as Chair of the Committee for the Maintenance of the Crystallographic Information File Standard (COMCIFS), or as Chair of the IUCr/OUP Book Series Committee. As in prior triennia, the work of the Commission was conducted primarily through the expert sub-committees and working groups it appoints. All recommendations arising thereby are reviewed by the Commission.

The Sub-committee on Atomic Displacement Parameter Nomenclature completed its 1994 charge of examining the merits of a uniform approach in reporting quantities that describe atomic displacement with a report entitled *Atomic Displacement Parameter Nomenclature*, which was published in *Acta Cryst.* (1996), **A52**, 770–781. Following a consideration of the inconsistent terms and symbols previously used for parameters denoting dynamic or static displacements of atoms in crystals, the report provides clear definitions for these quantities, discusses graphical representations of the Gaussian mean-square displacement matrix and the expressions used if the

Gaussian approximation is inadequate, and makes recommendations for symbols and nomenclature. It, as all other Commission reports, is now fully accessible on-line at the Commission's home page, see below.

The Sub-committee on the Nomenclature of *n*-Dimensional Crystallography, see *Acta Cryst.* (1996), A52, 91–124 for membership, completed its 1990 charge of assessing the extent to which the representational symbolism then in use may have become so non-uniform as to be unacceptably ambiguous with a report entitled *Symbols for Point-Group Transformations, Families, Systems and Geometric Classes* (in *n* Dimensions). The Commission accepted the revised report, with its unified notation and symbolism for crystallography in arbitrary dimensions, on 16 November 1998. It will appear in *Acta Cryst.*

J.-C. Tolédano was appointed Chair of the Working Group on Phase Transition Nomenclature in 1995 and R. S. Roth to membership in 1996 replacing R. L. Snyder who resigned; see *Acta Cryst.* (1996), A52, 91–124 for the remaining members. The Working Group completed its 1994 charge of studying the current multiple-choice nomenclature for naming the phases formed sequentially by a material as a function of temperature and/or pressure with a report entitled *Structural Phase Transition Nomenclature*, which was published in *Acta Cryst.* (1998), A54, 1028–1033. The resulting notation uses six separate fields to specify the essential crystallographic and physical characteristics of each phase in the sequence the first time the phase is named in a paper. Following first use it is recommended that if the phase is commonly associated with a trivial label such as α or I, then the first two fields only be used later in the paper to identify that phase; if not commonly associated with a label, then the second two fields should be used. Examples drawn from the sequence of phases formed by nine different materials are provided. After the revised report had been accepted, the Commission further charged the Working Group in 1998 with extending the recommended nomenclature to incommensurate, polytype, quasicrystal, magnetic and time-resolved phase transitions. Membership in the continued Working Group consists of J.-C. Tolédano (Chair), P. J. Brown, A. M. Glazer, R. S. Roth, R. S. Berry, R. Metselaar, D. Pandey, M. Perez-Mato and S. C. Abrahams.

A question concerning the definitions in the Commission report of 1989 entitled *Definition of Symmetry Elements in Space Groups and Point Groups* and another concerning Fig. 3 of the 1992 Commission report entitled *Symbols for Symmetry Elements and Symmetry Operations* led to the appointment of an *ad hoc* group consisting of H. D. Flack (Chair), Th. Hahn, H. Wondratschek and S. C. Abrahams. Following thorough examination, any corrections found necessary will be presented later as *addenda* to the original reports.

The Commission Observer [see *Acta Cryst.* (1997), A53, 822] has noted that COMCIFS was very active in the triennium, posting a modified version and then approving a new version of the core CIF dictionary, a new Powder CIF dictionary and a management group with responsibility for its development. There were no nomenclature issues in contention and cooperation with COMCIFS was harmonious.

The name of each member, the office on which *ex officio* membership depends, and the titles of all reports are listed on the Commission's home page at <http://www.iucr.ac.uk/iucr-top/comm/cnom/index.html> through the skilful efforts of B. McMahon. The page also provides general information about the Commission, links to each member, to the full content on-line of *all* Commission reports, and to a valuable group of sites containing nomenclature resources of interest to crystallographers.

S. C. Abrahams, Chair

4.9. Commission on Crystallographic Teaching

4.9.1. Visiting Professorship Programme. Visiting Professorships were granted to J. P. Glusker (see below) in 1997 and to D. Viterbo, who was a Visiting Professor at the University of La Habana, Cuba, 1–14 July 1998. Professor Viterbo presented several lectures concerning X-ray diffraction and crystal structure determination as an introductory part to an International School on Materials. A number of Visiting Professorships were awarded in 1997 and 1998 as part of a project to promote crystallography in Africa. UNESCO awards through ICSU helped to support this Programme.

4.9.2. Contributions to Schools of Crystallography. The Commission has taken an essential part in organizing the Fifth International School and Workshop of Crystallography: Teaching and Applications, which took place in Suez, Egypt, 5–11 April 1997. K. El-Sayed was the Chair of the Organizing Committee, and L. A. Aslanov, J. P. Glusker, C. M. Gramaccioli and Å. Oskarsson were members of the Programme and Scientific Committees, and some were also teachers there.

M. Laing has taken active part in organizing a School on Practical Applications of X-ray Powder Diffraction, which was held in Durban, South Africa, 22–26 September 1997. The Commission has also positively supported applications from some other International Schools asking for IUCr sponsorship and financial support: The Rietveld Summer School, Cieszyn, Poland, August 1997; Direct Methods, Erice, Italy, 22 May–2 June 1997; Electron Crystallography, Erice, Italy, 22 May–2 June 1997; Implications of Molecular and Materials Structure for New Technologies, Erice, Italy, 28 May–7 June 1998 (C. P. Brock, M. Gramaccioli and L. Riva di Sanseverino participated as teachers); International School on Data Mining in Crystallography, to be held at Erice, Italy, 12–23 May 1999.

4.9.3. Other activities. At the Seattle Congress, a session on Teaching Crystallography was organized by Å. Oskarsson and L. A. Aslanov. Several members of the Commission contributed to the session. M. B. Hursthouse and E. Makovicky organized a session on Computer-Based Teaching in Crystallography at ECM-17, Lisbon, Portugal, 24–28 August 1997. An Open Session on Teaching Crystallography was organized by Å. Oskarsson and D. Puscharowsky at ECM-18, Prague, Czech Republic, 16–20 August 1998. The Commission is presently organizing the Open Commission Session on Teaching at the Glasgow Congress.

C. M. Gramaccioli, Chair

4.10. Commission on Electron Diffraction

The Commission has been involved in a number of Schools on Electron Crystallography. One of these was held in Erice, Italy, in 1997 and directed by D. L. Dorset (Secretary of the Commission). There were 20 lecturers from 10 countries and 228 students from 24 countries. Joint sessions were held concurrently with the NATO Advanced Study Institutes on Direct Methods of Solving Macromolecular Structure. This school was supported by the IUCr as was a School on Electron Crystallography held in Stockholm, Sweden, in 1998. This school, organized by S. Hovmöller and X.-D. Zou, was also well attended and stimulating with a wide range of international participants and lecturers (one being J. W. Steeds, Chair of the Commission). Another similar school is being organized by S. Hovmöller and X.-D. Zou in Nantes, France, in 1999.

Members of the Commission have been influential in organizing and contributing to a large number of conference sessions related to electron diffraction. The list is too long to give in detail but includes two sessions of the Fourteenth International Congress of Electron

Microscopy in Cancun, Mexico, one on Electron Crystallography (S. Hovmöller) and another on Convergent-Beam Electron Diffraction (J. W. Steeds). Also worthy of report is the election of D. L. Dorset as a member of the US National Committee for Crystallography (1996–1998). D. L. Dorset contributed a paper to a special issue of *Acta Crystallographica*, entitled Electron Crystallography – Accomplishments and Challenges [*Acta Cryst.* (1998), **A54**, 750–757].

D. L. Dorset is a member of the Programme Committee for the Glasgow Congress. The Commission is organizing three micro-symposia on Quantitative Electron Diffraction and Microscopy (Chairs D. van Dyck and J. K. Gjønnnes), The Phase Problem in Electron Crystallography (D. L. Dorset and R. Vincent) and Structure Solutions from Powders using Electron and Powder Diffraction Techniques (S. Hovmöller with R. J. Cernik of the Commission on Powder Diffraction).

The decision for gas electron diffraction to be moved to the Commission on Structural Chemistry is regarded as a sensible rationalization. The Commission effectively covers three communities at present. First there is the dynamical diffraction community for high-energy electrons using convergent-beam techniques. Second, there are the former X-ray crystallographers who are transferring well developed techniques from that field to electron crystallography. Third, there is the surface electron diffraction community. The one important community not represented at present is biochemical electron microscopists largely in the field of membrane proteins who rely on Fourier transformation of averaged image intensities to solve crystallographic problems. It would be an interesting challenge to try to extend our dialogue to this community in the next few years.

J. W. Steeds, Chair

4.11. Commission on High Pressure

The triennium now ending has been the first for the Commission on High Pressure. The Commission was created at the Seattle Congress without prior preparation, and started out as the previously existing High Pressure Group of the Commission on Crystallographic Apparatus under a new guise, but with the same membership and no specific new remit. A substantial task of the triennium has thus been to metamorphose the Group into a Commission – with Terms of Reference, a broader remit, officers, and a clear role and identity in the IUCr – as well as continuing the regular programme of meetings established by the Group, starting in 1989.

To secure expertise over the wider range of science that it was felt appropriate for the Commission to cover, consultants were appointed in the areas of stress effects (A. K. Singh), and biological and other soft matter (S. M. Gruner). It was also decided that the Commission should have both a Secretary (J. B. Parise) and a Treasurer (W. F. Kuhs). It became clear in the first year that the Commission would benefit from taking time to frame its Terms of Reference. The change from the Group, with its focus on single-crystal and powder diffraction, to the wider role and responsibilities of a Commission led to considerable debate as to just how wide its scope should be. The matter was discussed at a meeting of the Commission held at Grenoble, France, in November 1997; the experience of mounting a Workshop, at Argonne, USA, in November 1998, covering the proposed full range of the Commission's activities, was used to test and finalize ideas; and the Terms as now approved by the Executive Committee were agreed at a meeting of the Commission held during that Workshop. The Commission has undertaken to work to strengthen the links between high-pressure crystallography and the wider field of high-pressure science, to make the scope of high-pressure crystallography as inclusive as possible without compro-

promising its crystallographic identity, to make information about high-pressure methods and facilities widely available, and where possible to assist young scientists and others new to the field. In pursuit of these and other aims, the Commission now also has an active web page under continuing development.

4.11.1. Symposia and workshops. The Commission's principal activity has been the organization of symposia and workshops. High-pressure crystallography is going through a period of rapid change and major development that seems set to continue for many years yet. Regular meetings are essential to keep the community in touch with the latest science and techniques, and also to keep the Commission abreast of growth in the community and to draw in new people. One sign of the level of innovation has been the difference in topics and speakers from one year's meeting to the next throughout this triennium. The Commission has been particularly concerned to encourage participation in its symposia and workshops by young scientists, and has been greatly assisted in this by funding from the IUCr.

The inaugural activity of the Commission was a one-day Symposium on 'Structural Study under High Pressure using X-rays and Neutrons' at the International Conference on High Pressure Science and Technology (AIRAPT-16) held in Kyoto, Japan, 25–29 August 1997. The organizer was Commission member O. Shimomura. The programme focused principally on synchrotron and neutron facilities around the world, and the latest high-pressure results obtained using them. There was an excellent attendance of some 50 participants throughout despite the competition from eight other symposia.

The Commission's first independent meeting was a three-day Workshop on Crystallography at High Pressure using Synchrotron Radiation; the Next Steps, held at ESRF, Grenoble, France, 21–23 November 1997. The organizer was Commission member D. Häusermann. The focus on synchrotron science was selected to celebrate the first few years of successful operation of ESRF, which had made a major impact on high-pressure techniques and research. Nearly 30 scientists selected from the main groups active in synchrotron techniques and associated fields from around the world gave invited talks. Over 80 participants from 18 countries included 11 young scientists who benefited from support for the workshop from the IUCr. The workshop also received generous financial support from ESRF, in addition to access to its meetings' facilities.

A four-day workshop held at Argonne National Laboratory, USA, 14–17 November 1998, on Synchrotron, Neutron and Laboratory Source Crystallography at High Pressure was the first attempt to hold a meeting encompassing the full range of the Commission's activities. The organizer was Commission member and Secretary J. B. Parise. The programme ranged over soft and biological matter, Earth and planetary science, new materials, physical and chemical properties including magnetism and superconductivity, structures and transitions in fundamental ionic, metallic and H-bonded systems, the latest in facility and technique developments around the world including work at extremes of pressure and temperature, with experimental methods ranging from diffraction – including from liquid and amorphous samples – through inelastic neutron and X-ray scattering to optical, Mössbauer and X-ray spectroscopy, and a substantial component of the latest computational work. Nearly 120 participants from 14 countries included 23 young scientists, 17 of whom benefited from support for the workshop from the IUCr. The workshop also received financial support from the Center for High Pressure Research at Stony Brook and the Carnegie Institution of Washington, the GeoSoilEnviro-Consortium for Advanced Radiation Sources (GSECARS) at the Advanced Photon Source (APS), and the APS

itself, as well as very considerable assistance with local arrangements from N. Lazarz and other GSECARS staff.

All members of the Commission put a large amount of effort into planning and running these meetings. Over the past year, they have also been actively engaged in shaping the Commission's sessions for the Glasgow Congress, particularly A. Katrusiak who is a member of the Programme Committee. All other members and consultants are acting as Chairs or Co-chairs for the Commission's microsymbiosia. There are to be six of these, two keynote lectures, and an Open Commission Meeting over four days of the Congress. The number of abstracts submitted shows a 40% increase over the Seattle Congress.

4.11.2. Meetings of the Commission. All members of the Commission have met on two occasions during this triennium, first at the 1997 Workshop in Grenoble and then at the 1998 Workshop in Argonne. The main items of business at the first meeting were the Terms of Reference, membership and the appointment of consultants, and future meetings. In addition to all the members, both consultants would also have been present at the second meeting but for A. K. Singh's absence due to a bar by the US Government on Indian scientists entering the Argonne site. The main items of business at this second meeting were the final Terms of Reference, future membership of the Commission, plans for sessions at the Glasgow Congress, and other future plans and activities.

4.11.3. Other events. The Chair represented the Commission at a workshop in honour of C. T. Prewitt and L. W. Finger, held at the Carnegie Institution in Washington DC, USA, 11–13 April 1999, to mark the retirements of these two outstanding high-pressure crystallographers. C. T. Prewitt was a former member of the pre-existing Commission on Crystallographic Studies at Controlled Pressures and Temperatures, and L. W. Finger was a member of that Commission and of the subsequent High Pressure Group of the Commission on Crystallographic Apparatus.

4.11.4. Future plans and activities. The Commission intends to organize workshops in 2000 and 2001, at venues yet to be finally agreed. Plans are also under way to organize a School on High Pressure Crystallography at Erice, Italy, in 2003. Commission member A. Katrusiak is acting as the Commission's contact with the organizers of the Erice programme. Work is currently in progress to compile a directory of high-pressure crystallographers and their research. The Commission also plans to collect and disseminate information on central facilities for high-pressure crystallography, and on how to access them.

The Commission thus reaches its first Congress fully fledged, but still developing. Just one of the significant developments of this triennium has been the successful introduction of the field of biology and soft matter into the Commission's activities. Further enlargements seem certain to follow. The interfacing of the core of high-pressure crystallography to the wider field of high-pressure science has been a key task and priority, and will remain so; there is good evidence that the Commission is being successful in attracting a growing number of that wider community to its fold. Much is owed to the hard and creative effort put in by Commission members and consultants, who have all been exceptionally active and reliable throughout this triennium in response to many requests for involvement in shaping workshop and Congress programmes, Terms of Reference and other Commission business, and in attending meetings of the Commission. The Commission looks forward to its second triennium aware of much yet to be done, but also confident that the effort will prove as rewarding as hitherto.

R. J. Nelmes, Chair

4.12. Commission on Neutron Scattering

The last three years have seen major developments in neutron scattering worldwide. On the one hand, there have been major plans developed for advanced neutron scattering facilities in Europe, North America and in the Asia–Pacific region and, on the other, the formation of strong neutron scattering associations in Europe and North America and the beginnings of such an association in Asia/Australasia/Oceania. The Commission on Neutron Scattering 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. This report will concentrate on these developments which have far-reaching consequences for structural and dynamic studies in chemistry, physics and biology as neutron beams with intensities of the order of 100 times those currently available may become accessible in the first years of the new millennium. This is not to forget, however, the very successful satellite meeting and microsymbiosium programme at the Seattle Congress, the ongoing interests of the Commission in international standards for neutron inelastic scattering cross sections (NISC) and the internationally agreed exchange format for neutron and synchrotron data as well as the preparations for the satellite and microsymbiosia, Open Commission Meetings *etc.* at the forthcoming Glasgow Congress.

4.12.1. International meetings. The firm foundation in neutron scattering research across a broad range of subject areas in Europe as a result of the domestic reactor neutron scattering programmes of European countries and their participation in the Institut Laue–Langevin, Grenoble, France, is well recognized. Since 1995 the establishment of the European Neutron Scattering Association (ENSA) has given form and organization to this community of scientists. The first major meeting of this association at Interlaken, Switzerland, was a resounding success and drew more than 800 participants. The next meeting of this group will be in Budapest, Hungary, 1–4 September 1999, and is again likely to be a 'Mecca' for neutron scattering practitioners worldwide.

In parallel with this, the Neutron Scattering Association has also gone from strength to strength with a very successful meeting in Toronto, Canada, 16–20 August 1997, and satellite meetings at the National Institute for Science and Technology, Gaithersburg, USA, as well as the Intense Pulsed Neutron Source, Argonne National Laboratory. Here about 200 scientists from the USA, Europe and other countries met and there was a strong participation of young scientists. The fields of interests, as in the European meeting, ranged from low-resolution biological structure determination using neutron contrast variation through chemistry and materials science to solid-state physics including superconductivity, ultra-low-temperature magnetism and soft-matter physics. It appears that the widening of applicability of neutron scattering techniques already demonstrated by the European experience is happening elsewhere, particularly as cold neutron sources and the new methods of neutron reflectivity and very high resolution neutron inelastic scattering become more widely understood and applied.

The formation of an Asia/Australasia/Oceania neutron scattering association mooted in the 1997 report has the strong support of the Japanese Neutron Scattering Association and the Australian National Committee for Crystallography. As mentioned in this year's report, the most tangible initial step was taken at the Asian Crystallographic Association's meeting in Malaysia (October 1998) with a significant part of the programme devoted to neutron scattering measurements. Major investments in new neutron sources likely to occur or already decided in the Asia–Pacific region (see below) should provide a boost

to these initiatives, similar in magnitude to that which has been seen in Europe and North America. It will be the task of the Commission and its members to facilitate these developments with other colleagues.

It would be remiss not to mention the lively participation of neutron scattering scientists in a variety of conferences over the last few years that have been devoted to particular scientific themes. One of the problems of the old International Atomic Energy Agency conferences, which many of us so much appreciated in the 1960's and 1970's, was that they became meetings where the 'converted preached to the converted'. Neutron scattering research now is an integral part, like nuclear magnetic resonance spectroscopy, of many scientific disciplines and the Commission sees it as quite healthy that there are now conferences speaking specifically of neutron and X-ray scattering from surfaces *etc.* – the techniques having become sufficiently mature to command specialist worldwide audiences at regular intervals in particular subject areas such as surface science.

4.12.2. New major neutron scattering facilities – international cooperation. The Mega-Science Forum of the Organization for Economic Cooperation and Development (OECD) produced a report in 1997 which surveyed the possibilities for international cooperation in the construction of major new facilities for neutron scattering, synchrotron radiation *etc.* The obvious intention was to rationalize development of these sources and maximize international cooperation, which institutes such as the Institut Laue–Langevin, Grenoble, France, have shown to be so valuable for facilitating new scientific developments. Another intention was to use most wisely the experience gained in the construction of one major facility to take the next step with its successor. In this way, a worldwide development of facilities could be promoted. The Mega-Science Forum discussions were also in response to the predicted 'neutron drought' likely to occur as the older generation of nuclear reactors become obsolete and are closed down in the early years of the next century, and also a response to the long maturing intentions for major source construction in Europe, North America and Japan.

The last three years have been an exciting period. In North America, the major project to create the Advanced Neutron Source (ANS) based upon the world's most powerful nuclear reactor project at the Oak Ridge National Laboratory in the USA was finally cancelled in 1996, to be replaced by the spallation neutron source (SNS) project, again at the Oak Ridge National Laboratory, USA, whose design characteristics to produce a 1 MW spallation neutron source target would make the next quantum leap beyond the existing world's best spallation source, the ISIS source at the Rutherford–Appleton Laboratory in the UK. This project has since been funded by the United States Congress.

In Europe, the continuous 1 MW spallation neutron source at the Paul Scherrer Institute in Switzerland has become available and shows the power of a spallation source built on those principles. The JRM-2 reactor project in Munich, Germany, is now under construction and is likely to be the world's most powerful medium flux reactor when it is completed in about two years. The future needs for neutron scattering facilities in Europe were reviewed at a meeting sponsored by the European Science Foundation at Autrans near Grenoble, France, in May 1996 and there are extensive discussions in Europe for a second phase development at the ISIS neutron scattering facility in the UK as well as in preparation for the projected European Spallation Source (ESS).

Nor is major instrument development lacking in the Asia–Pacific region. In Australia, the government decided to replace the ageing HIFAR nuclear reactor at Lucas Heights near Sydney with a modern 20 MW research reactor to be in operation by 2005 and, in Japan,

major projects were studied both at the KEK, Tsukuba, and in the Japanese Atomic Energy Research Institute (JAERI), Tokai, in 1997 and 1998. The Tsukuba project was for the Japanese Hadron project a 0.6 MW pulsed spallation target and associated instruments and the JAERI project was not only to build something approaching 2 MW in a spallation target useful for neutron scattering but also to begin the study of the destruction of transuranic nuclear waste using spallation. As reported in the 1997 and the 1998 reports, various members of the Commission have been involved in all of these developments giving advice to governments through national and international advisory committees. The Japanese project has recently come to a very exciting point where the KEK and JAERI projects may be combined in a joint project for the most powerful spallation neutron source in the world likely to be operating before 2004. It is expected that a decision on this project will occur within the next six months.

4.12.3. Conclusion. This report has attempted to reflect something of the way in which neutron scattering is developing worldwide. The development of the technique necessarily relies on initiatives taken at large institutes or through a combination of large institutes. These bodies and national bodies have to take the initiative as they have the budgets and the scientific strength to bring together the working parties and technical expertise needed to underpin proposals for finance ranging from hundreds of millions of dollars to more than a billion dollars. It is essential for the scientific intentions – the problems that need to be solved and the sifting of those problems to be sure that the best scientific and technical reasons for the investment are chosen – that the Commission and its members should continue to play a key role.

J. W. White, Chair

4.13. Commission on Powder Diffraction

The Commission had an ambitious programme of events and projects during the triennium. The mailing list for the *Newsletter* 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. 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 microsymbioses 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 largest meetings covering the areas of interest for the Commission were the European Powder Diffraction Conferences held in Parma, Italy, and Budapest, Hungary. These were excellent meetings organized by G. Artioli and

T. Ungar. Both conferences covered structure solution; refinement; QPA; *in situ* kinetics; catalysis; disordered structures; instruments; size/strain; accuracy; thin films and general materials. The focus of the Budapest meeting was more strongly concentrated on practical applications of the method. The Commission held business meetings in Parma (1995) and Budapest (1998). There was Commission involvement in the 17th Conference on Applied Crystallography and the 3rd Rietveld Summer School organized by D. Stroz (1997) and at the workshop to discuss the possibility of a Spanish powder beamline at the ESRF (1998). Commission member S. Sen-Gupta organized a meeting in Calcutta, India (1998), which included a wide variety of presentations, mostly practical. This meeting was very popular and included the President of the IUCr among the attendees. Shao Fan Lin obtained funding for visiting speakers to a powder workshop to be held in Kunming, People's Republic of China (1999). The Commission was also represented at the Stockholm School on Electron and Powder Diffraction (1998) organized by S. Hovmöller. Throughout the triennium there were a significant number of people participating in Commission events and the Denver meetings. In 1996, M. Delgado organized a powder diffraction course in Merida, Venezuela, and there was a School on Polycrystalline Diffraction in Frascati, Italy (1996), organized by G. Cappuccio.

4.13.2. Projects. Quantitative phase analysis. Four samples of carefully constituted multiple composition have been distributed to those people who volunteered for the study. All the results are back and have been analysed. The participants have all been informed of the real composition of the test samples. The original chemical specification has changed slightly since the original specification and is now better defined. The samples are (1) corundum + zincite + fluorite; (2), as (1) but with preferred orientation and brucite; (3), as (1) but with amorphous glass; (4) corundum + magnetite + zircon. Thanks are due to I. C. Madsen particularly but also to Commission consultant R. J. Hill, and to Commission member D. K. Smith. I. C. Madsen will present the results of the study in full at the Glasgow Congress.

Rietveld guidelines. Commission member L. B. McCusker has led the project to publish advice and guidelines for Rietveld refinement [*J. Appl. Cryst.* (1999), **32**, 36–50]. The paper has the endorsement of the Commission and we hope that it will spread better working practices amongst the powder community. This was felt to be necessary after the results of the first Commission round robin were published by R. J. Hill & L. M. D. Cranswick [*J. Appl. Cryst.* (1994), **27**, 802–844]. A copy has been distributed with the *Spring Newsletter*.

Industrial application notes. Commission member P. Scardi has begun research into the possibility of the Commission making further inroads towards industrial application notes. The aim would be to publish good practice in certain common industrial situations in a variety of languages. This project is not finished but has attracted a good deal of interest.

Software and the web. The Commission web site has been used to direct interested parties to freely available software in powder diffraction. Links now exist to the CCP14 and programme exchange banks. Further links on the Commission 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.

Newsletters. There have been five *Newsletters* published in this period edited by Commission members L. B. McCusker, R. Delhez, P. Scardi, S. Sen-Gupta and guest editor L. M. D. Cranswick. All editions have appeared on the web (<http://www.iucr.org/iucr-top/comm/cpd/index.html>).

R. J. Cernik, Chair

4.14. Commission on Small-Angle Scattering

The Commission was chartered at the Seattle Congress. During the three years since its inception, this Commission has focused on three topics: (1) community building, (2) education, and (3) standardization.

A web site (<http://www.nist.gov/sas>) has been built to serve as a 'community centre'. The associated list server (sa_scat@nist.gov) has attracted a fairly steady subscribership of 300+ individuals. The message traffic has been sparse, but many readers have found it to be a valuable resource for getting questions answered and activities publicized.

The series of triennial world congresses established in 1965 has long been a core component of the small-angle scattering (SAS) community. 1999 is the occasion for the eleventh such congress (see <http://sas99.bnl.gov/sas99>). This will serve as a formal occasion for obtaining feedback and enhanced participation from the members of the community.

On the education front, there has been a more or less steady series of workshops and organized sessions at national meetings. The Commission has worked with the American Crystallographic Association, the Society of Plastics Engineers, and the American Chemical Society in these efforts. These activities are aimed at increasing awareness of SAS methodologies in the broader world of materials science. Dates and titles are available in the Commission's Annual Reports for the relevant years.

It will be an uphill struggle for the Commission to get standardized SAS methodologies accepted into the community. The tradition of quantitative characterization of the performance of test methods is weak. Indeed, many users do not understand the concept of a 'SAS test method'. There is no widespread set of software tools for reducing and visualizing SAS data. There has been very little work devoted to putting data derived from different realizations of SAS experiments onto a common basis.

An interlaboratory test program for SAXS measurements in the moderate q range ($0.1 < q < 3 \text{ nm}^{-1}$) is in the design stages. We are soliciting suggestions for suitable samples for use in a comparable effort for SANS. We hope that the results from such objective assessments of test method performance will stimulate a desire for more rigorous approaches to these matters.

The Commission has taken some tentative steps in the direction of improved standardization by issuing a draft CIF for one-dimensional SAS data. We have been supporting other efforts to develop suitable standards for two- and three-dimensional SAS data. The hosts of software tool collections are being encouraged to expand their activities.

By increasing the awareness of SAS users, by promulgating appropriate standards, and by facilitating the development of appropriate analytical methods, the Commission hopes to help our little corner of crystallographic science realize its full potential.

The Commission would like to thank M. Hart and H. Fuess for their efforts on our behalf in their roles as liaison to the Executive Committee. The support of P. Coppens and W. L. Duax as we worked to establish the Commission and develop its agenda is also appreciated.

J. D. Barnes, Chair

4.15. Commission on Structural Chemistry

For many years, there had been a feeling among the members of this Commission that the title Commission on Small Molecules was no longer descriptive of the broad areas of research being pursued by

many non-macromolecular crystallographers. In recognition of the continuing evolution of this field, the Commission requested that its name be changed to the Commission on Structural Chemistry. The request was approved at the Seattle General Assembly. A single-crystal electron diffractionist was also added to the membership of the Commission.

The Commission members met twice during the Seattle Congress, once under outgoing Chair F. H. Herbstein and once under the incoming Chair C. Krüger. During the second meeting, the Commission members took advantage of the presence of J. A. K. Howard to extend early programme suggestions for the Glasgow Congress. The Commission also responded favourably to a request by Y. Ohashi for support of a meeting in Japan on Analysis and Design of Solid State Organic Reactions, 30 September–2 October 1996.

In 1997, the Commission supported three meetings: Indaba II – Intermolecular Interactions, held in Kruger National Park, South Africa, in August and organized by J. C. A. Boeyens; the 10th International Symposium on Organic Crystal Chemistry, also held in August in Poznan-Rydzyna, Poland; and the workshop Predictability of Crystal Structures of Inorganic Solids held in October and organized by the German Crystallographic Society and the German Chemical Society.

The annual meetings of the regional crystallographic associations continue to include sessions and workshops on topics of interest to the community represented by the Commission. In addition, we feel that it is important to reach out beyond the crystallographic meetings to introduce a broad-based chemical audience to the benefits of X-ray crystallography. Towards this goal, a session entitled Advanced Methods of Structure Determination by Diffraction and Related Methods was organized by A. Clearfield for the American Chemical Society meeting in Dallas, Texas, USA, in the spring of 1998. In 1998, the Commission also gave its support to a workshop on Modern Techniques in Structural Chemistry of Microcrystalline and Amorphous Compounds, which was scheduled for October in Germany. Unfortunately, this workshop was cancelled for lack of participation. Commission member V. Belsky was involved in the organization of the first Russian National Conference on Crystal Chemistry. During 1998, the Commission also made further contributions to the organization of the programme for the Glasgow Congress.

Throughout the triennium, the Commission endorsed a number of the NATO Advanced Study Institutes which are held every year in May in Erice, Italy. Reports on meetings of interest to structural chemists can be found at <http://www.geomin.unibo.it/orgv/erice/erice.htm>.

Even before the name change, the Commission had begun to broaden its scope and the process has continued during the triennium. It now represents not only the single-crystal X-ray and electron diffraction communities but also other topics of interest, such as crystal engineering, modelling techniques, and all theoretical aspects of structural chemistry. More details about Commission activities may be found on its new web home page as well as in the annual reports to the IUCr. Most of the symposia and workshops supported by the Commission have been reviewed in the *IUCr Newsletter*, the *ACA Newsletter*, or similar publications. The Commission has not yet interacted with crystallographers in South America and some parts of Asia but hopes to be able to do so in the future.

It is noted that the concerns of the Commission as pointed out in the last report to the IUCr have become even more severe during the last triennium: the disappearance of crystallographic education from standard university coursework, the tendency towards the use of 'black box' applications without any fundamental understanding of

the science of crystallography, and the increasing number of errors appearing in the crystallographic literature.

In addition to supporting symposia and workshops, it must be one of the tasks of the Commission to develop recommendations for the appropriate approval of crystallographic research results in publications of related fields. The Commission also intends to work with the Commission on Biological Macromolecules and the Committee on Crystallographic Databases to develop guidelines for deposition of structure factors for all structures.

J. L. Flippen-Anderson, Secretary

4.16. Commission on Synchrotron Radiation

The main activity of the Commission during the triennium has been to organize scientific meetings that cover the broad fields of crystallography involving the use of synchrotron radiation.

The Commission was heavily involved in the Seattle Congress. Three microsymbposia (Synchrotron Radiation I, II and III) were successfully organized. In the microsymbposia, topics were focused on Instrumentation and Techniques, Macromolecules and Applications; Time-Resolved, Micro-crystal, High Energy, respectively. In addition to the main Seattle Congress, a synchrotron-radiation satellite meeting at the Advanced Photon Source (APS) in Argonne, USA, was organized under the auspices of the Commission and the APS (4–7 August 1996). 150 people participated in the satellite. More than 30 invited leading synchrotron-radiation scientists presented the latest developments in the field. The impact of the new third-generation sources was reviewed. The satellite consisted of seven oral sessions and four poster sessions. The oral sessions covered Facility Report, Developments at Third-Generation X-ray Sources, Macromolecular Applications, Materials Science and Physics Applications (two sessions), High-Pressure Applications, and Detector, software and instrumentation. During the Seattle Congress, a meeting of the Commission was held, and the future plans of the Commission's activities were discussed.

In 1997, the Commission organized a scientific meeting on the crystallographic application of synchrotron radiation (1–2 August 1997) at the Photon Factory as a satellite meeting of the Sixth International Conference on Synchrotron Radiation Instrumentation (4–8 August 1997) which was held at Himeji, Japan. Y. Amemiya (University of Tokyo) and T. Matsushita (Photon Factory) co-chaired the satellite meeting. In the meeting, particular attention focused on time-resolved X-ray experiments. The satellite meeting consisted of the following six oral sessions: (1) New opportunities for time-resolved experiments (I) – third-generation synchrotron radiation sources; (2) New opportunities for time-resolved experiments (II) – new methods; (3) Time-resolved small-angle X-ray scattering; (4) Mössbauer spectroscopy in time domain; (5) Time-resolved XAFS; (6) Detectors for time-resolved measurements. About sixty people from ten countries participated in the satellite. Advanced techniques and new methods for time-resolved measurements were discussed in detail over a broad range. The role of second-generation sources was discussed in relation to the new third-generation sources in order to broaden experimental opportunities available and to activate further the field of synchrotron-radiation research. The collaboration of the Photon Factory staff for the organization of the satellite was greatly appreciated. The proceedings of the satellite meeting were issued as a KEK Proceedings (74–14, November 1997, M), which is available from the KEK library.

Since the end of 1997, the Commission has been discussing the satellite meeting of the Glasgow Congress. The venue will be Daresbury Laboratory on 2–3 August. R. J. Cernik will chair the

satellite meeting. The title for the meeting is From Source to Science and covers topics such as: (1) Coherence; (2) Polarization; (3) High resolution; (4) Dynamic studies; (5) Anomalous scattering. In addition, there will be two plenary lectures. The main aim is for a small, well focused, friendly meeting with a single set of sessions.

The Commission has been heavily involved also in the Glasgow Congress. Three members from the Commission (Y. Amemiya, R. Feidenhans'l and A. Yonath) are serving as members of the Glasgow Programme Committee.

Through the activities of the Commission, the interaction between users groups of synchrotron-radiation facilities all over the world has been enhanced.

Y. Amemiya, Chair

4.17. Commission on XAFS

The IUCr Commission on XAFS has existed for three years, since its approval at the Seattle Congress. Activities during this period have focused on education, aimed at improving the practice of XAFS, on operations of the International Conference on XAFS, and on building an effective interface with the International XAFS Society.

4.17.1. Background. Over the last twenty years, X-ray absorption fine structure (XAFS) has developed into an extremely useful technique for obtaining local structural information for non-crystalline systems, thus making it often the structural technique of choice when crystallography cannot be used. In recognition of this natural connection between XAFS and crystallography, the Executive Committee of the International XAFS Society proposed that a Commission on XAFS be established within the IUCr. The creation of this Commission was approved at the Seattle General Assembly.

One of the principal goals of the Commission is to promote stronger links between the IUCr and the International XAFS Society (IXS). The IXS is a relatively new organization that represents all scientists that utilize the fine structure associated with inner-shell excitation (near edge and extended) by various probes (e.g. X-rays and electrons), including those who utilize related techniques for which the data are interpreted on the same physical basis (more information about the IXS can be found at <http://ixs.csrii.iit.edu/IXS/>). It is hoped that the creation of a Commission on XAFS will promote closer interactions between the X-ray diffraction and the X-ray absorption communities.

4.17.2. Educational activities. Since its creation, the principal activity of the Commission has been the development of educational materials aimed at improving the practice of XAFS. The most visible of these is the IXS homepage (special thanks are due to B. Bunker, G. Bunker, and the Center for Synchrotron Radiation Research and Instrumentation for development of these pages). The IXS home page serves as a clearing house for communication within the XAFS community, including information about worldwide synchrotron sources and access to a variety of XAFS databases (archived spectra, publications and software).

The web page committee has recently been updating and expanding the web page. It now has on-line XAFS Society registration and a community listing as well as many links to other synchrotron and related sites. A listing of all committees is on the site and work is under way to add all committee reports. The data listing provided by F. Lytle continues to receive attention from the community as well as a listing of analytical software and some preliminary descriptions of the features they contain. There are plans to expand other features of the site including a newsletter, and the abstracts from XAFS X and, hopefully, XAFS XI.

The Commission works (in cooperation with the IXS Education Committee) to develop course notes that can be used for XAFS training workshops. The IXS Education Committee is led by G. Bunker. It hopes to coordinate with schools and courses which teach XAFS around the world regarding the content of their curricula, develop standard educational materials and, possibly, organize XAFS training courses at locations around the world which may not have the expertise or resources to run a course themselves.

4.17.3. Standards and criteria in XAFS. As part of its educational mission, the IXS has established a Standards and Criteria (S&C) Sub-committee. Prior to 1998, it consisted of three sub-groups: experimental, analytical, and error reporting. In 1998, a group of scientists in the area of X-ray magnetic circular dichroism asked to affiliate with the S&C Sub-committee. This idea was accepted and they are now actively working on a report dealing with standards for XMCD. Because their scope is broader than XAFS, the XMCD subgroup is working in a parallel and coordinated fashion with the main committee. It met in Seattle, USA, in July 1997 and again in Chicago, USA, just prior to XAFS X. An oral report and summary of recommendations for error reporting which are under consideration by the S&C Sub-committee was made to the meeting. A draft report of the activities for the past two years is circulating in the committee. It is hoped that a final version will be ready soon. When it is, it will be posted on the IXS web page. There is also a set of recommendations for error reporting under final consideration by the S&C Sub-committee. If approved by the S&C Sub-committee, they will be forwarded to the IXS Executive Committee for approval as official policy of the IXS. The mechanism for this is still being determined but will involve time for input and suggestions from the community. After adoption by the IXS, the recommendations will be posted on the IXS web page. Although not directly involved in the S&C activities, the Commission maintains close links to this committee. It is hoped that the Commission can assist in the wide dissemination of the S&C recommendations through links to the IUCr, particularly the IUCr web page and perhaps publication in an IUCr journal.

4.17.4. Conferences and meetings. On 10–14 August 1998, the Tenth International Conference on XAFS was held on the Illinois Institute of Technology campus in Chicago, USA. Approximately 360 scientists from 23 countries attended the conference. The programme consisted of 467 abstracts for plenary talks, invited talks, contributed talks and posters. The co-chairs for the conference were B. Bunker, S. Heald and T. Morrison and the Programme Chair was J. Penner-Hahn. The first IXS award for career contributions to the field was presented to F. Lytle who gave a plenary talk on The EXAFS Family Tree: History of the Development of X-ray Absorption Spectroscopy. In addition, awards were given for the best poster by a young scientist at each session. The winners were M. Duff, D. Cabaret and S. Rossano. The IUCr also sponsored poster prizes for the best posters in the areas of biology and instrumentation and methods. These winners were A. Templeton and M. Suzuki. The proceedings of XAFS X will be published in the *Journal of Synchrotron Radiation*.

At XAFS X, it was announced that XAFS XI, which had previously been awarded to Japan and was to be held in 2001, had agreed to change its dates to 27–31 July 2000. It will be held in Ako City near SPring-8 (the Japanese third-generation synchrotron source). The timing of the XAFS conferences was changed in 1998 from every 2 years to every 3 years in order to avoid periodic conflicts with IUCr meetings. The additional phase shift in meeting year (from 2001 to 2000) was made in order to avoid conflicts with a major VUV conference. The selection and time for XAFS XII was also made at this time. This meeting will be held in 2003 in Lund, Sweden, associated with MAXLab.

As part of the effort to increase the coupling of the XAFS community with the IUCr, a session on XAFS was organized by the Commission at the ACA meeting in St Louis, USA, in 1997. It is planned to continue to sponsor related sessions like this at other related meetings. It was hoped that a similar session could be organized at the IUCr meeting.

J. Penner-Hahn, Secretary

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

In the triennium, the Committee on Electronic Publishing, Dissemination and Storage of Information (CEP) constituted a small and very active technical working group. The Committee suffered a tragic loss with the death of Professor E. N. (Ted) Maslen on 2 February 1997. In his role as Chair of the Working Party on Crystallographic Information, then as Director of Archiving and Crystallographic Information and then as founding Chair of this Committee, Ted guided the IUCr's publication and archiving activity into the electronic era through a tangled maze of options and opinions. The CEP was reinforced on 21 December 1998 by the appointment of L. M. D. Cranswick as a member.

A publishing consultant's study of activities of the IUCr was received in January 1996. The consultant recommended the use of SGML favouring a DTD modelled on the Elsevier Art(icle) DTD and conforming to ISO 12083. This is now the manner in which documents are treated in the editorial offices.

During the Seattle Congress, a microsposium devoted to the Internet was organized by two members of the CEP, and the Committee's then Chair E. N. Maslen gave a very clear exposition of the Science, Technology and Economics of Electronic Publishing in Crystallography, and Y. Epelboin spoke on Internet Resources for Crystallography. The microsposium also contained a talk from G. D. Purvis, an outsider to crystallography, on The Role of the World-Wide Web in Computational and Pharmaceutical Chemistry, and finished with short presentations on two hot subjects on the Internet, Java and VRML, both likely to have impact on the area of electronic publishing. Further, a workshop on the Internet was run to give participants hands-on experience.

In the period 1996–1999, on-line services based on the Internet have followed such a rapid and widespread development that it was not considered necessary to organize similar events in association with the Glasgow Congress.

Within the triennium, the CEP has expended considerable effort on the implementation and deployment of the IUCr web information service. This has been nurtured into a system with a unified design with content arising from distributed sources of information. A high priority is set on providing up-to-date information of use to the whole crystallographic community. During its meeting in Lisbon, Portugal, in August 1997, the IUCr Executive Committee delegated editorial powers for IUCr web services to the CEP. The information service needs its content to be increased by input from collaborating providers from the crystallographic community.

Within the triennium, deployment of mirror servers for the IUCr information services has passed from the stage of the non-existent to that of a fully functional, highly optimized set of mirror sites. The development involved not only overcoming the technical difficulties and improving the efficiency of file transfer but also of producing the policy documents detailing the responsibilities of site managers and National Committees. This policy was approved by the IUCr Executive Committee at its meeting in Lisbon in August 1997. The

latest improvements involved a considerable restructuring of the file system at the Chester site. As part of this strategy for mirror sites, the IUCr has acquired the Internet second-level domain name *iucr.org*, permitting a unified naming of Chester and the mirror sites. The deployment of the mirror-site system depends on the good will and involvement of the IUCr members (*i.e.* the National Committees for Crystallography) in providing equipment with network connectivity to act as mirror sites for their country or region. Some regions of the world are inadequately covered at the moment, depriving crystallographers of a very important resource.

The CEP identified a need within the community for discussion forums operated by means of an e-mail list server. In early 1998, this became operational and the CEP drafted a Policy Document on Creation and Management of Discussion Lists, which received the approval of the IUCr Executive Committee. The IUCr list server provides facilities for e-mail-based discussion lists on topics relevant to the IUCr and the field of crystallography. At present, the server is only lightly used.

A major revision of the *World Directory of Crystallographers (WDC)* was started at the beginning of 1996 and the National Editors were invited to prepare their data to be ready before the end of 1996. Subsequently, the tenth edition of the *WDC* was published and made available in printed form through a limited print run. The *WDC* was also made available for on-line consultation using a web interface on an industry-standard public-domain directory service. It has become apparent on many occasions that the procedures for updating the *WDC* were obsolescent. Consequently, a functional specification for a new implementation of the *WDC* as a relational database using technology parallel to, but not directly integrated into, the IUCr editorial-office production database is currently at the discussion stage. The design of this database is centred around the need to allow rapid, but supervised, updating of records in a secure manner. It is intended that it should be possible to consult the database on-line by a variety of the most popular industry-standard protocols.

The conversion of the Chester editorial office to electronic publishing using full-text SGML mark-up is virtually complete (apart from *Acta Crystallographica* Section C, which uses an entirely different production stream). The in-house production relational database is fully operational. The electronic on-line distribution of the IUCr's six journals will require an infrastructure that the Chester office is not in a position to provide itself, indeed in the same way that the printing, mailing and subscription administration for the printed journals is subcontracted. The negotiations with the publisher (Munksgaard) for the electronic distribution of the IUCr's journals are continuing.

The CD ROM is an attractive medium for electronic publication. The CEP is supportive of L. M. D. Cranswick's NeXus project. In this, CD ROMs are produced just-in-time upon request in small quantities on a low-cost burner and are distributed to crystallographers in developing countries lacking a reliable Internet connection. The content contains a 'virtual' WWW of crystallographic information drawn from the IUCr information services and elsewhere, and a selection of public domain software of general use and for crystallographic applications. Over 40 CD ROMs have been distributed in this way. The CEP is collaborating in the project to produce the CD ROM for the Glasgow Congress. The CD ROM will contain the Congress Abstracts, material from the sponsoring organization, a selection of the IUCr information services and a digitized copy of an out-of-print book. The CD ROM will be distributed to participants and will also replace the three-yearly printed supplement to *Acta Crystallographica* Section A containing the Congress Abstracts. The project will afford valuable experience in the production of CD

ROMs and in the scanning and digitization of books by a commercial service. The latter will be useful for the digitization of all back numbers of the IUCr journals.

Contacts are being pursued with some other learned societies and publishers concerning the checking of their crystal structure data. It is projected that the web interface and criteria used for the checking of these data for *Acta Crystallographica* Section C could be adapted to the needs and requirements of the other interested parties as individual joint developments with participation in costs.

Three members of the CEP (Y. Epelboin, H. D. Flack and B. McMahon) accompanied by S. R. Hall and A. Authier attended the ICSU Press/UNESCO conference on Electronic Publishing in Science held in February 1996 in Paris. The conference brought together interested parties from learned societies, publishing houses and libraries in a series of formal presentations and working groups in which the technical, economic and social effects of electronic publishing in science were discussed. The CEP met during the Seattle Congress. H. D. Flack visited the IUCr Editorial Offices, Chester, UK, in November 1996, November 1997 and November 1998.

H. D. Flack, Chair

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

6.1. Purpose

The purpose of COMCIFS is to commission and approve new CIF dictionaries and to keep the crystallographic community informed of its decisions. COMCIFS is a Sub-committee of the Executive Committee.

6.2. Membership

The members of COMCIFS during the triennium were: I. D. Brown (Chair), P. R. Edgington, P. M. D. Fitzgerald, S. R. Hall, B. McMahon (Secretary), G. Madariaga, M. A. Spackman, B. H. Toby. In addition, COMCIFS has had a number of consultants and observers who have received COMCIFS mailings and made important contributions to the discussions.

6.3. Approval of dictionaries

During the triennium, three dictionaries were approved, one was a revision and two were new. These were:

The second version of the core dictionary (*core_cif.dic* 2.0), which is used, *inter alia*, for submission of papers to *Acta Cryst.* Section C.

The dictionary for macromolecular structures (*mm_cif.dic* 1.0), which is being adopted by the Protein Databank and the Nucleic Acid Databank.

The dictionary for powder diffraction (*pd_cif.dic* 1.0), which is being adopted for the Powder Diffraction File.

Support for these dictionaries is provided by Dictionary Maintenance Groups chaired by I. D. Brown (*core_cif.dic*), P. M. D. Fitzgerald (*mm_cif.dic*) and B. H. Toby (*pd_cif.dic*). These groups are charged with consulting with their respective communities and preparing revised versions of the dictionaries as required.

Revisions proposed by the Dictionary Maintenance Groups are presented to COMCIFS for final approval. Revised versions of the core (2.1) and macromolecular (1.1) dictionaries are at an advanced stage.

6.4. Preparation of new dictionaries

Six new dictionaries are in various stages of preparation. These are:

A modulated structure dictionary (*ms_cif.dic*) which will be shortly presented to COMCIFS for tentative approval. It is being prepared by a group under the direction of G. Madariaga.

A dictionary for images (*img_cif.dic*) which is also nearly ready for presentation to COMCIFS for tentative approval. This is designed for storing diffraction patterns from two-dimensional detectors, but it will be able to store any two-dimensional image with extension to higher dimensions. Because of the size of the files and the need to process them in real time, a binary version of this CIF is also being defined. The ASCII and binary standards are identical except for differences needed to write and read a binary file. A. Hammersley is in charge of this project.

A small-angle scattering dictionary (*sas_cif.dic*), which is being constructed by a group headed by M. Malfois. A draft has been prepared.

A dictionary for magnetic structures (*mag_cif.dic*), which is being prepared in conjunction with the Database of Magnetic Structures Determined by Neutron Diffraction, headed by W. Sikora.

A dictionary for crystallographic symmetry (*sym_cif.dic*), which is under construction by a group headed by I. D. Brown.

A dictionary for electron density CIFs (*rho_cif.dic*), which, after a slow start, is being prepared by a group under P. Mallinson.

6.5. Communication

All COMCIFS formal business is conducted *via* an electronic discussion group whose transactions can be viewed by the public at <http://www.iucr.org/iucr-top/lists/comcifs-l>. In addition, regular reports on COMCIFS activity have appeared in the *IUCr Newsletter*.

6.6. Other Projects

A group is exploring questions of intellectual property rights related to CIFs and CIF-based software.

We are also working on a scheme to allow the automatic concatenation of different dictionaries at run time in order to allow one dictionary to incorporate other dictionaries that may be necessary for its proper functioning. This raises the question of whether we should continue to carry the overhead of maintaining CIF dictionaries in two incompatible Dictionary Definition Languages (DDL) or whether we should standardize on one DDL.

Proposals are being prepared that may allow dictionaries to express functional relationships between the different archived items.

6.7. Acknowledgements

It is my pleasure to thank the members of the Committee, and others too numerous to mention, whose careful and often time-consuming efforts have made an essential contribution to the success of the CIF.

I. D. Brown, Chair

7. Appendix G: 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 eleven issues published during the triennium included extensive coverage of the Seattle Congress, preliminary information concerning the Glasgow

Congress, a cover story on the IUCr web site, and articles covering the development of CIF formats.

The aim is to cover all areas of crystallography, both in the text and with the choice of cover illustrations. Cover illustrations in the triennium included small-molecule crystallography, macromolecular structures, fibre diffraction, small-angle scattering, the IUCr web site, and the Glasgow Congress site. Several covers were composites combining small-molecule, materials and macromolecular applications to emphasise the broad range and remarkable power of crystallography.

Eleven issues of the *IUCr Newsletter* were published from 1996 through 1998. The issues ranged in length from 16 to 32 pages. Each contained a letter from the President, news of IUCr Commission activities, crystallographic meeting announcements and reports, obituaries of prominent crystallographers, notices of elections, awards to crystallographers, and information on books, web sites, resources and activities of interest to crystallographers. When available, information on meetings and advances in electron diffraction, neutron diffraction, amorphous materials and quasicrystals, and other related topics are published. Contributions from crystallographers everywhere are sought; material is gathered from newsletters of crystallographic associations and societies and from leading science news magazines. Photographs are provided by contributors or drawn from the personal collection of the Editor. Almost all contributions are published and all material is edited to varying degrees.

A significant portion of the support for the publication and distribution of the *IUCr Newsletter* comes from advertising revenue. The average number of pages of advertising per issue rose from eight in 1996 to twelve in 1998.

The staff of the editorial office in Buffalo, New York, USA, are 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

8. Appendix H: IUCr/Oxford University Press Book Series

The launching of this Series was reported to the General Assembly at Perth (1987). The agreement between the IUCr and the OUP was finalized soon afterwards. The Series has consisted of three sub-series:

IUCr Crystallographic Symposia (IUCr CS)

IUCr Monographs on Crystallography (IUCr MC)

IUCr Texts on Crystallography (IUCr TC)

The above arrangement continued over the initial seven years of the Series but was revised by the Executive Committee in 1994, when it was decided that, with the exception of the series on Crystallographic Computing, The Symposia Series (IUCr CS) could be dropped because it had become possible for that type of publication to be handled by Special Issues of the IUCr journals. Thus the Book Series consists now of Monographs and Texts only, except for the books on Crystallographic Computing.

The Book Series Committee membership currently is: P. Coppens (USA; Chair), A. A. Chernov (Russia), G. R. Desiraju (India), J. Drenth (The Netherlands), A. M. Glazer (UK), J. P. Glusker (USA) and J. R. Helliwell (UK), with M. Levitt as the *ex officio* representative of the OUP and the President and the General Secretary of the IUCr as *ex officio* members. This Committee considers proposals for new publications and makes recommendations to the IUCr Executive Committee and to the Delegates of the Press (the body responsible for approving all publications handled by the OUP).

During the reporting period, the Committee interacted with a considerable number of prospective authors and with representatives of Oxford University Press (OUP). Collaboration with OUP has been easy and effective. While the Committee has attempted to facilitate rapid publication of approved manuscripts, there is a large variation in the length of time between the initial contact and publication, generally caused by circumstances beyond the Committee's control. Several volumes initiated by the previous Committee have appeared during the reporting period. Of the volumes handled by the present Committee, a Conference Proceedings and a Monograph are scheduled to appear before the Glasgow Congress. Two additional Monographs are under OUP contract and being written, while two other manuscripts are in the negotiating stage. The field of crystallography is by no means fully covered by the books that have appeared or are to appear in this Series. Prospective authors are invited to discuss their plans with any of the members of the Book Series Committee.

P. Coppens, Chair

9. Appendix I: Promotion Committee

In 1996, the Executive Committee decided to set up a special Promotion Committee, with the aim of improving the financial position of the IUCr. The first task of the Committee was to appoint a Promotions Representative. As a result Miss A. J. Sharpe was appointed to this post in early 1998. Since then, a campaign to market the IUCr journals and services more aggressively to the crystallographic community as well as to structural science communities in biology, chemistry, materials science and physics has begun.

Increased participation at meetings, whether it be with an exhibition stand, the supply of promotional material for delegates' wallets, or as part of an informal joint marketing agreement with Oxford University Press, has raised the profile of the IUCr and its publications. An initiative to highlight journal articles within the *IUCr Newsletter* is designed to tempt individuals to petition their libraries for subscriptions, and an on-line order form now provides a convenient way to subscribe.

While it is important to promote all IUCr journals, particular attention has been given to the relatively new *Journal of Synchrotron Radiation*. Early results show that the number of personal subscriptions has risen owing to increased exposure at relevant conferences and users' meetings. The emphasis is now on increasing institutional subscriptions by targeting synchrotron and neutron sites. The imminent on-line appearance of *Acta Cryst.* Section D and the journal's recent redesign and doubling of frequency present exciting promotional opportunities for that publication.

Attractiveness and value in the market place are areas that need constant monitoring, and innovation is the buzzword for mature journals. Market research and competitor tracking may reveal ideas for new sections and presentation.

Special Issues, whether milestone-celebrating compilations or conference proceedings, are important in increasing the impact of a journal. They are, however, expensive to produce. The sale of advertising space and of extra copies of these issues *via* conferences and advertising campaigns in the journals, the *IUCr Newsletter* and on the IUCr web site has gone some way to recovering costs.

To give some idea of the impact at this early stage of the Promotions exercise, the total advertising revenue generated (January 1998 to March 1999) is USD 50,694. Most of the income has resulted from the following Special Issues: SRI '97 Proceedings (May 1998 issue of *Journal of Synchrotron Radiation*) USD 10,940; Fiftieth Anniversary

of *Acta Cryst.* and the IUCr (November 1998 issue of *Acta Cryst.* Section A) USD 20,340; CCP4 Proceedings (November 1998 issue of *Acta Cryst.* Section D) USD 5,607. Additional revenue has come from sales of the *World Directory of Crystallographers* database and mailing lists compiled from this (USD 2,152) and from the sales of other Special Issues (USD 4,800).

The Promotion Committee membership is currently A. M. Glazer (Chair), F. H. Allen, P. W. Coddington, M. H. Dacombe, W. L. Duax, H. D. Flack, S. R. Hall, J. Harada, S. J. Maginn, A. J. Sharpe (Promotions Representative) and P. R. Strickland, with the President and General Secretary of the IUCr as *ex officio* members.

A. M. Glazer, Chair

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

The Sub-committee on the Union Calendar is a sub-committee of the Executive Committee. A summary of its activities is given in this Appendix for the information of delegates.

During the period since the last General Assembly, the Sub-committee 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 Seattle Congress and the Glasgow Congress. The financial support given to assist young scientists totalled CHF 64,409 in 1996, CHF 91,816 in 1997 and CHF 76,399 in 1998. This support has helped several hundred young scientists attend a scientific meeting during the triennium.

Powder Diffraction, Denver, Colorado, USA, 3–8 August 1996 (satellite meeting of Seattle Congress)

Synchrotron Radiation, Argonne, Illinois, USA, 4–7 August 1996 (satellite meeting of Seattle Congress)

Neutron Scattering, Gaithersburg, Maryland, USA, 5–7 August 1996 (satellite meeting of Seattle Congress)

Summer School on Crystallographic Computing, Bellingham, Washington, USA, 17–22 August 1996 (satellite meeting of Seattle Congress)

Fifth International Symposium on Protein Structure Function Relationship and Workshop on Protein Structure Elucidation, Karachi, Pakistan, 6–9 and 11–16 January 1997

BCA/CCG Sixth Intensive Course in X-ray Structure Analysis, Durham, UK, 7–14 April 1997

26th International School of Crystallography: Electron Crystallography, Erice, Italy, 22 May–2 June 1997

School on Direct Methods for Solving Macromolecular Structures, Erice, Italy, 22 May–2 June 1997

Fifth European Powder Diffraction Conference (EPDIC 5), Parma, Italy, 25–28 May 1997

ACA Annual Meeting, St Louis, Missouri, USA, 20–25 July 1997

Sagamore XII Conference, Waskesiu, Saskatchewan, Canada, 27 July–4 August 1997

Structural Chemistry Indaba II – Intermolecular Interactions, Skukuza, South Africa, 3–8 August 1997

Symposium on Organic Crystal Chemistry, Poznan-Rydzyna, Poland, 17–21 August 1997

Seventeenth European Crystallographic meeting (ECM-17), Lisbon, Portugal, 24–28 August 1997

International Conference on Aperiodic Crystals (Aperiodic '97), Alpe d'Huez, France, 27–31 August 1997

Seventh International Conference on the Application of Density Functional Theory in Chemistry and Physics, Vienna, Austria, 2–6 September 1997

Rietveld Summer School '97-PL (RSS97-PL), Cieszyn, Poland, 5–7 September 1997

Fifth Oxford Summer School on Neutron Scattering, Oxford, UK, 8–18 September 1997

Conference on X-ray Scattering from Surfaces, Interfaces and Thin Layers, Smolenice, Slovakia, 1–4 October 1997

Current Challenges on Large Supramolecular Assemblies, Athens, Greece, 31 October–4 November 1997

Crystallography at High Pressure: the Next Steps, Grenoble, France, 21–23 November 1997

Implications of Molecular and Materials Structure for New Technologies, Erice, Italy, 28 May–7 June 1998

IV Latin American Workshop on Magnetism, Magnetic Materials and their Applications, São Paulo, Brazil, 7–11 June 1998

Seventh Annual ACA Summer Course for Crystallographers, Athens, Georgia, USA, 5–18 July 1998

ACA Annual Meeting, Arlington, DC, USA, 18–23 July 1998

Twelfth International Conference on Crystal Growth (ICCG-12) in conjunction with Tenth International Conference on Vapor Growth and Epitaxy (ICVGE-10), Jerusalem, Israel, 26–31 July 1998

International Workshop on Science of Crystal Growth Technology, Beatenberg, Switzerland, 5–16 September 1998

International School on Powder Diffraction, Calcutta, India, 7–10 October 1998

Third Conference of Asian Crystallographic Association (AsCA '98), Selangor, Malaysia, 13–15 October 1998

II Workshop on Optoelectronic Materials and their Applications (including Solar Cells), Havana, Cuba, 2–6 November 1998

Meeting on Synchrotron, Neutron and Laboratory Source Crystallography at High Pressure, Argonne, Illinois, USA, 14–17 November 1998

Symposium on Protein Structure Function Relationship, Karachi, Pakistan, 16–19 December 1998

BCA/CCG Seventh Intensive Course in X-ray Structure Analysis, Durham, UK, 8–15 April 1999

School on Data Mining in Crystallography, Erice, Italy, 12–20 May 1999

School on Crystal Engineering: From Molecules and Crystals to Materials, Erice, Italy, 12–23 May 1999

XI International Conference on Small-Angle Scattering, Upton, New York, USA, 17–20 May 1999

The organizers of all IUCr-sponsored meetings are requested to recommend the journals of the IUCr as a suitable channel of publication for the original papers presented at the meeting.

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. Schenk. A new Chair will be appointed in Glasgow.

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

11.1. American Crystallographic Association (ACA)

The ACA continues to be a vibrant organization. A new Special Interest Group (SIG), the General Interest Group, has been formed and the Elizabeth A. Wood Science Writing Award has been instituted for Science Writing, for which all ACA members can submit material that has appeared in a newspaper or a popular magazine. A statement on Ethics in Crystallography has been adopted by the ACA Council and published in the *ACA Newsletter*. The yearly ACA meetings continue to be highly successful. Though many aspects of crystallography continue to be represented, the emphasis on the life sciences is evident from the distribution of the contributed papers. The ACA, which includes both US and Canadian crystallographers, continues to be a very strong Regional Associate of the IUCr.

P. Coppens, Representative

11.2. Asian Crystallographic Association (AsCA)

The Asian Crystallographic Association has made a significant contribution in promoting crystallography in the region during the past three years. In one aspect, AsCA encourages its member societies to have more and effective academic activity to promote the development of crystallography in their country and/or region; meanwhile, AsCA itself concentrates on its main task of organizing the AsCA conference series. These conferences are held every three years in different countries and regions.

Thanks to the rapid development of science and technology in Asia, crystallography has its chance to prosper. Each member society of AsCA has made its contribution in materials science, life science and other related disciplines. In these countries and regions, crystallographic societies made every effort to promote students and young scientists by helping them to participate in more workshops, symposia, and conferences organized by these societies. AsCA also encourages its member societies to give more help to those in less developed countries and regions by providing information, collaboration and even some research facilities.

The Third AsCA Conference (AsCA '98) was a major activity in the past three years; AsCA '98 was held in Hotel Equatorial, Bangi, Malaysia, 13–15 October 1998. More than 300 scientists and students from 14 countries and/or regions participated in this conference. During the three-day programme, all the participants had a successful academic exchange and helpful discussions. There were 4 plenary lectures and 14 microsymbiosia. The topics ranged from Diffraction Theory, Structure Refinement, Aperiodic Structures, Biocrystallography and Proteins *etc.* to Instrumentation and Other Categories. To celebrate the Fiftieth Anniversary of the IUCr, a microsymbiosium was held during AsCA '98. In addition to the symposia, a small instrumentation exhibition was held. AsCA '98 received contributions from seven professional bodies and institutions, such as the IUCr, the Crystallography Society of Japan, the University of Kebangsaan, Malaysia, *etc.* Financial support from Rigaku International (Japan), MAC Science, the International Centre for Diffraction Data, Bruker AXS and Marresearch are gratefully acknowledged.

The Fourth AsCA Conference will be held in 2001 and the Organizing Committee and venue will be determined at the Glasgow Congress.

AsCA is very grateful to the IUCr for support and guidance and hopes to continue to play an important role in promoting crystallography in Asia.

M. Tanaka, Representative

11.3. European Crystallographic Association (ECA)

The European Crystallographic Association (ECA) has been established as the Regional Associate of the International Union of Crystallography replacing the rather informal European Crystallographic Committee (ECC). The ECA is registered in The Netherlands following Dutch legislation. Three categories of members are admitted: National Members represented by their Adhering Bodies, Affiliate Members and Individual Members. Statutes and By-Laws were adopted by Council during its meetings in Lisbon, Portugal, in 1997 and Prague, Czech Republic, in 1998. The National Members are European and some neighbouring countries from the Mediterranean area and Africa. An Executive Committee was elected in 1997 based on the new statutes. Those elected are: C. Giacobozzo (President), J. Bernstein (Vice-President), P. Beurskens (Secretary), S. Harkema (Treasurer) and A. M. Carrondo, P. Paufler and F. H. Allen (members).

Two very successful European Crystallographic Meetings were held. ECM-17 in Lisbon, Portugal, and ECM-18 in Prague, Czech Republic, attracted between 800 and 1000 participants. Forthcoming meetings will be ECM-19 in Nancy, France, 25–31 August 2000, and ECM-20 at Cracow, Poland, in 2001.

H. Fuess, Representative

11.4. International Centre for Diffraction Data (ICDD)

The last three years have seen major changes at the International Centre for Diffraction Data (ICDD). First, the membership has grown from 98 to 266 with the infusion of many new overseas members. At present, the ICDD has 133 USA members and exactly the same number of non-USA members. The second major change is that it has actively pursued joint activities with other database organizations, notably Fachinformationszentrum (Inorganic Crystal Structure Database) and the Cambridge Crystallographic Data Centre (Cambridge Structural Database). ICDD has drawn up contracts with both of these organizations that allow the ICDD to calculate powder patterns from the crystallographic data. In addition, each of the three organizations has pledged to add cross references in their databases thus allowing user interaction between several databases – permitting new extensions of Computational Materials Design. The Sub-committees and task groups are actively engaged in screening and reviewing all new and historical data. The Technical Committee has established Co-chairs on each of the world's continents and is looking forward to operating as a truly international organization. The ICDD is currently sponsoring about 45 different institutions in various parts of the world for assistance in producing high-quality experimental powder data. It also sponsors scholarship programmes and gives financial support to selected national and international meetings. Last year, the ICDD took over the administration of the Denver X-ray Conference and continues to support domestic and overseas clinics and training courses. The ICDD was closely involved in the establishment of an X-ray Analytical Society.

R. J. Cernik, Representative

11.5. International Organization of Crystal Growth (IOCG)

During the triennium, the activities of the IOCG were mainly governed by the preparation and performance of the following scientific meetings:

Tenth International Summer School on Crystal Growth (ISSCG-10), Rimini, Italy, 1–6 June 1998. Chairs: R. Fornari (MASPEC Parma) and C. Paorici (University of Parma).

Twelfth International Congress on Crystal Growth (ICCG-12). Chair: A. Horowitz (Beer Sheva, Israel).

Tenth International Congress on Vapour Growth and Epitaxy (ICVGE-10). Chair: M. Roth (The Hebrew University of Jerusalem).

The two latter conferences were jointly held in Jerusalem, Israel, 26–31 July 1998 and were attended by 570 registered participants, which is considerably less than the 700 attendees of ICCG-11 held in The Hague, The Netherlands, in June 1995. About 25% of the participants came from Eastern European countries. Roughly 900 abstracts were accepted and about 650 papers and posters presented. Three satellite workshops (W1: Crystallization Phenomena in Food, Pharmaceuticals and Bio-related Materials; W2: Phase Field Models of Solidification Processes; W3: Room Temperature Semiconductor Detectors for Remote, Portable and *In Situ* Radiation Measurement Systems) were run in parallel with the main conferences. About 240 papers presented during both conferences and the three workshops were published in the Conference Proceedings [*J. Cryst. Growth* (1999), **198/199**, 1–1394].

During ICCG-12, meetings of the IOCG Executive Committee, of the IOCG Council and of the General Assembly were held under the Chair of its President, T. Nishinaga. The following resolutions, among others, have been approved: The Chinese Crystal Growth and Materials Sub-Society (CCGMS), affiliated to the Chinese Ceramic Society, and the Australian Association for Crystal Growth (AUSACG) were formally accepted into the IOCG. The offers made by the French Association for Crystal Growth to organize ICCG-14 during 2004 in France, and by the German Association for Crystal Growth to organize ISCCG-12 during 2004 in Germany, were accepted. The offer made by the American Association for Crystal Growth to hold ICCG-15 in Washington, DC, in 2007 was noted. The President and the Executive Committee were asked to explore (a) the possibility of the IOCG becoming an International Scientific Associate affiliated to ICSU, with a possible change of name to International Union for Crystal Growth, and (b) ways of raising funds appropriate for IOCG activities.

The following officers and Executive Committee members are elected for the period 1998–2001: President: T. Nishinaga (Japan), Vice-Presidents: K. W. Benz (Germany), R. F. Sekerka (USA), Secretary: T. E. Kuech (USA), Treasurer: C. F. Woensdregt (The Netherlands), Past President: B. Cockayne (UK), Honorary Principal Founder IOCG: M. Schieber (Israel). Executive Committee members: J. J. Favier (France), A. Horowitz (Israel), Jiang Min-Hua (People's Republic of China), T. Ohachi (Japan), V. V. Osiko (Russia), C. Paorici (Italy), H. J. Scheel (Switzerland), J. N. Sherwood (UK). *Ex officio* members of the Executive Committee: J. Buttrey (USA), P. M. Dryburgh (UK) (IOCG representative to the IUCr), H. Klapper (Germany) (IUCr representative to the IOCG), J. P. van der Eerden (The Netherlands) (IOCG representative to IUPAC); J. N. Sherwood (UK) (IOCG representative to IUPAC), and others. In addition, 35 Councillors representing 18 national associations, five Councillors representing nations who do not have a national association, and four *ex officio* Councillors representing International Unions were approved. The *ex officio* Councillor representing the IUCr is M. H. Dacombe, the Executive Secretary of the IUCr.

The following IOCG Prizes, sponsored by the ICCG-12/ICVGE-12 Organizing Committee, were awarded: The Frank Prize to K. A. Jackson (USA) and the Laudise Prize to I. Akasaki (Japan). The Thirteenth International Congress on Crystal Growth (ICCG-13) and the Eleventh International School on Crystal Growth (ISSCG-11) will be held in Kyotanabe, Japan, 29 July–3 August 2001.

H. Klapper, Representative

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

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

IDCNS is responsible for all recommendations concerning matters of nomenclature and symbols originating within the International Union of Pure and Applied Chemistry (IUPAC), with an emphasis on maintaining proper standards and resolving interdivisional nomenclature conflicts prior to publication in *Pure Appl. Chem.* The IUCr representative and his alternate evaluate each document, providing critical comment as appropriate crystallographically. IDCNS meets annually to facilitate communications between Commissions, Divisions and International Organizations with common interests.

The meetings this triennium were held in Sèvres, France, in August 1996, in Geneva, Switzerland, in August 1997 immediately preceding the 39th IUPAC General Assembly, and in Durham, North Carolina, USA, in August 1998; the first meeting followed the Seattle Congress so closely that neither the representative nor his alternate were able to participate. Sèvres is the location of the Bureau International des Poids et Mesures (BIPM); in 1994, the Comité Consultative d'Unités (CCU) of BIPM proposed that the ångström be formally deprecated. The strong objections presented by the IUCr at earlier IDCNS meetings to this proposal were set forth so effectively by the chair of IDCNS at the April 1996 meeting of CCU that the ångström (Å) was included in Table 8, Chapter 4 of the definitive 7th edition (1998) of *Le Système International d'Unités* (SI) as “a non-SI unit currently accepted for use with the International System, although ‘its use is not encouraged’”. The practical result of this decision is that the ångström continues to be in conformity with the SI provided only that it is defined in relation to the SI in every document in which it is used. IUCr journals follow this *proviso* by printing an appropriate statement in each issue of its journals. It is noted that authority to act in all matters between nations concerning measurement standards has been given jointly to the Conférence Générale des Poids et Mesures, the CIPM and the BIPM by the Convention du Mètre. This Convention, which dates to 1875, is a diplomatic treaty with legal consequences that is currently subscribed to by 48 nations.

Among IDCNS matters of interest to the IUCr is the revised list of atomic weights through atomic number 111 (symbol Uuu, name Ununium, atomic weight ~272) published in *Pure Appl. Chem.* (1997), **69**, 2471–2473. Uuu and the element with atomic number 110 (symbol Uun, name Ununilium, atomic weight ~269) are the only elements with three-letter symbols. The revised list of atomic weights for atomic numbers 1–111 may be found at: <http://www.chem.qmw.ac.uk/iupac/>. A proposal by the International Electrotechnical Commission to adopt the following prefixes for binary systems: 2^{10} = kibi (kilobinary), symbol Ki; 2^{20} = mebi (megabinary), symbol Mi; 2^{30} = gibi (gigabinary), symbol Gi; and 2^{40} = tebi (terabinary), symbol Ti is under consideration. The class of supplementary SI units will be deleted, so that there are now only base and derived units. The proposal to extend the range of SI prefixes from the present $10^{\pm 24}$ to $10^{\pm 48}$ is also under consideration, and important progress has been made toward a new and fundamental definition of the kilogram. The International Standardization Organization (ISO) practice for displaying dates is to use the order year/month/day, thereby eliminating the present ambiguity between the European order day/month/year and the US order month/day/year. Both ISO and IUPAC recommend that numerical values of physical quantities in tables and figures be labelled by their international symbol divided by the SI unit; for example λ/nm , not λ (nm) [the IUCr would use

$\lambda/\text{\AA}$, not λ (\AA)]. The reason is to allow manipulation of physical quantities, numerical values and units by the ordinary rules of algebra and to eliminate possible ambiguity by representing numerical quantities with an unambiguous dimension of unity.

All provisional and all final IUPAC nomenclature recommendations, also all IUPAC books, are in the process of becoming accessible on-line at <http://www.iupac.org> as IUPAC moves toward full electronic publishing.

Among recent IUPAC publications of interest to many crystallographers are *Principles of Chemical Nomenclature, a Guide to IUPAC Recommendations* by G. J. Leigh, H. A. Favre & W. V. Metanomski [(1998), Oxford: Blackwell], and *Compendium of Chemical Terminology, IUPAC Recommendations*, 2nd ed., by A. D. McNaught & A. Wilkinson [(1997), Oxford: Blackwell]. The 3rd edition of IUPAC's Green Book *Quantities, Units and Symbols in Physical Chemistry*, currently in preparation, will contain a new list of fundamental constant values, a new section on uncertainties, new material on surface science, NMR and non-linear spectroscopy and will be published in computer-readable format.

A major concern of IDCNS was the recent Report of the IUPAC Strategy Development and Implementation Committee (SDIC), which proposes to terminate most of the long-term Commissions of IUPAC and replace them by short-term Task Groups to carry out scientific projects. IDCNS prefers more evolutionary means for improving the less-effective Commissions to the SDIC's revolutionary proposals. V. Metanomski of *Chemical Abstracts* became the new Secretary of IDCNS on 1 January 1998. T. Cvitas of Zagreb will succeed I. Mills as Chair in January 2000. The IUPAC Secretariat has moved from Cambridge, UK, to Research Triangle Park, NC, USA.

S. C. Abrahams, Representative

12.2. International Council for Science (ICSU)

ICSU (though it has retained its acronym) is now the International Council for Science (formerly International Council of Scientific Unions). The emphasis is to reach society outside its natural community of scientists and researchers, and also to become more of a 'player' in the 'new global system of international cooperation among governmental, regional and international bodies'. As a result, interaction between Scientific Unions, which was an important aspect of ICSU in the past, has been de-emphasized.

P. Coppens, Representative

12.2.1. ICSU Committee on Data for Science and Technology (CODATA). No report was received from the IUCr Representative.

12.2.2. ICSU Committee on Science and Technology in Developing Countries – Incorporating International Biosciences and Other Scientific Networks (COSTED–IBN). COSTED is continuing its discussions on technology management, coping with hazardous wastes, facilitating technology transfer, leadership development for science and technology in developing countries, and undertaking natural resource surveys for economic development.

P. Coppens, Representative

12.2.3. ICSU Committee on Space Research (COSPAR). The formal COSPAR activities in the triennium were governed by the biannual international congresses, the 31st and the 32nd COSPAR Scientific Assembly and Related Events held in 1996 in Birmingham, UK, and in 1998 in Nagoya, Japan. Following a decision of the COSPAR council during the 31st Assembly in Birmingham, the COSPAR Charter and By-Laws were modified in order to create a

new category of affiliates for organizations or individuals willing to support financially the COSPAR activities. The changes of the Charter and By-Laws, allowing the installation of these 'COSPAR Associated Supporters', were subject to voting by correspondence and accepted.

The 32nd COSPAR Assembly was held 12–19 July 1998 in Nagoya, Japan, with Y. Kamide as Chair, Solar-Terrestrial Environment Laboratory, Nagoya University. It was connected with the 40th Anniversary of COSPAR, which was established by ICSU in October 1958. In addition, the 58th COSPAR bureau meeting and the 32nd COSPAR council meeting were held. The most important item of the agenda was the election of the President, the Vice-Presidents, the remaining Bureau members and the Finance Committee members for the period 1998–2002. The presiding President G. Haerendel (Germany) as well as the Vice-Presidents L. J. Lanzerotti (USA) and A. Nishida (Japan) were re-elected.

Another item on the agenda concerned the election of the Nomination Committee. Under current COSPAR By-laws, a new Nomination Committee must be elected every two years, whereas the COSPAR officers are elected for a period of four years. In order to homogenise the rules, a modification of the By-laws allowing an extension of the term of Nomination Committee members from two to four years was discussed and subjected to voting by correspondence.

The 33rd COSPAR Scientific Assembly (COSPAR 2000) will be held in Warsaw University of Technology, Warsaw, Poland, 16–23 July 2000 with K. Stepień of Warsaw University Astronomical Observatory as Programme Chair. In 2002, the 34th COSPAR Assembly will be held jointly with the International Astronautical Federation (IAF) and in combination with the Second World Space Congress (WSC-II) in Houston, Texas, USA, 11–20 October 2002. The American Institute for Aeronautics and Astronautics (AIAA) will serve as Local Organizing Committee.

H. Klapper, Representative

12.2.4. ICSU Programme on Capacity Building in Science (PCBS). No significant meetings occurred during the triennium but the IUCr's Visiting Professorship Programme, which receives support from the ICSU/UNESCO subvention, continues.

C. Gramaccioli, Representative

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

With the utmost sadness we have to report that the IUCr representative to ICSTI since 1993, E. N. (Ted) Maslen, died suddenly on 2 February 1997. H. D. Flack, as Chair of the Committee on Electronic Publishing, Dissemination and Storage of Information, assumed *ad interim* responsibility until appointment, following his resignation as the IUCr's representative to CODATA, in mid-July 1997. This sequence of events has unfortunately had the consequence that the IUCr's interaction with ICSTI has been slow in getting under way and partially undocumented during the first part of the triennium. The web site <http://www.icsti.org> gives public information on ICSTI's activities, including the quarterly newsletter *Forum*.

ICSTI held Annual General Meetings in Pretoria, South Africa, in May 1996 (E. N. Maslen present), in Philadelphia, USA, in June 1997 (no IUCr representative present) and on the banks of Loch Lomond, UK, in May 1998 (H. D. Flack present). Winter committee and discussion meetings have been held yearly over a weekend in Paris or London but the IUCr representatives did not attend these. Themes presented and discussed in these meetings pertinent to the interests

of the IUCr include: (i) recent developments in copyright law in the European Union and in the USA, (ii) the electronic publications archive, (iii) the EBLIDA/ECUP/STM (European Bureau of Library, Information and Documentation Associations/the European Copyright User Platform/International Association of Scientific, Technical, and Medical Publishers) interim joint statement on guidelines for incidental digitization and permanent storage of scientific, technical and medical journal articles, (iv) electronic libraries – relationship between suppliers and customers, (v) restructuring/rationalisation in the information industry, and (vi) the DOI (Digital Object Identifier).

Current activities include: (i) a networking survey of user needs, (ii) an international classification scheme for physics, and (iii) the addition of information on A&I services to the ISSN register. A group is active in the area of legal issues, which surveys developments in copyright, database and patent law throughout the world. The Information Policy Committee has given considerable attention to the problem of the electronic archive and this subject will form the theme of ICSTI's contribution *Sharing Scientific Knowledge* to the World Science Conference in collaboration with ICSU Press and CODATA.

New projects include collaboration in an IUPAC/CODATA project on standardization of physico-chemical property electronic data files (IUCOSPED). The goal of this project is to develop standards for the publication, dissemination and storage of numerical data files in electronic form and thereby avoid the proliferation of incompatible formats as journals move to dissemination on the Internet.

ICSTI has undertaken a drive to improve its finances by reducing staff at the secretariat, by switching from print to electronic distribution for its quarterly newsletter and by charging a registration fee for its Annual General Meeting and opening the discussion sessions to non-members. A considerable effort has also been undertaken to increase the membership. It is intended that some future meetings will be joint efforts with associated organizations. ICSTI's membership is drawn from diverse sectors of learned societies, the commercial publishing industry, national and academic libraries, patent offices, intellectual property consultants, secondary services *etc.* Over the years, ICSTI's links with ICSU have weakened and within its membership the user community is now poorly represented. Only those scientific unions directly involved in the publishing field are members.

During this triennium, ICSTI has reoriented its mission away from the consideration of purely technical issues so prevalent with the

onset of the era of electronic publishing into that of the strategy of the scientific and technical information industry as a whole. ICSTI is a most useful source of information and contacts for the IUCr with regard to its considerable involvement in publication for the crystallographic community.

H. D. Flack, Representative

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

13.1. 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 1999–31 December 2001.

	CHF	CHF
Income		
Subscriptions from Adhering Bodies	456,000	
Yield from investments and banking accounts	750,000	
Subventions from UNESCO through ICSU	60,000	1,266,000
Expenditure		
Administration	783,000	
Subscriptions to ICSU and bodies of ICSU	30,000	
Administrative meetings	255,000	
Scientific meetings	194,000	
Transfers to other accounts	100,000	1,362,000
Estimated profit or deficit		-96,000

13.2. Unit Contribution

According to Statute 5.10(k), the General Assembly has to determine the Unit Contribution to be paid by the Adhering Bodies for the period to the next General Assembly. The Executive Committee recommends to the General Assembly that the Unit Contribution should remain at its present level of CHF 1,000 for the years 2000–2002.