international union of crystallography

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Report of the Executive Committee for 2000

1. Meetings

The IUCr sponsored the following meetings held during 2000:

1. Structural Characterization of Amorphous and Nano Crystalline Materials, Suez Canal University, Egypt, 22–29 January.

2. Seventh European Powder Diffraction Conference (EPDIC-7), Barcelona, Spain, 20–23 May.

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

4. Ninth Annual ACA Summer Course for Crystallographers, Athens, Georgia, USA, 7–19 July.

5. ACA Annual Meeting, St Paul, Minnesota, USA, 22–27 July.

6. Eleventh International Conference on X-ray Absorption Fine Structure, Ako City, Hyogo, Japan, 26–31 July.

7. Indaba 3: Structure and Symmetry, Skukuza, South Africa, 6–11 August.

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

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

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

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

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

The Executive Committee met in Nancy, France, in August. The Finance Committee met twice, in Copenhagen, Denmark, in March, and then in August in Nancy, immediately before the Executive Committee meeting, to prepare its advice and recommendations on finances, establishment and staff matters. The most important items of business dealt with by the Executive Committee at its meeting, and in postal ballots, were:

(1) editorial policy, pricing policy and subscription rates, approval of appointments of new Editor for *Journal of Synchrotron Radiation*, approval of appointments of Co-editors, electronic publishing, Special Issues, launch of *Acta Crystallographica* Section E, and other matters concerning the IUCr journals;

(2) approval of the audited accounts for the previous year;

(3) the General Fund estimates and the level of the unit contribution;

(4) the status of membership subscriptions;

(5) investment policy;

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

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

(8) progress with Volumes A, A1, B, C, D, E, F and G of *International Tables* and development of associated software;

(9) the *IUCr Newsletter*;

(10) the *World Directory of Crystallographers*;

(11) promotion of journals, other publications of the IUCr and crystallography in general;

(12) the Ewald Prize;

(13) discussion of the arrangements for the 2002 General Assembly and Congress.

Other items dealt with in this way were:

(14) the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* and other uses of CIF, trademark applications, work of the Committee for the Maintenance of the CIF Standard (COMCIFS), provision of checking services to other publishers;

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

(16) crystallography in Africa

(17) use of financial support through ICSU;

(18) the Inter-Union Bioinformatics Group;

(19) review of the activities of the Commissions;

(20) review of the activities of Regional Associates;

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

Items concerning the Chester office were:

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

(23) upgrading of office technology in the IUCr office in Chester, provision of Internet services.

2. Publications

Volume 56 of *Acta Crystallographica*, Volume 34 of *Journal of Applied Crystallography* and Volume 8 of *Journal of Synchrotron Radiation* were published.

3. Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Annex IV to the Report of the Eighteenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (2001), A**57**, 741–795].

4. Work of the Commissions

4.1. Commission on Journals

4.1.1. Overview. In 2000, a number of developments for the IUCr journals should be highlighted.

A new electronic journal, *Acta Cryst.* Section E, has been prepared, for launch in January 2001. The Section Editors, Professor W. Clegg and Dr D. G. Watson, and their Co-editors have been appointed. A

new mechanism for subscribers involving a member's (*i.e.* author's) subscription is being piloted. The chemical crystallography IUCr journal outlets of *Acta Cryst.* Section B (*Structural Science*), *Acta Cryst.* Section C (*Crystal Structure Communications*) and *Acta Cryst.* Section E (*Structure Reports Online*) provide an outstanding service to the chemical structure community.

The biological community expands apace and *Acta Cryst.* Section D (*Biological Crystallography*) completed its second year of being published monthly. This has been very well received and supported by the community. Crystallization papers are also very popular and account for as much as 50% of the printed pages in any one issue. Since these are such a buoyant category of papers, and a resulting high work load on the Editorial Board, three new *Acta Cryst.* Section D Co-editors in the field of protein crystallization have been appointed to the Board (Dr N. Chayen, Dr A. Zagari and Dr M. Pusey). These papers are likely to be further fuelled by the new field of structural genomics.

The *Journal of Applied Crystallography* has been delivering bumper sized issues through the year 2000. It attracts papers from all subject areas, namely, biology, chemistry, materials and physics, and where the general interest in developments in one subject area are of keen interest to other subject specialists.

The *Journal of Synchrotron Radiation* saw the appointment of a new Main Editor, Dr D. M. Mills from the APS. The journal published the Proceedings of the Synchrotron Radiation Satellite Meeting of the Glasgow Congress. Work was also carried out on the Proceedings of the XAFS XI Conference, which are to be published in March 2001.

The IUCr web coverage of the journals, including the services to authors and Co-editors for manuscript tracking, is extensive. This now includes the provision of electronic proofs as a service to authors. Web access to the full text of the journals themselves was made 'subscribers only' during the year. An e-mail alerting service of the contents of each issue is available, however, free of charge as are the non-article contents of the journals.

Highlighting of IUCr journal articles *via* mini-reviews within the *IUCr Newsletter* has been undertaken regularly in close cooperation with the *IUCr Newsletter* Editor (Professor W. L. Duax). These have been well received. The *Newsletter* opens a channel to 15,000 readers.

Digitization of all the IUCr journals back to 1948 is under way and is expected to be completed by the end of 2001. Sample issues in pdf format are accessible *via* Crystallography Journals Online. Possible candidates for themed CD-ROMs are being considered within the IUCr Promotion Committee (Chair Professor A. M. Glazer).

The Commission on Journals (JComm) met in Nancy, France, on the occasion of the ECM. A smaller meeting of Co-editors took place at the ACA. JComm input at the Finance Committee was taken at meetings in Copenhagen, Denmark (March 2000) and Nancy (August 2000), and in Nancy also at the Executive Committee meeting. Substantive issues have been the financing of Conference Proceedings, the financial deficit of *Journal of Synchrotron Radiation*, and the general decline of subscriptions across all our titles (which has continued, year on year, for the last 15 years). In 2000, possible new subscription models have been extensively discussed, *e.g.* for the option of electronic access that is now possible *via* **Crystallography Journals Online**. There is now also a Journals Working Group which meets approximately every two months in Chester and five such meetings were held in 2000. Its principal deliverables are marketing leaflets. These include a leaflet covering the full suite of journals, distributed to 5000 people, and the *Acta Cryst.* Section E launch leaflet. Finally, I personally mention that as the Editor-in-Chief I have received or generated some 1500 e-mails on IUCr JComm business through the year. I warmly acknowledge the excellent working relations with the IUCr Chester office, especially Peter Strickland (Managing Editor), Mike Dacombe (IUCr Executive Secretary) and Andrea Sharpe (Promotions Officer). I wish to highlight as well the work of my Editorial colleagues, who give so generously of their time and expertise in the service of the community. I offer my appreciation also to members of the Executive, Finance and Promotion Committees and the *IUCr Newsletter* staff for their collaboration.

A survey of the contents of the IUCr journals is given in Table 1. Details of each journal can be found in the accompanying reports below. The overall publication times (including review and technical editing) fell for all journals. The current times are: *Acta* Section A 6.8 months, *Acta* Section B 8.5 months, *Acta* Section C 5.2 months, *Acta* Section D 5.7 months, *Journal of Applied Crystallography* 9.8 months and *Journal of Synchrotron Radiation* 6.3 months.

J. R. Helliwell, Chair

4.1.2. *Acta Crystallographica* Section A. Section A published 649 pages in 2000, comprising 68 full research papers and 2 Short Communications. These numbers represent a sharp decrease with respect to preceding years. The number of submitted manuscripts has fortunately recovered: 117 manuscripts were received by Co-editors in 2000 against 88 received in 1999. The number of manuscripts published in 2001 should approach the numbers published in previous years.

The efforts by the Editorial Board of Section A to reduce the handling time are paying off since it has been brought down on average from about 4.1 months in 1998 to 3.1 months in 2000. This reduction is due in part to the fact that more and more authors have already started submitting their manuscripts electronically and it is to be expected that there will be a further decrease when electronic submission is generalized. It is to be hoped that the reduction of the time between submission and publication, which results from the combined efforts of the Chester staff and the Co-editors, will encourage authors to send more manuscripts to Section A in the future.

A. Authier, Editor of Section A

4.1.3. *Acta Crystallographica* Section B. Section B published 1127 pages in 2000, its content being dominated by the 123 full research papers published during the year. This figure continues a steady upward trend from 101 in 1998 and 112 in 1999. In 2000, Section B also published one Topical Review, two Short Communications, and two contributions that were categorized as Scientific Comment and a Letter to the Editor.

The chemical systems covered by the research papers can be broadly classified as inorganics and metal-organics (51% of papers) and organics (49%), and these data continue the steady annual increase in the organic content of Section B from the 38% recorded in 1997. Across these chemical categories, Section B continues to serve the needs of those working on charge-density studies, neutron diffraction, structural systematics from the inorganic and small-molecule databases, modelling and prediction of crystal structures, powder diffraction methodologies, studies of phase transitions *etc.* The international nature of the journal is reflected in contributions from 373 individual authors from 32 countries.

During 2000, Co-editors of Section B have made a very significant effort to reduce publication times, particularly speeding up the review process, and by requiring that all revisions of manuscripts shall normally be completed within two months, with minor revisions being completed within one month. Continued improvements in the in-

Table 1
Survey of the contents of IUCr journals.

Acta Crystallographica

Vol.	Year	Number of pages§		Number of papers		Full Articles† Number		Full Articles† Average length		Short Communications‡ Number		Short Communications‡ Average length	
A52¶	1996	1010	6596	96	1702	85	320	10.4	9.1	11	98	1.8	2.5
B52		1078		130		126		8.3		4		1.9	
C52		3262		1289		1284		2.5		5		0.5	
D52		1246		187		109		9.1		78		2.8	
A53	1997	863	4733	86	1201	76	273	10.7	9.1	10	59	1.8	2.7
B53		1045		113		111		9.0		2		4.5	
C53		2004		872		869		2.3		3		1.0	
D53		821		130		86		7.7		44		2.9	
A54	1998	1049	5518	113	1332	103	419	9.7	9.1	10	59	1.7	2.6
B54		943		106		103		8.8		3		2.3	
C54		2026		884		874		3.1		10		1.2	
D54		1500		229		213		6.3		26		3.5	
A55	1999	1073	6472	122	1571	99	567	9.7	7.0	23	80	4.3	3.2
B55		1128		126		113		9.6		13		1.6	
C55		2192		929		924		2.4		5		4.4	
D55		2079		394		394		5.4		39		3.1	
A56	2000	649	5678	82	1501	68	4927	8.2	6.5	14	418	6.0	1.6
B56		1127		137		124		8.6		13		1.2	
C56		2179		943		591		2.8		352		1.3	
D56		1723		339		300		5.3		39		2.4	

Journal of Applied Crystallography

Vol.	Year	Number of pages§	Number of papers	Full Articles Number	Full Articles Average length	Short Communications†† Number	Short Communications†† Average length	Short items‡‡ Number	Short items‡‡ Average length
29	1996	759	131	84	7.5	27	3.0	20	2.3
30	1997	1191	209	162	6.2	32	3.4	15	1.2
31	1998	988	162	104	7.7	33	3.4	25	2.2
32	1999	1208	192	126	7.9	28	4.5	38	1.9
33	2000	1468	259	190	6.1	43	4.1	26	1.3

Journal of Synchrotron Radiation

Vol.	Year	Number of pages§	Number of papers	Full Articles Number	Full Articles Average length	Short Communications Number	Short Communications Average length	Short items‡‡ Number	Short items‡‡ Average length
3	1996	326	45	43	6.9	2	3.5	0	0
4	1997	405	51	49	7.6	2	2.5	0	0
5	1998	1431	371	86§§	6.0	285§§	3.0	0	0
6	1999	1209¶¶	69	57	8.1	2	2.0	10	2.2
7	2000	419	65	58	6.6	4	2.8	3	1.3

§ Numbered pages excluding contents pages. Indexes are also excluded for *Section C*. † Including Lead Articles and Topical Reviews for *Sections A*, *B* and *D*, and Crystallization Papers for *Section D*. ‡ Including Fast Communications, Addenda & Errata, Letters to the Editor, IUCr Notices, Notes & News, Book Reviews, Books Received, Obituaries, Scientific Comments and Editorials. ¶ Volume A52 includes, in addition, 688 pages of abstracts communicated to the Seattle Congress. †† Including Addenda & Errata, Fast Communications, Computer Programs and CIF Applications ‡‡ Including Letters to the Editor, Laboratory Notes, Meeting Reports, Cryocrystallography Papers, Computer Program Abstracts, IUCr Notices, Notes & News, Book Reviews and Books Received. §§ 34 Full Articles and 280 Short Communications were published in Part 3 of Volume 5 as the Proceedings of SRI '97. ¶¶ Proceedings of XAFS X were published as Part 3 of Volume 6 (687 pages).

house typesetting of manuscripts and the routine provision of proofs *via* the Internet also speed the overall process.

During 2000 also, a variety of changes to the presentation of Section B was agreed for 2001, and are now being reflected in published papers. Chief among these is that atomic coordinates will no longer be printed, but can readily be downloaded from the IUCr CIF archive in an immediately useable form. It is a pleasure to record thanks to the IUCr Editorial staff in Chester for the high-quality work carried out, and for the continuing technical improvements being made to the journal.

F. H. Allen, Editor of Section B

4.1.4. *Acta Crystallographica* Section C. Section C published 2179 pages in 2000 comprising 591 Full Papers and 334 Electronic Papers. With the advent of the electronic journal, *Acta Crystallographica* Section E, in January 2001, all Electronic Papers accepted after 24

Table 2
Some of the macromolecular crystal structures reported in 2000 in *Acta Cryst.* Section D.

Structure	Resolution
0.9–1.0 Å	
Charge-density studies on a toxin	0.96 Å
Toxin bucandin	0.97 Å
1.0–1.5 Å	
Porcine pancreatic elastase	1.1 Å
Lantibiotic mersacidin twinned crystal	1.06 Å
Serratia endonuclease	1.1 Å
Bacillus chorismate mutase catalytic homotrimer	1.30 Å
m-Carboxyphenyl-α-D-galactopyranoside plus enterotoxin	1.3 Å
Retinoic acid nuclear receptor plus detergent	1.3 Å
Lysin monomer and dimer	1.35 and 2.07 Å
Feline immunodeficiency virus dUTP pyrophosphatase plus substrates	1.40, 2.3 and 2.5 Å
1.5–2.0 Å	
β-Mannanase	1.5 Å
Streptomyces aminopeptidase plus product analogue	1.53 Å
Pseudoazurin	1.55 Å
Alga cyctochrome c_6	1.57 Å
Spinach acetohydroxy acid isomeroreductase plus reaction product	1.6 Å
Human α-thrombin plus inhibitor plus hirugen	1.7 Å
Alcaligenes azurin II	1.75 Å
Neurotoxin	1.76 Å
Jack bean chitinase	1.8 Å
β-1,4-Xylanase	1.8 Å
Human deoxyhaemoglobin and mutant	1.8 Å
Haemoglobin genetically cross-linked	1.8 Å
Streptomyces xylose isomerase	1.85 Å
Human MRP8 plus calcium	1.9 Å
Human pepsin and transition-state analogue	1.96 Å
2.0–2.5 Å	
FKBP12.6 with rapamycin	2.0 Å
Bovine interferon-γ	2.0 Å
Lysin monomer and dimer	1.35 and 2.07 Å
Jack bean canavalin	2.1 and 2.0 Å
Antigen-binding fragment plus single-strand DNA	2.1 Å
Iron superoxide dismutase	2.1 Å
Monoclonal anitbody Fab hGR-2 F6 against human glucagon receptor	2.1 Å
δ-Chymotrypsin plus inhibitor	2.14 Å
Inhibitor of trypsin and α-amylase	2.2 Å
Family IIIa cellulose-binding domain of scaffoldin	2.2 Å
Water channel AQP1	2.2 Å
Moloney murine leukaemia virus reverse transcriptase plus DNAmers	2.3 Å
Thrombin plus various inhibitors	2.3, 2.7, 2.3, 2.0 and 2.1 Å
Plasmodium Rab6 in GDP-bound form	2.3 Å
Feline immunodeficiency virus dUTP pyrophosphatase plus substrates	1.40, 2.3 and 2.5 Å
Ferredoxin-NADP + reductase and ferrodoxin	2.4 Å
2.5–3.0 Å	
Dienelactone hydrolase plus inhibitor	2.5 Å
Nucleosome core particle	2.5 Å
Mutant human thrombin plus fibrinopeptide	2.5 Å
Wild-type and mutant HIV proteases plus inhibitors	2.5 Å
5-Aminolaevulinate dehydratase and metal sites	2.5 Å
Naphthalene 1,2-dioxygenase	2.6 Å
Porcineβ-trypsin and inhibitor	2.7 Å
Trichosanthes lectin 1, type 2 ribosome-inactivating protein	2.7 Å
Human acetylcholinesterase native and mutant plus toxin	2.7 and 2.8 Å
Human erythrocyte catalase	2.75 Å
Bovine heart cytochrome *c* oxidase	2.9 Å
Human aldose reductase plus inhibitor	1.7 and 2.9 Å
3.0 Å and lower resolution	
Hepatitis B surface antigen Fab fragment from F124	3.0 Å
Pf1 protein capsid	3.0 Å
Buffalo lactoferrin	3.3 Å
E. coli cytochrome bo_3 ubiquinol oxidase (membrane protein)	3.5 Å
Influenza virus hemagglutinin trimer with neutralizing antibody	3.5 Å
Bacteriophage PP7	3.7 Å
Porphobilinogen synthase metalloenzymes	
Hexameric insulin plus resorcinol	
Human cytomegalovirus protease and its inhibitor	

October 2000 were transferred for publication in Section E. Section C now only accepts Full Structural Papers for publication. As established in 1999, only submissions with a significant *Comment* section (as decided by Co-editors and referees) are accepted for publication in Section C. Authors of papers submitted to Section C and recommended for transfer to Section E still have the option of reworking their structural *Comment* section so that it can be judged to be acceptable to Section C.

With the January 2000 issue of Section C, a new format was adopted for all papers, with each starting on a new larger page. Authors are now asked to collect their proofs electronically *via* the Crystallography Journals Online web site; this is working well. Authors are also able to download reprints of their papers from the Crystallography Journals Online web site. As Editor, I am also able to download and review all Section C proof pages from the web site at the same time as the authors. This has allowed any of my comments on the proofs to be acted upon in a timely manner with no significant delays to the publication process.

The decision to appoint deputies for the Editor and Data-Validation Editor proved to be farsighted. Dr A. J. Linden (Data-Validation Editor) and I were both unavoidably absent for some time in 2000; Dr C. Glidewell took over from me as Editor with no interruption to services and Dr A. J. Blake was able to take over seemlessly from Dr Linden.

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

G. Ferguson, Editor of Section C

4.1.5. *Acta Crystallographica* Section D. Section D continued as a monthly journal and printed 324 scientific articles throughout the year 2000. Two were Topical Reviews, one on porphobilinogen synthase (5-aminolaevulinate dehydratase) crystal structures, with emphasis on metal-ion utilization. The other was a full description, with experimental results, of the nucleosome core particle with marvellous illustrations and analyses of structure. There was also a debate on the density of proteins within crystals (the subject of two back-to-back Scientific Comment articles). Again we were delighted to be able to publish the reports of a CCP4 Study Weekend; the subject this year was Low-Resolution Phasing. J. Wilson, H. Saibil and J. Grimes were the editors for this issue of 17 articles. The journal also contains Book Reviews and Meeting Reports.

Rules on the deposition and release of macromolecular structural data (atomic coordinates and structure factors, required to be deposited before publication is approved) can be found in the *Notes for Authors*.

A selection of macromolecular crystal structures reported in 2000 is given in Table 2; these represent proteins and nucleic acids with a

wide range of molecular weight. The resolution of structures presented in Section D continues to improve. Of 84 structures reported in research papers, 38 had a resolution of better than 2.0 Å, and 12 of these had resolutions higher than 1.5 Å. Higher resolution was shown to allow for more precise pictures of hydrogen-bonding interactions, distinction between amide and carboxylate groups and suggestions on enzyme mechanisms. Experimental methods of data collection articles include those on neutron Laue diffraction studies, the first protein structure from powder diffraction data (on mechanically ground material), camera modification so that very low resolution data can be obtained, single-wavelength anomalous dispersion, flash-cooling recycling experiments, and the suppression of ice formation on crystals. In the area of phase determination, many articles on direct methods were published together with papers on a new vector-search rotation function, an alternative molecular replacement program, cryo-soaking with halides for phasing, and different density constraints in low-resolution phasing. With respect to later stages such as model refinement, there are articles on phase refinement, *R* free, solvent flattening, bulk-solvent corrections, selenium atom arrangements in Se-Met-substituted proteins, the enhancement of Se-Met anomalous signals by oxidation, solving data from twinned crystals, electron-density map quality, mass spectroscopy as an aid in identification and in screening heavy-atom derivatives, and the validation of protein crystal structures. Many analyses of structure (beta-sheet propensity, side-chain conformations, metal-binding modes) and of crystal perfection (defects, mosaicity, temperature effects, radiation damage, effects of humidity changes) were also reported. There were also several articles on combinations of experimental techniques such as X-ray diffraction and electron microscopy or EXAFS.

Three crystallization Co-editors (N. Chayen, M. Pusey and A. Zagari) have been appointed. They will oversee the publication of crystallization papers (of which there were 180 in 2000), and we envisage the possible eventual publication of an electronic version of this part of the journal. Studies on the optimal crystallization procedures, effects of microgravity on crystal quality, critical nuclear size in protein crystallization, and crystal growth in magnetic fields have been described this year.

Illustrations are wonderful and the journal producers are to be complimented on the fact that colour pictures are free to the authors. The result is evident in each issue of the journal and also on the covers which each month portray an interesting structure or item of information from the contents. The assistance of reviewers is again acknowledged and they, together with the staff at Chester, ensure that this is a high-quality journal. My thanks to all of you.

J. P. Glusker, Editor of Section D

4.1.6. *Acta Crystallographica* Section E. In early 2000, it was decided to establish a new electronic-only journal, *Acta Crystallographica* Section E: *Structure Reports Online*. This represents the IUCr's first production of a purely electronic journal, and may pave the way for further moves in this direction. It is a joint venture of the IUCr and the Cambridge Crystallographic Data Centre (CCDC); the involvement of other database organizers is being sought. Throughout the year, planning meetings took place at Chester and in Cambridge. These were largely concerned with the drafting of *Notes for Authors* and the role of the CCDC in providing check facilities aimed at detecting duplicate publications, together with a software editor for the preparation of papers in CIF format; this should be available during 2001 and will help to attract new authors. A team of ten Co-editors was established, covering inorganic, metal-organic and organic structures. The decision was taken to terminate the publication of Electronic Papers in Section C, with effect from January 2001. This meant that papers, originally destined for Section C, were diverted to Section E starting in October/November 2000. A small number of the editorial team, with extensive experience of editing papers for Section C, processed these papers so that the launch of Section E took place, as planned, in the first week of 2001. The first issue reported the structures of 68 compounds. The new journal has been promoted through the newsletters of various crystallographic associations and at several scientific meetings, as well as directly by the IUCr through its own journals, the *IUCr Newsletter*, web site, and leaflets. Promotion includes attractive subscription packages.

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

4.1.7. *Journal of Applied Crystallography*. *JAC* published 1468 pages in 2000, up from 1208 in 1999. This included 190 full research papers and 69 shorter papers. A special issue containing the proceedings of the Eleventh International Conference on Small-Angle Scattering, held at Brookhaven National Laboratory, USA, in May 1999, was published in June 2000. Although the manuscripts were submitted at the conference, a long delay resulted owing to the review handling process. Publication in *JAC* of the proceedings of future small-angle scattering meetings is desirable, as this gives high visibility to the authors and highlights one of the major subject areas of the journal. For the front cover, the Editor provided a selection of keywords based on the articles and other material in each issue. This procedure has, to the Editor's knowledge, not provoked any comments so far. Although several keywords appear regularly, the procedure seems to make sense and may alert some readers to look at a specific item.

G. Kostorz, Editor of *JAC*

4.1.8. *Journal of Synchrotron Radiation*. We would like to acknowledge the outstanding contribution to the journal of Professor J. R. Helliwell who retired as a Main Editor in September 2000; he has been replaced by Dr D. M. Mills of the APS, Argonne, USA. *JSR* published proceedings from the Daresbury Laboratory Satellite Conference of the IUCr Glasgow Congress entitled From Source to Science. The Guest Editor was Professor R. J. Cernik. The Commission on Synchrotron Radiation are thanked most warmly for their input coordinated by Professor Y. Amemiya (Chair). The XAFS XI Conference took place at SPring-8 in August 2000 and subsequently a very large number of papers have been handled by the Co-editors through the latter half of 2000 for publication in March 2001. Again these are being handled as camera-ready copy and the articles are fully refereed. The special Guest Editors are Professors T. Ohta and M. Nomura.

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

4.2. Commission on *International Tables*

The main activity during the year 2000 was the SGML conversion, typesetting and proof-reading of text and data for several volumes of *International Tables*. For the remaining volumes, the preparatory work continued. The *International Tables* home page was continually updated by U. Shmueli in Tel Aviv, Israel, and B. McMahon at the IUCr office in Chester, UK.

The proposed new Volume A2 on Relations between the Wyckoff Positions of the Space Groups and their Maximal Subgroups, Editor U. Müller, was approved by the Executive Committee. Volumes A1 and A2 will be printed in one book.

4.2.1. Volume A. *Space-Group Symmetry*; Editor Th. Hahn. All text sections for the Fifth Edition of Volume A were printed as galley

proofs and proof-reading by the authors continues. The LaTeX files of the space-group tables, prepared by M. Aroyo, P. Konstantinov and their colleagues in Sofia, Bulgaria, are complete and proof copies with the scanned space-group diagrams inserted are awaited. Publication of the Fifth Edition of Volume A is envisaged for the latter part of 2001.

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

4.2.2. Volume B. *Reciprocal Space*; Editor U. Shmueli. The year 2000 was marked by a most significant progress in the preparation of the Second Edition of Volume B. The distribution of the galley proofs among the authors was completed, and their corrections were received. There followed an extensive correspondence between the Editor, the Technical Editor and the authors regarding the galley proofs which contributed greatly to a successful preparation of the page proofs. The effort invested in this careful examination of the galley proofs and an expert implementation of the corrections turned out to lead to a very small number of corrections in the page proofs. At the time of writing this report, the corrections for all the page proofs are with the Technical Editor, who has already implemented all or most of them. It was announced in the IT home page that the Second Edition of Volume B would be published in early 2001, and the present status of the Second Edition certainly confirms this expectation.

4.2.3. Volume C. *Mathematical, Physical and Chemical Tables*; Editor E. Prince. The publication, in June 1999, of the Second Edition of Volume C essentially completed the volume as originally conceived in 1981. The activity in 2000 was therefore limited to collecting lists of misprints and ideas about things that would need to be added or updated in a future edition.

4.2.4. Volume D. *Physical Properties of Crystals*; Editor A. Authier. Parts 1 and 2 are complete and have been in the Chester office since November 1999. Typesetting has begun.

4.2.5. Volume E. *Subperiodic Groups*; Editors V. Kopsky and D. B. Litvin. The volume is being prepared for an anticipated 2001 publication.

4.2.6. Volume F. *Crystallography of Biological Macromolecules*; Editors M. G. Rossmann and E. A. Arnold. This volume was commissioned in recognition of the extraordinary contributions that knowledge of macromolecular structure has made, and will make, to the analysis of biological systems, from enzyme catalysis to the workings of a whole cell. The volume covers all stages of a crystallographic analysis from preparation of samples using the techniques of molecular biology and biochemistry, through crystallization, diffraction data collection, phase determination, structure validation, and structure analysis. Although the book is written for experienced scientists, it is recognized that the modern structural biologist is more likely to be a biologist interested in structure, rather than a classical crystallographer interested in biology. Thus there are chapters on the fundamentals, history, and current perspectives of macromolecular crystallography, as well as the availability of useful programs and databases including the Protein Data Bank. Each chapter has been written by an internationally recognized expert.

Macromolecular crystallography is undergoing a revolution. Just as crystallography became central to the study of chemistry, macromolecular crystallography has become a core science in biology. Macromolecular crystallography has shaped our view of biological molecular structure, and is providing a broader understanding of biological ultrastructure and the molecular interactions in living systems. As reflected by the exponential increase of entries in the Protein Data Bank over the past decade, there has been an explosion in the number of macromolecular structures determined, the majority by X-ray crystallography. Knowledge of the sequences of entire genomes, from bacteria through human, has sparked a structural genomics effort that aims to determine 10000 new macromolecular structures in the next decade. Crystallography is expected to yield the largest share of this new crop of structures. The field of macromolecular crystallography is still evolving rapidly, and capturing its essence in a single volume is a challenge. Therefore the volume emphasizes durable knowledge, but also contains articles on somewhat more volatile topics.

As of February 2001, the editing of galley proofs for all 85 articles in the volume is nearly complete. The overall quality of the articles received is very high, and we are very grateful for the high level of commitment that so many have given to this project. Volume F will be published in 2001.

4.2.7. Volume G. *Crystallographic Information*; Editors B. McMahon and S. R. Hall. With the submission of a draft of a major chapter on the macromolecular CIF dictionary, the important first phase of covering the topic areas originally envisaged is essentially complete. However, additional chapters have been commissioned to cover the recently approved image CIF (imgCIF) dictionary. This is a dictionary of data names required by the Crystallographic Binary File (CBF) image representation project. The imgCIF/CBF initiative extends the CIF approach to cover efficient storage of two-dimensional area detector data and other large data sets. The chapters on this topic are expected by summer of 2001. Other work to be done during 2001 will be the rigorous reviewing of the chapters already in hand and the collection of the remaining chapters on technical matters.

4.2.8. Volume A1. *Maximal Subgroups of Space and Plane Groups*; Editor H. Wondratschek. For the Contents of Volume A1, see *Acta Cryst.* (1996). A**52**, 962. During a meeting of the authors at the end of the year 2000, partly financed by the IUCr, the final editorial decisions were taken. The checking of the data has been completed. The Chapters Guide for Users and Mathematical Background of the Subgroup Tables are approaching completion. Volume A1 will be bound together in one book with the new Volume A2.

4.2.9. Volume A2. *Relations between Space Groups*; Editor U. Müller. The Wyckoff positions of a space group show up in well defined Wyckoff positions of its subgroups. These relations are important for the consideration of structural relationships between crystal structures and play an important role in phase transitions of crystals. The corresponding relations have been listed for all Wyckoff positions of all space groups and their maximal subgroups. This includes the infinity of all isomorphic subgroups. The tables have been complete for two years. However, some alterations were performed in order to obtain a presentation consistent with Volume A1.

[*Note:* Volumes A1 and A2 have subsequently been designated Volume A1, *Symmetry Relations between Space Groups*, edited by H. Wondratschek and U. Müller.]

Th. Hahn, Chair

4.3. Commission on Aperiodic Crystals

In 2000, the Commission was involved with the organization of the international conference Aperiodic2003. This meeting will be held in Belo Horizonte in Brasil, 21–26 July 2003. It will be organized by N. N. Speziali. See http://www.fisica.ufmg.br/~ap2003/ for futher details.

There were no other specific activities of the Commission.

S. van Smaalen, Chair

4.4. Commission on Biological Macromolecules

The recommendations for the publication and release of coordinates and structure factors have been published [*Acta Cryst*, (2000). D**56**, 2]. The editors of more than 15 journals that publish crystal structures of biological macromolecules have been contacted to acquaint them with the new guidelines and to seek their cooperation in adopting these as at least minimum standards. Of the journals approached, only three had requirements which met or exceeded the IUCr guidelines.

The IUCr Executive Committee has approved a suggestion from the Commission to nominate a representative on the Protein Data Bank Advisory Committee (PDBAC) following an invitation from the Director of the Protein Data Bank. The Commission's nominee, Professor E. N. Baker, has been appointed to the PDBAC as the first nominee of the IUCr.

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

Plans are well advanced for a Symposium on Crystallography and Bioinformatics in Structural Biology to be held in Bangalore, India, in November 2001, following the meeting of the Asian Crystallographic Association.

M. Guss, Chair

4.5. Commission on Charge, Spin and Momentum Densities

The Commission held open and closed meetings during the Sagamore XIII Meeting on Charge, Spin and Momentum Densities (Stare Jablonki, Poland, 3–9 September 2000). The Sagamore meetings remain the most important 'outcome' of the Commission, and this particular meeting was an outstanding success. The thirteenth in this series of triennial meetings took place at Hotel Anders, in the Taborskie Woods beside the wonderful Lake Szelag Maly in the Mazurian lakes and woods region of north-eastern Poland. The Sagamore meetings focus on aspects of charge, spin and momentum distributions, their determination from a wide variety of experimental techniques, and their detailed analysis and comparison with theory, and have a considerable history, recently documented by M. J. Cooper (http://alpha.uwb.edu.pl/sagamore/page_history.html).

The meeting attracted just over 100 participants, with nearly 50% of those in attendance from either France or Poland. L. Dobrzynski and his Local Committee did a truly superb job of organizing the meeting, impressing all with their warm hospitality and the ease with which they assisted with all manner of requests. As expected, the oral and poster presentations contained more physics than chemistry, but that did not distract from some wonderfully lively discussions, even if there was always the perception that most present worked and thought in either direct space or momentum space, and had some difficulty traversing the landscape in between!

Many presentations dealt with the use of synchrotron radiation in various forms, and this was reflected in the large number of participants from ESRF, France, and Japan. However, there was a disappointing turnout from the charge-density, neutron and electron diffraction communities, and the discussions could have benefited from a few more theoreticians. A number of talks described quite substantial and dramatic improvements in methods and measurements (shorter times and increased accuracy and precision), and it was clear that maximum-entropy methods are being employed to great effect in all aspects of charge, spin and momentum density research.

Discussion at Commission meetings in Poland centred on upcoming conferences relevant to the Commission's community, as well as updates on projects sponsored by the Commission. Planning for the next triennial Gordon Research Conference on Electron Distributions and Chemical Bonding is well under way. The meeting is being organized by J. C. H. Spence and C. Lecomte, both Commission members, and will be held 8–12 July 2001. An International Conference on Inelastic X-ray Scattering will be held in Haikko, Finland, 22–26 August 2001, and is being organized by K. Hämäläinen, S. Manninen, and P. Suortti, all present or past Commission members. The next European charge-density meeting is proposed for Denmark in 2002.

Progress on the Density Matrix, Fermiology, Maximum Entropy (MEM) and Multipole Refinement Projects was outlined. W. Weyrich is keen to return to activity on the Density Matrix Project, and is planning to involve a number of new participants; A. Bansil indicated that interest and participation in the Fermiology Project was increasing rather than decreasing; M. Sakata would like to see some interaction between the MEM and Multipole Refinement Projects, and is keen for others to look at the standard data sets; according to C. Lecomte, there was a disappointing number of takers for the Multipole Refinement Project, but S. Pillet has recently analysed all data sets and this work has been submitted for publication; P. Mallinson attended the recent COMCIFS meeting, and is now actively seeking input from the charge-density community, particularly *XD* users, in order to refine further a CIF dictionary for charge-density analysis; V. Tsirelson's proposed Project on Topological Features was described and considered best as part of the Multipole Refinement Project (in the sense that one must obtain a model electron density before any topological analysis). With more than 70 subscribers worldwide, *XD* is no longer a Commission project.

As an interesting footnote, the Commission was formed in 1975 as an outcome of the Sagamore meetings, and to this day the Commission is actively involved in the planning and execution of these conferences. An offer to host the next Sagamore meeting in Australia was endorsed at an open meeting of the Commission, so those with an interest in charge, spin and momentum distributions should pencil in Sagamore XIV for mid-August 2003, hopefully on an island off the southern Queensland coast! Updates on this and other Commission activities can be found at the Commission website: http://www.iucr.ac.uk/iucr-top/comm/csmd/index.html.

M. A. Spackman, Chair

4.6. Commission on Crystal Growth and Characterization of Materials

The Commission focused its activity on two main events during 2000: (i) organization of the International School on Crystal Growth of Materials for Energy Production and Energy-Saving Applications and (ii) promotion and support of an International Workshop on Preparation and Characterization of Technologically Important Single Crystals. Both meetings have been sponsored by the IUCr with young scientist support.

The School was initially planned to be held in Monastir, Tunisia, in November 2000 but due to local organization problems it had to be moved to Trieste, Italy, in March 2001. The organization proceeds

well and over 50 students from different countries have so far enrolled. The School is chaired by R. Fornari and four other members of the Commission are involved as lecturers or members of the Scientific Committee.

The Workshop will be held at the National Physical Laboratory, New Delhi, India, 26–28 February 2001. The Workshop, in addition to dealing with growth and characterization of single crystals (in particular oxides), will also serve to celebrate the 60th birthday of K. Lal, an eminent scientist who has contributed for more than three decades to the development of new crystallographic methods for the characterization of defects in crystalline materials. He was also a member of the Commission for three triennia between 1987 and 1996. Four members of the Commission are included in the International Advisory Committee.

The Commission examined the application of K. Sato for IUCr sponsorship of the 11th International Summer School on Crystal Growth that will take place in Doshisha, Japan, in July 2001, and confirmed its support to this traditional and important school. The Commission advanced two suggestions for microsymposia to be held during the forthcoming 2002 Congress. First a symposium on High-Resolution X-ray methods for Characterization of Thin Layers and second a symposium on Preparation of Crystals for Medical Applications, which could include detectors for X-, γ- and other ionizing rays, piezoelectric crystals for echography *etc.* Decisions about these proposals will soon be taken by the Programme Committee of the Congress.

Finally, in the last months of 2000, the Commission also established some contacts with colleagues in Romania and Egypt to verify their interest in organizing new schools/workshops in 2002/2003.

R. Fornari, Chair

4.7. Commission on Crystallographic Computing

During 2000, the Commission has been almost solely involved in affairs in Europe. We would have appreciated leads to enable us to become involved in the USA, Asia or Australasia.

4.7.1. ECA Computing Special Interest Group (SIG). The principal event for us in 2000 was the inaugural session of the European Crystallographic Association Computing Special Interest Group. This was convened under the interim chairmanship of D. Viterbo at the ECM in Nancy, France. A significant number of crystallographers turned up for the session, covering all domains of current crystallography. A. L. Spek (Netherlands) was nominated as first full Chair, A. Urzhumtsev as Secretary and L. M. D. Cranswick as Vice-Chair. I am involved as the IUCr Commission Representative.

The compilation of the programme at Nancy for sessions involving computing once again revealed the problems of the relationship between macromolecular and other crystallographers. Two sessions were organized with the intention that each should contain contributions from all crystallographic domains. This was not entirely successful, with a fair amount of disturbance in the lecture rooms as the topics moved from one domain to another.

A. L. Spek has negotiated a different format for the ECM in Crakow, Poland, in the hope that he can create more continuity within each session, noting that the cost of separating macromolecular crystallographers from the rest is that opportunities for cross-fertilization of ideas may be lost.

4.7.2. 2002 Congress. We are keen to organize a school as a satellite for Geneva. The outline format we would like to try will aim to be attractive across the whole range of the interface between computing and crystallography. The pattern proposed would be along the lines of a mini-Congress, with both joint and parallel sessions. I have no doubt that a Programme Committee can be formed to generate an exciting and profitable scientific programme.

The thing that worries me most is the practical logistics. The costs of schools, conferences and meetings of all kinds continue to escalate at a rate that makes it increasingly difficult for young students to attend. Costs, however, would be a major concern if a school in Geneva is to be widely accessible.

4.7.3. Other activities. For many years there has been discussion amongst the changing members of the Commission about the setting up of a database of intensity data, similar to those once available as part of *XTAL*. At one point we had much e-mail discussion about setting up a database of experimental intensity data for use by software developers or for use by teachers needing an example of specific problems. Several interesting data sets were identified and permission sought for their inclusion in the database, but in the end we perceived no external interest in this work, and further work has been put in abeyance.

D. J. Watkin, Chair

4.8. Commission on Crystallographic Nomenclature

The principal concerns of the Commission in 2000 were the nomenclature of phase transitions and of crystallography in n dimensions, as they have been over the last several years. All communications within the Commission and its sub-committees were conducted electronically this year. No new nomenclature problems in the crystallographic literature were brought to the Commission's attention in 2000, continuing the trend established in recent years.

The first Report of the Working Group on Phase Transition Nomenclature, with J.-C. Tolédano as Chair, was accepted by the Commission in May 1998 and appeared in *Acta Cryst.* (1998). A**54**, 1028–1033. The Working Group, see *Acta Cryst.* (2000). A**56**, 199 for membership of the renewed group, was thereupon charged with extending its recommendations for a six-field structural phase transition nomenclature to other classes of phase transition. These eventually included magnetic, incommensurate, morphotropic, polytypic, radiation-induced and quasicrystalline phase transitions. Extension was straightforward for the first three categories of phase transitions. Recommendations for the nomenclature of the remaining classes, with their less-clearly established relevance to standard schemes of transition in equilibrium systems, are more tentative. The second Report is expected to be complete early in 2001.

The first Report of the Sub-committee on the Nomenclature of n-Dimensional Crystallography, entitled I. Symbols for Point Group Transformations, Families, Systems and Geometric Classes, appeared in *Acta Cryst.* (1999). A**55**, 761–782. The Sub-committee, with T. Janssen as Chair and membership as in *Acta Cryst.* (2000). A**56**, 616, was renewed by the Commission and charged with proposing a set of recommendations that would supplement those presented in the first Report, thereby completing the recommended nomenclature and symbolism for use in n-dimensional crystallography. Considerable discussion of alternative notations and symbols for lattice centrings and Bravais and arithmetic crystal classes in four- and six-dimensional space has led to general agreement on the symbols for arithmetic crystal classes, centrings and Bravais classes. A similar degree of consensus has developed concerning the generalization of the Hermann–Maugin symbols to higher dimensions.

The Commission Observer to COMCIFS, see *Acta Cryst.* (1997). A**53**, 822, reported that the Committee has been very active, mainly with the formulation of CIF dictionaries. Version 2 of the mmCIF (macromolecular) dictionary is now formally approved; the imgCIF/CBF dictionary, designed for the transmission and archiving of

images from array detectors and suitable for any multidimensional image, has been reviewed; the sasCIF (small-angle scattering), rhoCIF (electron densities) and magCIF (magnetic structures) dictionaries are at advanced states of preparation. These, along with the powder diffraction dictionary, which has been adopted as the standard of the powder diffraction file, show that a large number of IUCr Commissions have now adopted the CIF standard.

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

S. C. Abrahams, Chair

4.9. Commission on Crystallographic Teaching

During 2000, there has been intensive discussion using the Commission e-mail listserver. The discussion was mainly centred on the forthcoming workshop to be held at Ismailia, Egypt, in November 2000. The Commission agreed on the title of the workshop, the topics of the lectures and the invited speakers. Moreover, the Commission supported the idea of producing computer-based teaching materials in printed form for those who cannot access the web site and at the same time have limited computing facilities, producing teaching materials for school children (printed and on CD-ROM) and also producing teaching materials in applied crystallography for the general public.

A. Hunter who has wide experience in teaching was appointed as a consultant.

A microsymposium on teaching crystallography was organized by R. Neder who is a member of the Commission at ECM-19, Nancy, France, 25–31 August 2000. Five lectures were given and there were 70–100 attendees. In connection with the microsymposium, an informal meeting chaired by Å. Oskarsson, the Secretary of the Commission, was held with the Commission members attending the Nancy meeting. They were able to suggest the following: (1) people should be appointed to be responsible for regions; (2) a list on educational resources should be available on the web site; (3) a teaching mailing list should be created; (4) some of the interactive programs should be on the IUCr server. Most of these suggestions are being implemented.

Most of the members and consultants are really active in serving the goal of the Commission either by producing teaching materials or by organizing teaching sessions. To see the different activities of the members and consultants, see the e-mail discussion list on the teaching web site.

K. Al-Sayed, Chair

4.10. Commission on Electron Diffraction

There has been considerable activity by members of the Commission in the year following the Glasgow Congress. D. L. Dorset has replaced J. C. H. Spence as Co-editor of *Acta Crystallographica* Section A to represent the interests of electron diffraction and electron crystallography. Since D. L. Dorset has relocated to another workplace, responsibility for the Commission web page has been taken over by the Secretary, S. Hovmöller, from his location at Stockholm University, Sweden (svenh@struc.su.se).

Commission members have organized and/or presented invited talks at crystallographic or microscopy meetings related to electron crystallography or diffraction. These include: the 21st Meeting of the Society of Crystallographers in Australia (February 2000, Thredbo, NSW, conference talk by D. L. Dorset); Microscopy 2000, February 2000, Canberra, ACT, Australia (session on atomic architecture organized by R. Withers with presentations by J. C. H. Spence and D. L. Dorset); EUREM 2000, Brno, Czech Republic, July 2000 (workshop on electron crystallography organized by I. G. Voigt-Martin and J. R. Fryer – contributions by H. Zandbergen, D. Van Dyck, J. Gjønnes, and D. L. Dorset); International Kunming Symposium on Microscopy, Kunming, People's Republic of China, July 2000 (entire meeting on electron diffraction and electron microscopy, organized by Li Fang-Hua); 19th European Crystallographic Meeting, Nancy, France, August 2000 (session on electron crystallography organized by I. G. Voigt-Martin, also a contribution by J. Gjønnes). For the European Crystallographic Association, a special-interest group on electron crystallography has been organized, initially chaired by S. Hovmöller and J. Gjønnes.

Education has always been a strong theme for the Commission, exemplified, for example, by the annual schools on electron crystallography organized by S. Hovmöller in Stockholm, Sweden, or at other sites in Europe, wherein other members of the Commission have been invited as lecturers. The most recent school was a Euro Summer School held at the Central Facility for Electron Microscopy at the Aachen University of Technology in Germany. Additionally, small informal meetings on electron crystallography have been organized by H. Zandbergen at TU Delft, Netherlands, in December for discussion of practical issues related to structure determination. The first was held in December 1998 and the most recent was held during December 2000.

D. L. Dorset, Chair

4.11. Commission on High Pressure

High-pressure crystallography continues to develop very rapidly through the influence of modern synchrotron and neutron sources, with new techniques and areas of science opening up every year. The Commission sees as its principal activity the organization of symposia and workshops to keep the crystallographic community in touch with the latest developments, and to create opportunities to extend the boundaries of the Commission's activities and draw in new people from the wider field of high-pressure science.

The principal activity of this year was the organization of an international workshop focused on the topic of Crystallography at High Pressure and High Temperature using X-rays and Neutrons. Nearly 80 high-pressure scientists from 13 countries gathered at the picturesque site of the third-generation synchrotron facility SPring-8 at Hyogo, Japan, for the four days from 30 September to 3 October 2000. The workshop was jointly organized by the Commission, the SRRC Japan Atomic Energy Research Institute (JAERI), and the Japan Synchrotron Radiation Research Institute (JASRI). The local organizer was Commission member O. Shimomura. The major topics of the oral sessions included structures and transitions in molecular and elemental liquids; novel (and often complex) structures in simple systems – like lithium, oxygen and xenon; theoretical studies of liquid carbon, molecular hydrogen and alkali metals under pressure; a wide variety of geoplanetary science – mineral phases and equations of state, the Earth's lower mantle and core, and planetary ices; high P–T synthesis of new materials like cubic boron carbonitride and 3D polymerization of C_{60}; and high P–T experimental techniques using X-ray synchrotron and neutron sources. Altogether, there were 25

oral and 43 poster presentations. The participants included 13 young scientists supported jointly by the IUCr and JAERI, from Germany, India, Russia, Switzerland, USA, UK and Sweden, and a further three young scientists were invited speakers. Considerable assistance with the excellent local arrangements was given by JAERI and JASRI staff.

In addition, Commission members have been involved during this year in the early stages of preparing an international workshop covering the full range of its activities to be held at Orsay, France, in September 2001 with Commission member I. Goncharenko as the local organizer. A preliminary bid has been prepared and submitted for sessions at the 2002 Congress. Planning has also continued for a School on High-Pressure Crystallography to be held at Erice, Italy, in 2003 with Commission member A. Katrusiak as Director.

The Commission maintains a regularly updated mailing list and an active web site, including a list of forthcoming meetings of interest to high-pressure crystallographers and detailed reports on past meetings. Work has been in hand to fulfil the one further undertaking of the Commission's terms of reference by adding a listing of 'current information on central facilities for high-pressure crystallography, and on how to access them', and this will soon appear. These services to the community depend on the much appreciated efforts of J. Parise, J. Loveday and M. Kunz.

R. J. Nelmes, Chair

4.12. Commission on Neutron Scattering

In the last fall, a series of international meetings were held on neutron scattering. The First ICFNS (International Committee on the Future of Neutron Sources) under WGFCMP (Working Group on Facilities for Condensed Matter Physics) of IUPAP (International Union of Pure and Applied Physics) was held at Mito, Japan, 3–4 November 2000 to explore a way to promote international collaboration for planning, construction and exploitation of large facilities for condensed-matter physics such as neutron sources. Several IUPAP Commission Chairs, members of the OECD Neutron Source Working Group, representatives of the regional users community, major neutron facilities and other organizations involved all over the world, 28 members in total, gathered together. The status reports from the existing facilities (ILL/Grenoble, LLB/Saclay, FRJ-2/Jülich, HMI/Berlin, FRM-II/München, ISIS/RAL, HFIR+SNS/ORNL, NBR/NIST, LANSCE/LANL, RRR/ANSTO, JRR-3M/Tokai, KENS/Tsukuba), planning facilities (ESS, JSNS) and regional users groups (NSSA: the Neutron Scattering Society of America, ENSA: the European Neutron Scattering Association, NSAJ: the Neutron Scattering Association of Japan) were presented and discussed. A strong concern about the unforeseen closures of neutron sources such as HFBR/BNL, USA, and DR-3/Risø, Denmark, was shown so that the timely provision of new facilities and the upgrade of existing facilities were strongly recommended. Y. Fujii reported the status of the Asian–Oceanian Neutron Sources as the President of NSAJ and activities of this Commission as its Chair. Strong support for a plan to form the Asian–Oceanian Neutron Scattering Association (tentatively designated AONSA) to complement ENSA in Europe and NSSA in the USA was expressed by the attendees. Finally it was concluded that the strong growth of the neutron scattering community such as ENSA, NSSA, AONSA and these overarching organizations should be supported not only by IUPAP covering physics but also by other organizations from the ICSU bodies such as the IUCr covering other broader fields.

ICANS-XV (International Collaboration on Advanced Neutron Sources) at Tsukuba, Japan, 6–9 November 2000, was co-hosted by KEK and JAERI. This meeting has traditionally focused its topics on accelerator-based neutron sources and related science/technology, but this time it partly included reactor-based sources so that participants from the Asian–Oceanian region presented their activities and future plans to build/refurbish research reactors for neutron beam utilization. By taking such an opportunity, Y. Fujii (Commission Chair) organized an evening session on Asian–Oceanian Neutron Sources and made a summary report at the plenary session. In contrast to other regions such as Europe and North America, a large number of new neutron sources are built, funded or planned as follows: Australia began construction of a new 20 MW reactor (RRR) funded in 1999 at Lucas Heights and it will be completed in 2005; China has already started construction of a 60 MW reactor (CARR) with a high flux of 8×10^{14} n cm^{-2} s^{-1} in Beijing and it will be completed in 2006; Korea is building several spectrometers for a 30 MW reactor (HANARO) recently completed in 1997; Taiwan is in the middle of refurbishment of its 40 MW old reactor to a 20 MW higher flux reactor (TRR-II) at Lungtan to be completed in 2006; and Japan has proposed a spallation neutron source as strong as 1–5 MW to be built in Tokai jointly by KEK and JAERI. Later in December, the Japanese Government funded this project so that the construction will start in April 2001 and its first phase aiming at 1 MW will be completed in 2006. At the evening session, representatives from the users community and major facilities as well as general participants discussed the possible formation of the Asian–Oceanian Neutron Scattering Association and they agreed that both Australia and Japan having strong users communities already established would take the initiative in progressing this, possibly by taking an opportunity at the fourth Conference of the Asian Crystallographic Association Meeting (AsCA) at Bangalore, India, 18–21 November 2001. Toward such a target, users representatives and large facility representatives in the Asian–Oceanian region are being contacted by Y. Fujii). During this meeting, a few of the Commission members who had attended met for an exchange of information.

This Commission's project to file the 'Catalogue of Neutron Sources' is now under way. A full list of contact persons and neutron sources, both reactor and accelerator all over the world, is now being prepared while the format of the Catalogue is refined. The International Conference on Neutron Scattering (ICNS-2001) is to be held at München, Germany, 9–13 September 2001, where the Commission business meeting is planned. Also planned is a Microsymposium on Neutron Scattering organized by the Commission at the fourth AsCA meeting in Bangalore.

Y. Fujii, Chair

4.13. Commission on Powder Diffraction

Several important events and activities concerning Powder Diffraction (PD) took place during 2000, including congresses, workshops, schools and round robins. The Commission always played an important role, fostering the participation of scientists and trying to increase the number of people and different countries interested and involved in PD. This support role included a continuous consulting activity, to endorse meetings and schools, but also an active participation in the organization of most of the important events related to PD. Commission round robins and the Commission *Newsletter* increased their popularity, and are now appreciated by a large public of PD experts and novices. The Commission *Newsletter*, whose mailing list currently includes more than 2000 names and is available also on the web, is now regarded as an important forum where PD specialists can present their views on new methods and developments in PD. It is also read by a steadily increasing number of

people that are interested in PD applications, even if not strictly expert in the field. This wider community, including engineers, materials scientists, chemists and physicists, is particularly attracted by the editorial style, based on a main topic, changing for every new issue, reports on activities and events, and information on commercial products and available software. The web site and Commission *Newsletter* are now actively used as rapid and effective means to discover the state-of-the-art on the various applications of PD.

4.13.1. Meetings/workshops/schools. The major event of 2000 was EPDIC-7, held in Barcelona, Spain, in May 2000. This was also the site of the Commission meeting in 2000. The Commission was deeply involved in the programme of EPDIC-7, concerning both organization and chairmanship of sessions and had an active participation in the speaker list. The conference was endorsed by the Commission and sponsored by the IUCr. The Commission also took part in the planning activity for the next EPDIC conference (Sweden, 2002); the Commission Chair is now an *ex-officio* member of the EPDIC Committee and related ECA-SIG. Also of importance for PD were the Denver conference in the USA and ECM-19 in Nancy, France. Commission members were involved in session organization of ECM-19 for topics related to PD. Of particular interest were the two microsymposia on Advanced Methods for Structure Determination from Powder Data (Chairs: D. Loüer, B. M. Kariuki) and Microstructure Analysis by Powder Diffraction (Chairs: P. Scardi, R. Kuzel).

A further activity related to Congress organization concerned Accuracy in Powder Diffraction III, which will take place 22–25 April 2001 at the NIST facility of Gaithersburg, Maryland, USA. The Commission looks towards this event with considerable interest, in the hope that it will match the high success and interest of the two preceding conferences, and also as the site for the 2001 Commission meeting.

The CPD gave support to the International Workshop on the Rietveld Method (RW2000-PL), Wisla, Poland, 7–10 September 2000, and to the Workshop on Powder Diffraction, Bayreuth, Germany, 4–8 October 2000. Both events were successfully held and were characterized by the participation of numerous young scientists. Detailed reports are to appear in the forthcoming issue of the CPD *Newsletter*.

4.13.2. Projects. The two Commission projects carried out during 2000 are the round robins on phase analysis and on size–strain determination. Full details and extensive reports can be found on the web pages.

1. *Quantitative phase analysis*. The task was concluded during 2000 with an advanced report prepared by I. Madsen and co-workers. This important contribution, also available through the web in an extended form, summarizes the work carried out so far, with an interesting statistical analysis of the results. In the near future, a publication should appear in an IUCr journal, and the Commission has already allocated a budget to buy and to distribute (together with the Commission *Newsletter*) a large number of reprints.

2. *Size–strain analysis*. The Commission started this project at the end of 1999, when a preliminary description of the project was presented by the promoter, D. Balzar, in *Newsletter* No 21. During 2000, D. Loüer prepared a large number of ceria powder samples (the Commission contributed economically to the purchase of chemicals), which were distributed to several test laboratories (A. Le Bail, J. I. Langford, P. Stephens, A. Fitch, B. Toby, M. Daymond) for PD data collection using different techniques and methods. D. Loüer presented convincing details on the preparation procedure and powder microstructure during the 2000 Commission meeting. Eventually the data were made available *via* the Internet, and a large number of round-robin participants were freely allowed to download the data collected by means of different geometries. Results were returned and the large mass of data is currently being analysed by D. Balzar: the first report should appear in the Spring 2001 issue of the Commission *Newsletter*. The current status of the size–strain round robin is reported on the web pages of the CPD and linked URLs.

4.13.3. Web site. The Commission web site is now a well known reference for powder diffractionists around the world. It offers numerous links and information on events related to PD and any other activity of interest, including the Commission round robins, just concluded or in progress. Full details are available. An important point is the Commission *Newsletter* archive. Downloading of recent issues in pdf (Acrobat) and in doc (Word) format is freely allowed, and has resulted in a tremendous increase in the number of readers.

4.13.4. Newsletters. Two Commission *Newsletters* were published in 2000 (see http://www.iucr.org/iucr-top/comm/cpd/index.html for downloading). The spring issue (No. 23) was edited by R. J. Cernik and I. Madsen and focused on synchrotron-radiation PD and non-ambient techniques; it also contained an extended report on the Round Robin on Quantitative Phase Analysis, recently concluded. The fall 2000 *Newsletter* (No. 24), edited by D. Balzar, addressed the study of materials' microstructure by powder diffraction, and reported several contributions on line-profile analysis and full information on forthcoming events for the year 2001. In both issues of 2000, the computer software pages were taken care of by L. M. D. Cranswick, and were highly appreciated by readers for their quick and effective presentation. News from ICDD was reported in the dedicated pages, as is now a tradition of the Commission *Newsletter*. Starting with the next issue (Spring 2001), the Commission *Newsletter* will be given an ISSN number for official record (ISSN 1591-9552).

P. Scardi, Chair

4.14. Commission on Small-Angle Scattering

During 2000, the Commission has followed up on its previous activities in data standardization, education and meeting organization.

Commission member D. Svergun has led the data-format standardization activity. The details of the resulting sasCIF dictionary can be found at http://www.embl-hamburg.de/ExternalInfo/Research/Sax/sascif.html. M. Malfois, a postdoctoral fellow in Dr Svergun's laboratory, presented a talk on sasCIF at the NOBUGS 3 meeting in Daresbury, UK, in June 2000. This activity focused on the handling of one-dimensional small-angle scattering (SAS) data, and its CIF dictionary should prove to be a valuable resource for other members of the community who are attempting to standardize data formats for two dimensions and higher (time-resolved SAS, three-dimensional SAS, temperature-jump SAS *etc.*). The main leadership for these activities is provided by a group who call themselves 'Computer Aid for Nomadic Small-Angle Scatterers (CANSAS)' and meeting about every 18 months. Their home page is at http://www.ill.fr/lss/canSAS/main.html.

Commission member J. S. Pedersen has been active in the education area as a co-organizer of the 5th European School on Scattering Methods Applied to Soft Condensed Matter, which took place in Bombannes, Gironde, France, 28 May–3 June 2000. Dr Pedersen presented additional lectures on the analysis of SAS data in Les Houches, France, and Leoben, Austria. Dr Pedersen deserves to be congratulated on his recent move to a Chair at the University of Aarhus, Denmark. His lectures and publications on the subject of SAS data analysis are a real resource for the entire community.

D. Svergun is a principal organizer of the EMBO Practical Course on Solution Scattering from Biological Macromolecules scheduled

for August/September 2001. Further information may be found at http://www.embl-hamburg.de/ExternalInfo/workshops/2001/EMBO/index.html.

The Commission has worked on the subject of meeting scheduling since the last community-wide gathering at Brookhaven, USA, in May 1999. This triennial series of SAS Congresses has been a mainstay of scientific communication in the SAS community since 1965. Before the founding of this Commission the IUCr provided significant support in the publication of the Proceedings of the various SAS Congresses in the *Journal of Applied Crystallography*. The people who organize the SAS Congresses have, however, been basically autonomous, which has created difficulties in scheduling because their schedule has tended to overlap the IUCr's own three-year cycle of summertime Congresses. The findings of a survey conducted in early 2000 failed to uncover any factors that would prevent this Commission from taking a more active hand in assisting the organizers of these SAS Congresses. While the next SAS Congress is already set for August 2002 in Venice, Italy, the Commission will be working to promote the development of its successor in such a way as to minimize scheduling conflicts and to enhance IUCr support. All of the current members of the Commission are members of the Scientific Advisory Board for the Venice Congress. It is hoped that these efforts will lead to a more public and open process that will better serve the needs of the entire community.

The community notes with considerable sadness the passing of two of its most prominent members: A. Guinier (July 2000) and H. Brumberger (November 2000). Dr Guinier is often credited, along with P. Debye, with being a founder of the field of small-angle scattering. The Guinier model of scattering from dispersed particles is a crucial element of many SAS analyses. Dr Brumberger was a founder of the triennial series of SAS Congresses and edited the Proceedings book that came out of the Syracuse Conference in 1965. Both of these individuals had long and distinguished careers that contributed greatly to the SAS community. Their careers will be celebrated in upcoming meetings at Los Angeles, USA (July 2001) and in Venice, Italy (August 2002).

The issue of leadership succession will receive considerable attention from the Commission between now and August 2001. The current Chair will not be eligible for re-election and replacements will have to be found for at least two departing members. The Commission has been in existence for nearly five years and has become a mature body. We hope that new blood and a new purpose will contribute to the community's vitality in the coming years.

The Commission has moved its home page on the web to http://www.iucr.org/iucr-top/comm/csas/. Complete details about the Commission's agenda and instructions for subscribing to its listserver may be found there.

J. D. Barnes, Chair

4.15. Commission on Structural Chemistry

In 1999, the Commission endorsed Indaba 3 Symmetry Breaking, Chirality and Disorder in Molecules and Crystals. This very successful symposium was held in August 2000 in Skukuza, South Africa. Commission member D. Levendis served as Chair of the Organizing Committee and two Commission members, J. Flippen-Anderson and G. Desiraju, were among the invited speakers. J. Flippen-Anderson also served on the Programme Committee. A report describing the meeting has been posted to the Commission web page. Commission member V. Belsky was the Programme Chair for the second Russian National Conference on Crystal Chemistry that was held in May 2000 in Chernogolovka, near Moscow, Russia. There were about 300 posters and oral presentations divided into six sections – organic, inorganic and coordination crystal chemistry, structure–properties correlation, chemical bonding, solid-state reactions, and dynamic crystal chemistry.

In 2000 the Commission endorsed three microsymposia to be held in 2001. The first, entitled Symposium on Organic Crystal Chemistry, will be held in Poznan-Rydzyna, Poland, immediately preceding the ECM meeting in August. The leading subject of the symposium is Weak Interactions in Crystals and their Implications. The Symposium is being organized by T. Borowiak and two Commission members, V. Belsky and J. Flippen-Anderson, are among the invited speakers. The second symposium endorsed by the Commission is entitled Horizons in Hydrogen Bond Research and will be held in Torino, Italy, in September immediately following the ECM meeting in Poland. A wide variety of topics relating to hydrogen bonding will be discussed from both crystallographic and quantum-mechanical perspectives. Former Commission member G. Gilli is one of the organizers of this symposium. Thirdly, the Commission endorsed Crystallography in Drug Design, which will be held in Lódz, Poland, following the ECM meeting. The speakers at this symposium will be mainly crystallographers. The audience, however, is intended to be heavily weighted towards medicinal chemists and pharmacologists so that researchers in these areas can become acquainted with crystallography and begin to understand the critical role it plays in the field of drug design. The Commission feels strongly that this sort of interdisciplinary interaction should be well supported.

With the Commission membership being distributed over six of the seven continents, almost all our business is transacted *via* e-mail. Further to facilitate communications within the Commission and with the greater structural chemistry community, we have set up a small listserver just for Commission members and plan to apply to the IUCr to have a more general discussion list added to the IUCr site. While e-mail can be efficient and timely, it does not permit members to experience the way crystallography is carried out in different settings. The Chair had an opportunity during a recent South American vacation to visit with Commission member G. Punte at her university in La Plata, Argentina. It was a fascinating and educational experience to learn how some colleagues in South America function as crystallographers. Other activities involving members of the Commission included reviewing the notes for authors for *Acta E*, serving as α and β testers for the new CONQUEST search engine for the Cambridge Structural Database, and keeping the Commission web site up-to-date.

J. Flippen-Anderson, Chair

4.16. Commission on Synchrotron Radiation

The Commission has been active in a number of areas over the past year.

A workshop on Recent Developments in Medium Sized Synchrotron Radiation Sources was held 19 August 2000 at the ANKA synchrotron in Karlsruhe, Germany. The meeting was attended by about 45 people with the following invited and keynote talks: The Mission for ANKA (V. Saile); Machine Design Considerations and Commissioning Report (D. Einfeld); ANKA Beamlines, Experimental Stations and Beyond (H. Moser); SPEAR III (H. Winick); Swiss Light Source (T. Schmidt); Canadian Light Source (E. Hallin); Diamond Project (C. Nave); Boomerang (J. Boldeman); Development of In-vacuum Mini-Undulators (H. Kitamura). This field of synchrotron radiation (SR) machine design is a very fruitful one at present as medium-sized machines are being designed and commissioned with performance in the energies of interest to crys-

tallographers that are comparable with performance from the mega machine facilities. Much useful discussion occurred on machine design, costs of components, compatibility and standardization of ring components as well as a keen desire for individual facilities to find ways of collaborating in the area of medium-size synchrotron machine design. A keen wish was expressed to have similar meetings on a regular one to two year cycle and to form a network for aiding collaboration between facilities operating in this area.

An opportunity was also afforded to tour the newly operating ANKA facility and to admire various aspects of instrumentation, especially a multi-purpose beamline. The kind hospitality of ANKA GmBH and V. Saile, D. Einfeld and H. Moser in hosting this meeting is gratefully acknowledged.

A meeting of the Commission was held at SRI-2000 in Berlin, Germany, and a number of issues were discussed, especially relating to possible satellite meetings that might be held in conjunction with the 2002 Congress, encouragement of young scientists to see SR research as a career, expansion of the Commission web site and a number of other matters.

Letters of support for major proposed new SR facilities were written including those in connection with: The Australian Synchrotron Radiation Program (ASRP) in support of Boomerang (to J. Boldeman); Proposed New Third Generation VUV/SX Storage Ring at the University of Tokyo (UTSOR or VSX), Japan (to T. Oshima, Minister for Education, Science, Sports and Culture); The Australian National Synchrotron Facility (Boomerang) (to the Rt Hon Mr John Howard, Prime Minister of Australia).

S. W. Wilkins, Chair

4.17. Commission on XAFS

No report has been received from the Chair.

5. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 2000 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 2000 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2001, but approved in 2000, are listed below:

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

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

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

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

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

6. Meeting on Crystallography and Drug Design, Lódz, Poland, 1–3 September 2001.

7. Asian Crystallographic Association Meeting AsCA '01, Bangalore, India, 18–21 November 2001.

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. If organizers intend to publish proceedings, they should consider either a special issue of one of the journals of the IUCr or, for computing schools, the IUCr Crystallographic Symposia Series, which is published jointly by the IUCr and Oxford University Press.

Organizers of meetings wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the meeting, writing to the Chair of the Sub-committee. The present Chair is Professor H. Fuess, Technische Universität, Darmstadt, FB 11 Materialwissenschaft, Fachgebiet Strukturforschung, Petersenstrasse 23, D-64287 Darmstadt, Germany (e-mail: hfuess@tu-darmstadt.de).

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

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

H. Fuess, Chair

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

6.1. Information services

The CEP has continued its task as editorial body for the on-line information services of the IUCr. The highest priority is set on providing up-to-date information of use to the whole crystallographic community. The rebranding and restructuring of the site as a preliminary for the restyling of the existing pages is approaching completion. The information services are now under the general name **Crystallography Online** in tune with **Crystallography Journals Online**. The style and structure of **Crystallography Online** emphasizes the different aspects of crystallography and projects of the community rather than the IUCr as an institution. This change has also entailed a considerable amount of work, almost complete, by the Executive Secretary to produce a modernized set of web pages for the purely institutional part of the IUCr. It is hoped that the restyling can be completed during 2001 and a new, young and enthusiastic editor appointed to continue the work on this much-appreciated service. An important goal is to move towards an integrated approach to the dissemination of information and news within the crystallographic community by print and electronic means. To this purpose, the CEP maintains contact with other important players in the field, such as the editor of the *IUCr Newsletter*, to ensure the diffusion of valuable sources of information by all means available. In 1998, the R&D group at Chester made a relational data analysis for a new version of the *World Directory of Crystallographers* allowing a large degree of automation in the maintenance of this important facility. Owing to the heavy work load in 1999, caused by the introduction of **Crystallography Journals Online**, it was not possible to implement the redesigned *Directory* until now. It is intended that this work should be carried out early in 2001.

6.2. NeXus CD-ROM

Under the continued leadership of L. M. D. Cranswick, 1000 copies of a new version of the Crystallographic NeXus: Virtual Crystallographic Internet on CD-ROM were produced. These CD-ROMs are distributed free of charge to laboratories and scientists with an interest in crystallography lacking adequate connection to the internet. The CD-ROMs contain public domain software and copies of web sites of interest to crystallographers. The CD-ROMs were publicized through many channels in such a way that scientists have to apply to receive a copy. Distribution at some meetings to participants from the developing world was also undertaken. The IUCr is most grateful to ICSU for financial help for this project but regrets that the change in ICSU policy has meant that no funding is available from this source in 2001. It is nevertheless intended to continue this project and to report that almost all of the 1000 CD-ROMs have now been distributed.

6.3. Crystallography Journals Online

The online journal service has continued to evolve. From 1 September 2000, online access was available only to subscribers of the print journals. The IUCr has become a member of CrossRef, the organization offering a viable system which enables article cross referencing between journals of different publishers to be implemented. Individual online article sale was implemented during 2000 and subsequently put into service. The scanning of back issues of all IUCr journals is advancing well and it is hoped that all back articles will be online late in 2001 or early 2002. During 2000, a policy document concerning the archiving of IUCr journals was drafted and discussed amongst the CEP and other interested parties. It has now been submitted to the Executive Committee for discussion and approval.

6.4. Meeting attendance

H. D. Flack (IUCr Representative to ICSTI) and Y. Epelboin attended the ICSTI/ICSU Press interactive workshop on Digital Archiving: Bringing Issues and Stakeholders Together, held 30–31 January 2000 in Paris, France. As a result of attending this meeting, the first draft of a proposed IUCr policy on archiving was composed for deliberation and discussion by the CEP. Moreover, this meeting brought to our attention the initial report of an international working group convened by the IASTMP (International Association of STM Publishers) concerned with defining and certifying electronic publication in science. It is in the interest of the IUCr that this work be completed and finalized (there are severe difficulties of vocabulary in the initial report) as it will prove useful in achieving viable IUCr policies in two domains. The first concerns archiving and the second is in the field of acceptance standards for article submission to journals as concerns their prior distribution in print or electronic form as a preprint.

In May 2000, H. D. Flack (IUCr Representative to ICSTI), P. R. Strickland and B. McMahon attended the annual ICSTI meeting in Columbus, Ohio, USA. The collaboration of H. D. Flack and B. McMahon in the ICSTI review of the OAIS (Open Archival Information System) enabled an improved version of the proposed IUCr archiving policy to be drafted. (Details of the ICSTI meetings are given in the report of the ICSTI Representative.) The same persons made a day visit to CAS (Chemical Abstracts Service) following the ICSTI meeting. The in-house processes for producing abstracts, attributing registry numbers, chemical names and diagrams by CAS were explained and the CAS ChemPort facility was demonstrated. Discussions centred around the electronic delivery by IUCr to CAS of electronic headers for abstracts and came to a satisfactory conclusion. In the course of the discussions, the problem of publications in electronic-only journals was raised as it appeared that these were not integrated into the CAS system.

In October 2000, B. McMahon (IUCr Representative to CODATA) attended the CODATA 2000 conference in Baveno/Stresa, Italy. As the worlds of electronic publishing and scientific data overlap considerably, it is a significant advantage to the CEP that amongst its members one now finds the representatives both to ICSTI and to CODATA. In November 2000, H. D. Flack visited the IUCr editorial office in Chester. This provided an excellent opportunity for discussions both within the CEP and with the Executive Secretary, the Editor-in-Chief, the Promotions Officer and numerous other members of staff in Chester. In February 2001, H. D. Flack, B. McMahon, P. Strickland and J. R. Helliwell will attend the ICSU–UNESCO meeting entitled Electronic Publishing in Science, Paris, France.

H. D. Flack, Chair

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

7.1. Mandate

COMCIFS is the Committee appointed by the Executive Committee to maintain the Crystallographic Information File (CIF) standard owned by the IUCr.

7.2. Committee structure

COMCIFS consists of a small number of voting members appointed by the Executive Committee and a much larger number of non-voting members appointed by the Chair of COMCIFS. The latter are on the COMCIFS mailing list and are invited to comment on any COMCIFS business. Most business is carried out by e-mail and, to ease the load on the small number of COMCIFS voting members, much detailed work is carried out by Committees such as the Dictionary Maintenance Groups, the Dictionary Review Committee, the Publicity Committee, the Software Development Committee and the Dictionary Definition Language Committee. Many of these groups run formal e-mail discussions maintained by the staff in Chester. COMCIFS Committees collaborate with the IUCr Commissions as appropriate and CIF users are normally welcome to join the discussion list of any group in which they have an interest. All approved dictionaries, and some dictionaries close to approval, are posted on the IUCr web site where many of the CIF discussions can also be viewed

7.3. Membership

Members are appointed following each General Assembly. Current voting members are: I. D. Brown (Chair), B. McMahon (Coordinating Secretary), H. M. Berman, H. J. Bernstein, S. R. Hall, G. Madariaga. In 2000, P. Edgington resigned from his position as a voting member of COMCIFS and from his Committees as a result of a change in his position at the Cambridge Crystallographic Data Centre (CDCC). His place on the Committees has been taken by O. Johnson of the CCDC.

7.4. Dictionaries

Approval of new and revised CIF dictionaries continues to be a major part of COMCIFS activities. Each new dictionary is compiled by a working group, often in conjunction with the appropriate IUCr

Commission, and each existing dictionary is maintained by a Dictionary Maintenance Group. Recommendations from these groups are closely examined by a Dictionary Review Committee to ensure CIF compliance before being passed to the voting COMCIFS members for formal approval. Compiling a dictionary is a challenging and time-consuming occupation and several drafts are usually exchanged between the Dictionary Review Committee and the dictionary compilation group before a new dictionary is ready for approval. We are fortunate to have a number of volunteers willing to contribute a significant amount of their time to this effort.

In September, formal approval was given to Version 2 of the mmCIF dictionary which is now in use at the Protein Data Bank. This approval was combined with a formal lifting of the 80 character line restriction for files written using this dictionary.

In November, COMCIFS approved the imgCIF/CBF dictionary used to record and transfer information on images, specifically the images produced by two-dimensional detectors. This project broke new ground for COMCIFS because it also contains a specification for an equivalent binary file format: the Crystallographic Binary File (CBF). Approval of this dictionary was followed by the appointment of a Dictionary Maintenance Group consisting of H. M. Bernstein, R. Sweet and J. Westbrook, who were all closely involved with the original version of this dictionary. This group already has a draft of version 2 which can be found at http:// www.bernstein-plus-sons.com/software/CBF.doc/cif_img_1.1.3.html and which is expected to be approved in 2001.

A number of minor changes in the coreCIF dictionary have also been approved in the light of experiences gained in the submission of reports of crystal structures to the primary journals and databases.

Currently under final review by the Dictionary Review Committee are the modulated structure dictionary (msCIF) and a dictionary containing the basic symmetry concepts used in crystallography (symCIF).

Draft dictionaries for electron density (rhoCIF), magnetic structures (magCIF) and small-angle scattering (sasCIF) were submitted to the Dictionary Review Committee and are currently undergoing revision to bring them into conformity with CIF standards.

The increase in the number of dictionaries, many of which draw on definitions supplied in other dictionaries, has led to the development by B. McMahon, H. J. Bernstein and J. Westbrook of a protocol for merging two or more dictionaries into a larger virtual dictionary. This protocol will also allow official CIF dictionaries to be merged with local dictionaries to allow individual laboratories to customize their CIF applications.

7.5. Software

Developing the necessary software for manipulating CIFs is currently a major concern. While the crystallography community has the expertise needed to prepare new dictionaries, it has a relatively small pool of expertise in the type of sophisticated software that can exploit the full potential of the dictionaries. One approach, pursued by H. J. Bernstein, has been to exploit the information-handling techniques of extensible markup language (XML) by writing programs to interconvert CIF and XML. However, while XML is provided with a rich set of tools for managing and manipulating document structure, it still has rather few domain-specific applications, and is not an automatic candidate for mining the full information content of CIFs. Nevertheless, until there is more generic software available for processing STAR files such as CIF, the CIF language will not be able to achieve its full potential. COMCIFS encourages writers of crystallographic software to make full use of the capabilities built into the standard.

Most of the software currently available for CIF is in the form of toolboxes to help others write CIF applications. However, there is an urgent need to provide the user community with the tools for preparing and editing CIFs. The program enCIFer, to be released by the Cambridge Crystallographic Data Centre in late 2001, has many features that crystallographers will find useful. These include a browser that provides clear error markup, an alphabetic view of data names, data entry panes containing the dictionary definitions, buttons for the special character sequences frequently used in CIF text, spreadsheet loop displays, text searching, a text editing window, user templates and a crystal structure visualizer. EnCIFer is based on the DDL1 core dictionary and is designed for use by the small-structure community. A similar editor, ADIT, has been written for the DDL2 mmCIF dictionary and is designed primarily for users of the Protein Data Bank.

7.6. Relationships with other bodies

The Chair of COMCIFS sits *ex officio* on the Commission on Crystallographic Nomenclature, who also appoint a member to monitor COMCIFS activities. Many of the dictionary Committees are either sponsored by or have close ties with the corresponding IUCr Commission. Several members of COMCIFS are working on the text for Volume G of *International Tables for Crystallography*, the volume which describes the CIF standards. The secretary of COMCIFS has been appointed IUCr Representative to CODATA, and gave a presentation on IUCr publishing and data activities involving CIF at the CODATA conference at Lake Maggiore, Italy, in October 2000.

In order to simplify data exchange, the macromolecular crystallography community has been successfully lobbying other molecular biology groups to adopt the STAR file structure, the syntax used by CIF. As a result of the efforts of J. Westbrook, D. Greer and others, mmCIF has been recognized by the Object Management Group as providing the Common Object Request Broker Architecture standard (CORBA) for the exchange of macromolecular information between databases.

7.7. Future developments

Although CIF was originally developed as a simple file structure for recording information on crystal structures, it is developing into a fully featured language for manipulating crystallographic information. The purpose of the CIF dictionaries is to provide computer access to that information. Most of the attributes of a data item described in the dictionaries, *e.g.* whether a particular value is expressed as a number or as a character string, can already be parsed by a computer. Computers are, of course, unable to interpret the crystallographic definitions which remain only accessible to humans. However, the relationships between different data items can be described in machine-readable terms, and thus allow computers to build more detailed models of complex crystallographic objects. One of the current exciting extensions proposed for CIF is the development of a Dictionary Relational Expression Language (dREL) which will provide algorithmic expressions that allow values for each item in the dictionary to be derived from other items, *e.g.* the calculation of the density from the cell mass and cell volume. If values of these latter items are not present in the CIF, the computer will use the algorithms in the dictionary to calculate the cell volume from the lattice parameters and the cell mass from the list of atoms. A preliminary account of dREL has been given by Spadaccini, Hall & Castledean [*J. Chem. Inf.* (2000). *Comput. Sci.* **40**, 1289–1301]. While a dictionary

written in dREL is primarily intended to allow a computer to calculate derived values not currently stored in a given CIF, it will incidently provide precise definitions of, and relationships between, crystallographic concepts, allowing it to be used as an on-line crystallographic encyclopaedia.

7.8. IUCr support

It is my pleasure to express COMCIFS thanks to the IUCr office for its support, particularly in supplying web sites and discussion groups, and the services of B. McMahon as our very effective Secretary.

I. D. Brown, Chair

8. Committee on Crystallographic Databases

Members of the Committee have kept in touch by e-mail, personal visits and at major crystallographic meetings.

H. Behrens has retired as Head of the Inorganic Crystal Structure Database (ICSD) at FIZ, Karlsruhe, Germany. He is succeeded in that role by P. Luksch, and we welcome him to the Committee as the ICSD representative. Dr Luksch visited the IUCr Chester Office and the Cambridge Crystallographic Data Centre (CCDC) in the UK in late 2000. ICSD continue their software collaboration with NIST (Washington DC, USA).

R. Jenkins will step down as Executive Director of the International Centre for Diffraction Data (ICDD) in 2001, and his successor is now being sought. ICDD are now completing their holdings of powder data on metals and alloys through a collaborative agreement with NIST.

At the European Crystallography Meeting, held in Nancy, France, in August 2000, several members of the Committee had informal talks with members of the IUCr Executive Committee. Arising from these discussions, it was proposed that the IUCr web pages should contain a page devoted to the Committee on Crystallographic Databases, detailing its membership, and providing links to the web pages of the major crystallographic databases. It is expected that this page will be implemented early in 2001.

The Protein Data Bank (PDB) at the Research Collaboratory for Structural Bioinformatics (RCSB) have produced their first Annual Report. It reports completion of a seamless transition of the PDB from Brookhaven three months ahead of time, a total of 12 592 PDB entries as at 27 June 2000, and an average of 90 000 hits per day accommodated by the main PDB web site alone.

The CCDC released a completely new search interface for the Cambridge Structural Database (CSD) in April 2000. ConQuest brings the CSD to the PC Windows environment for the first time, and also operates under various flavours of Unix. A new licensing policy and protocols were also introduced at this time.

CRYSTMET remains fully up to date and is processing data on a current basis. Toth Information Systems has now developed a generalized software environment, the Materials Toolkit, within which both CRYSTMET and the ICSD (*via* an agreement with FIZ, Karlsruhe) can be loaded.

F. H. Allen, Chair

9. Promotion Committee

The Journals Working Group started off the year by inviting the Editors to reveal plans for their journals for the coming triennium to the wide readership of the *IUCr Newsletter*, and the Working Group's promotional work continued to build on that strong and positive foundation. For the first time, a full-colour brochure advertising the journals and the innovative features of Crystallography Journals Online was produced. The 2001 version will include details of the new member of the family, *Acta Crystallographica* Section E: *Structure Reports Online*, and the imminent launch of this, the IUCr's first online-only journal, necessitated a strong promotional effort. Publicity at the summer crystallographic meetings in the form of leaflets and posters was followed in the autumn by a direct-mail campaign to the participants of the Glasgow Congress, which was reinforced in the winter with substantial coverage in the crystallographic newsletters.

The Promotion Committee, which met at ECM-19 in August, also continued to publicise the new editions of *International Tables for Crystallography* Volumes A, B and C, and stepped up its promotion of the eagerly anticipated Volume F: *Crystallography of Biological Macromolecules*.

The IUCr's extensive range of publications and online services were exhibited at the major crystallographic meetings, and its profile was raised further by the presentation of prizes for posters that best promoted the understanding of crystallography.

The above initiatives were efficiently and effectively implemented by the Promotions Officer, Andrea Sharpe.

A. M. Glazer, Chair

10. *IUCr Newsletter*

Four issues of the *IUCr Newsletter* were printed in 2000. Each contained 32 pages, a 33% increase over the previous year's content. The content covered IUCr activities, Regional Associates, news concerning crystallographers and crystallography, notices, awards, elections, resources, obituaries, meeting reports, future meeting announcements, and a general calendar. The amount of material contributed from different countries, especially Japan, India and Africa, grew significantly.

Each issue devoted two or three pages to brief summaries of selected articles recently published in IUCr journals. Articles of particular note in Volume 8 (2000) were reports of the Scientific Sessions at the Glasgow Congress, reports of IUCr Committee activities including current developments with CIF files, a report on the IUCr Executive Committee meeting in Nancy, France, in August 2000, and extensive coverage of the new electronic-only *Acta Cryst.* Section E: *Structure Reports Online*. Other special topics included a discussion of structural proteomics, an exchange of views on the state of the art of electron-density determination by electron and X-ray diffraction, a feature article on Dorothy Hodgkin and women in science and crystallography, and contributions from the Mineralogical Society of America. 18 meeting reports from 14 different countries and 10 obituaries of prominent crystallographers in 6 countries were published.

The mailing list was maintained with little change in total circulation. Eighteen countries continued to assist in the effective and economic distribution of the *Newsletter*. Sustained advertising volume coupled with efficient production has reduced the total cost to the IUCr for production and distribution in the past year in spite of the 33% increase in newsletter content.

W. L. Duax, Editor

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

The Book Series Committee continued its activities during 2000. A second edition of *The Basics of Crystallography and Diffraction* by C. Hammond was published. Three other *Monographs*, covering dynamical theory, powder diffraction and bonding in inorganic compounds, are now in production and should appear in the near future, while two other manuscripts are being completed or in the negotiating stage. Prospective authors are encouraged to contact the Chair of the Committee. Manuscripts covering specific aspects of crystallography and related fields are most welcome.

P. Coppens, Chair of Book Series Committee

12. Regional Associates and Scientific Associates

12.1. American Crystallographic Association (ACA)

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

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

Two volumes of the ACA Transactions, Structural Informatics, Volume 32, and Two Decades of Synchrotron Radiation Research, Volume 33, were published and distributed. The ACA contributed financial support to the 2000 Summer Crystallography School in Athens, Georgia, and the 2000 Physics Olympiad.

The final total membership for 2000 was 1890 (1483 regular, 170 student, 209 retired and 28 corporate). Four issues of the *ACA Newsletter* were published.

Scheduled future ACA meeting include Los Angeles, California (21–26 July 2001), San Antonio, Texas (25–30 May 2002) and Cincinnati, Northern Kentucky (26–31 July 2003).

W. L. Duax, IUCr Representative

12.2. Asian Crystallographic Association (AsCA)

AsCA has begun the preparation for its 2001 meeting and the International Programme Committee for AsCA '01 was inaugurated in April 2000, with C. J. Howard (Australia) as Chair. In August, the International Organizing Committee was inaugurated, with Chair Z. Rao (China). The President proposed a new system for AsCA as follows: (*a*) the timing of the AsCA meeting may be changed to June/July; (*b*) the election of new Council and Executive members may be made at the AsCA meeting instead of at the IUCr Congress.

This proposal will be discussed at the AsCA meeting. AsCA sent a letter to the USA Civilian Research & Development Foundation (CRDF) to ask for support of crystallographers in the Central Asian region in September: The President visited Taiwan and held a meeting on the operation of AsCA with the Treasurer S. L. Chang . In October, the AsCA home page on the web opened: http://neon.otago.ac.nz/chemistry//asca/2000/home.html. The AsCA *Newsletter* will be published on this web site. The President and Rigaku held discussions about the Rigaku fund for AsCA '01, which will be used to support scientists from developing countries. The First Circular of AsCA '01 was published in November. M. Vijayan (India) was appointed Chair of the Local Organizing Committee. Preparations for AsCA '01 are proceeding smoothly.

M. Tanaka, IUCr Representative

12.3. European Crystallographic Association (ECA)

The ECA Executive Committee nominated the ECA Prize Committee, which was chaired by ECA Vice-President J. Bernstein. This Committee had to select among several nominations from different fields of crystallography and the first winner of this award was A. Yonath from the Weizmann Institute of Science for her work with the ribosome structure. The prize was awarded during the opening ceremony of ECM-19 in Nancy, France.

According to the ECA Statutes, representatives to the ECA Council of Affiliate and Individual Members (IM) should be elected on the basis of one representative for 100 Affiliate and Individual Members, from a list of nominations signed by at least six Affiliate or Individual Members. An Election Committee was nominated and a very efficient e-mail voting procedure and counting were organized by ECA Secretary P. T. Beurskens. From seven candidates and with more than 400 IMs, four new councillors were elected (C. Mealli, K. Wilson, P. Spadon and P. Gilli) and they later participated in the Council meeting in Nancy.

During the opening ceremony of ECA-19, the ECA President gave an oral report of his activity since the establishment of the ECA in 1997. This report was later made available to the Council, in written form.

The ECA Council met during the meeting and analysed its activity during the past year. The report by the Secretary was approved by the Council and the report by the Treasurer was presented and approved after being audited by an *ad hoc* Commission nominated by the Council. Reports from nine Special Interest Groups (SIGs), on Macromolecular Crystallography, Charge, Spin and Momentum Density, Aperiodic Crystallography, Electron Crystallography, Mineralogical Crystallography, Instrumentation and Experimental Techniques, Molecular Interaction and Recognition, Powder Diffraction, and Crystallographic Computing, were presented and approved. The organizers of ECM-18 presented the final report in the form of a CD-ROM and announced that the book of Proceedings would soon be published. The Chair of ECM-19, C. Lecomte, reported that this meeting had had more than 1000 registered participants and reported also on the quality of the scientific programme, with 12 plenary lectures, almost 60 microsymposia with about 300 oral presentations and 600 posters. The organization and programme for ECM-20 to be held in 2001 in Krakow was presented and discussed. The South Africa representatives presented the only proposal to host ECM-21 in 2003. The proposal was accepted after some discussion of the associated financial matters.

To conclude the meeting, a new President and other officers were elected. The new Committee consisted of C. Lecomte as President, P. T. Beurskens as Vice-President, G. Filippini as Secretary, M. T. Duarte as Treasurer and E. Dodson, M. Jaskolski and D. Viterbo as members.

M. A. Carrondo, IUCr Representative

12.4. International Organization of Crystal Growth (IOCG)

During 2000, the IOCG Executive Committee set the guidelines for the International Conference on Crystal Growth (ICCG-13), which will take place in Doshisha University, Kyoto, Japan, 30 July–4 August 2001, in conjunction with the International Conference on Vapour Growth and Epitaxy (ICVGE-11). The International Summer School on Crystal Growth (ISSCG-11) will also take place in Japan in the week 24–29 July 2001. Information regarding these events may be found at URL http://iccg.gakushuin.ac.jp/.

The IOCG Executive Committee has selected the venue for the 2004 ICCG and ISSCG meetings. Both will be held in Europe, the school in Berlin, Germany, and the conference in Grenoble, France.

The President and Executive Committee of IOCG have also started exploring the possibility of IOCG becoming an International Union to be affiliated to the International Council for Science (ICSU).

The IOCG Committee for Crystal Growth Awards, which had the task of selecting two scientists who gave outstanding contributions to either fundamental (Frank Prize) or technological (Laudise Prize) aspects of crystal growth, concluded its work. Nominations for the awards were mostly advanced by National Associations for Crystal Growth and the Committee had a very difficult task since the nominees were all of high standard. The conclusion was that the Frank Prize would be jointly awarded to D. T. J. Hurle and S. Coriell for their great contribution on the fundamental aspects of crystal growth, especially on cooperative research leading to the quantitative understanding of the role of convective flows and electric fields in crystal growth and morphological stability. The Laudise Prize will be assigned to G. Mueller for his outstanding contributions to the development of methodical and technological aspects of crystal growth and for his leading contribution to the development of global computer modelling of crystal growth processes. Both awards will be presented during ICCG-13 in Kyoto, Japan.

The triennial reports (period 1998-2000) prepared by the National Crystal Growth Associations were collected by the President of IOCG, T. Nishinaga, and distributed to members of the Council and Executive Committee. It appears that National Associations for Crystal Growth are very active in promoting crystal growth science in their own countries as well as in collaborating in the organization of international events.

During the General Assembly, which will take place in Kyoto, the new President and officers will be elected. In view of this event, T. Nishinaga asked the National Associations to submit proposals for the new President, Executive officers and councillors. These proposals will be reviewed by an Election Committee before being discussed at the Assembly in August.

R. Fornari, IUCr Representative

12.5. International Centre for Diffraction Data

R. Snyder represented the ICDD at the Commission on Powder Diffraction meetings, and now also the newly born International X-ray Analytical Society (IXAS), reporting on the many powder diffraction related activities carried out by the two organizations (see the ICDD web site: http://www.icdd.com/; and the IXAS web site: http://www.ixas.org/). Fruitful and active collaborations are steadily maintained.

P. Scardi, IUCr Representative

13. Representatives on Other Bodies

13.1. IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS)

The IUCr and six other international organizations are represented on IDCNS, the body charged by the International Union of Pure and Applied Chemistry (IUPAC) with responsibility for ensuring that all recommendations made in its name that are concerned with nomenclature and symbols are consistent with international standards. IUPAC recommendations are published in *Pure and Applied Chemistry* following revision and final acceptance. A total of 41 such documents passed through IDCNS hands during the year. IDCNS meets annually each August at a time that often coincides with a major crystallographic meeting. The meeting of 28–29 August 2000 in Sèvres, France, completely overlapped the Nineteenth European Crystallographic Meeting. It was not possible for either the IUCr Representative or his Alternate to attend, hence the report to IDCNS on IUCr nomenclature activities was communicated in writing.

Several matters were discussed in Sèvres of interest to crystallographers. The IUPAC *Compendium of Chemical Technology* (corrected and revised version of 2nd print edition) is available online at: http://www.iupac.org/publications/compendium/index.html and access to current values of the fundamental physical constants is available at: http://www.physics.nist.gov/cuu/Constants/. Major progress has been made with a new manual to replace the present IUPAC 'Blue Book' by a manual on organic nomenclature that will provide *unique* IUPAC chemical names. A third edition of *Quantities, Units and Symbols in Physical Chemistry*, covering the condensed state, is in preparation and is planned to be available on the web. Other recent IUPAC publications of interest include *Definition of Terms for Diffusion in the Solid States*, *Nomenclature of Organometallic Compounds of the Transition Elements* and *Names for Inorganic Radicals*. The International Standard *Prefixes for Binary Multiples* has been published; see *Acta Cryst.* (2000). A**56**, 625 for the new names and prefixes. New useful online chemical naming services are: http://www.iupac.org/nomenclature/index.html, http://www.acdlabs.com/ and http://www.beilstein.com/. The Bureau International des Poids et Mesures (BIPM) is working toward a redefinition of the kilogram linked to fundamental or atomic constants and also toward an extension of the International Temperature scale below the present lower limit of 0.65 K; BIPM approved katal (symbol 'kat') for the SI unit mole per second in the expression of catalytic activity.

The IUPAC Council confirmed the Strategic Plan of 1998–1999 for restructuring IUPAC management of projects, with all Nomenclature Commissions officially terminated by the end of 2001. However, IUPAC policy is not to discontinue or interrupt the collection and critical assessment of useful data in areas on which the international reputation of IUPAC has been established, and approved an *ad hoc* Committee to develop a long-range strategy for IUPAC's work in chemical nomenclature.

S. C. Abrahams, IUCr Representative

13.2. International Council for Scientific and Technical information (ICSTI)

The winter committee and discussion meeting was held in ICSU headquarters, Paris, France, 29–30 January 2000. This meeting enabled the business of ICSTI to advance and provided an opportunity for reviewing the state of the various technical activities and issues concerned with information policy. An important task concerned the policy to adopt for the replacement of the ICSTI

Executive Secretary due for retirement in September 2000. In the event, the secretariat was put out to tender and from the offers received the ICSTI bureau selected the offer of IIA (Information International Associates), a specialized consultancy established in the USA with whom ICSTI has had contacts for a considerable number of years. The arrangement involves the services of a part-time Executive Director experienced in scientific technical and medical (STM) publishing and a part-time Secretary in Paris.

The above meeting was followed directly on 30–31 January by an ICSTI/ICSU Press Interactive Workshop on Digital Archiving: Bringing Issues and Stakeholders Together. Y. Epelboin, member of the IUCr's Committee on Electronic Publishing, Dissemination and Storage of Information (CEP), also attended the workshop, which had such success that it had to be held in the UNESCO building as the ICSU headquarters proved to be too small. The principal speaker at the workshop was G. Hodge of IIA on Beyond the ICSTI/CENDI Study: Setting the Stage, and this was followed by sessions on Models for Digital Archives (T. van de Werf and C. Lupovici on The Open Archival Information System Framework as applied to Deposit Libraries in the NEDLIB project, C. Lynch on Open Archives: E-journal and E-print perspectives, F. Pelle and S. Rozenfeld on Electronic Archive Registry: The Results of a URN-based Experiment), The Economics of Sustainable Archives (J. T. Scott and T. Ingoldsby on The AIP Experience, L. Pope on The PubMedCentral Initiative and K. Hunter on The Elsevier Experience) and Policy and Standards Issues (D. Marcum on State of Legal Deposit Legislation, P. Gatenby on Developing Policy and Best Practice Procedures at the National Library of Australia and J. Rumble, Emerging Practices in the Data Community). A presentation was also made by E. Sandewall on the initial deliberations of an international working group convened by the IASTMP (International Association of STM Publishers) concerned with defining and certifying electronic publication in science. This apparently rather dry subject is really of the utmost importance to a learned society publisher such as the IUCr. The intention is to define clearly the relationship between an electronic preprint and a final peer-reviewed publication in such a way as to achieve a balance between the rapidity of the first with the authority and stability of the second. Such considerations are more than useful in defining an archiving policy for the IUCr. The meeting as a whole provided a wonderful introduction and status report to electronic archiving in scientific publication and moreover the presentation of the AIP was used by the Chair of the IUCr's CEP to produce the first draft of a proposed IUCr policy on archiving.

13.2.1. AGM 2000. The annual meeting was held 19–22 May in Columbus, Ohio, USA, hosted by CAS (Chemical Abstracts Service). The IUCr's Representative was accompanied to this meeting by the IUCr's Managing Editor and the IUCr's Research and Development Officer. The three also paid a working visit to CAS after the ICSTI meeting. The main discussion session entitled Economic Impacts of Electronic Publishing on 19 May was addressed by: R. J. Massie, CAS Director; M. Blume, AIP Editor-in-Chief; R. D. Bovenschulte, ACS Director; E. Pentz, CrossRef Executive Director; T. Ingoldsby, AIP; J. Jordan, OCLC President; M. Wallin, KTHB; G. Giroud, EPO; T. Sanville, Ohiolink Executive Director. Owing to the extremely poor weather conditions around Detroit on 18 May, this fascinating programme was marred for the IUCr's Representative by his absence at the morning session and advanced fatigue in the afternoon. Some of ICSTI's projects are of particular relevance to the IUCr. One should mention the IUPAC–CODATA–ICSTI project on the Standardization of Physicochemical Property Electronic Datafiles (IUCODIX) which seeks to bring to the world of physical chemistry the advantages that CIF has brought to crystallography. An INGENTA/ICSTI study will make an update to the 1996 ICSTI comparative study of access to journals through subscriptions and document delivery. It will investigate the effect on journal subscriptions of individual article sales and look to other aspects of user behaviour in an electronic environment. The IUCr Representative and R&D Officer, amongst others, participated in the review of the OAIS (Open Archive Information System) reference model. This involved reading the voluminous OAIS report and providing comments concerning its relevance and usefulness to the IUCr. These were collated and presented by G. Hodge at the meeting and transmitted to the OAIS Committee. OAIS is now well on its way to becoming an ISO standard. It is our opinion that this model is highly relevant to the IUCr's electronic publication and archiving activity. Indeed, the Chair of the CEP benefited directly from this experience by producing a second draft of the proposed IUCr archive policy using the vocabulary and terms of OAIS. This increases the clarity of the document immensely. At their annual meetings, ICSTI invites short presentations from member organizations. The IUPAC Representative presented their recent developments including a commitment to CML (chemical markup language) and IChIP, the IUPAC chemical identifier project. IUPAC has taken the bold step of abolishing all Commissions and now organizes its activities entirely around projects. The undersigned presented the IUCr, and especially its publishing activities, using the excellent slide presentation prepared in Chester. JST presented JSTAGE, their Electronic Journal Publication and Dissemination Center, which proved to be a system with several novel and interesting features.

13.2.2. Publications. ICSTI maintains both a public web site at http://www.icsti.org/ where the newsletter *ICSTI Forum*, published four times in 2000, and other general information are made available. A private section is available only to members, the IUCr Representative sharing this opportunity with the IUCr's CEP. Of particular interest to the IUCr, *Forum* No. 33 of March 2000 presented some very interesting articles resulting from the ICSTI/ICSU digital archiving workshop held in Paris in January 2000. *Forum* No. 34 presents information on digital libraries in Canada, No. 35 focuses on CAS (Chemical Abstracts Service) and No. 36 is concerned with distance learning projects at DTIC and a presentation of the National Library of Medicine in the USA.

In 2001 the ICSTI winter committee meetings will be held in January in Paris, France, and the annual meeting will take place in the premises of the European Patent Office in Münich, Germany, 3–7 May. For the record, the 2002 annual meeting will take place at KTHB, Stockholm, Sweden, and CISTI will host the 2003 meeting in Ottawa, Canada.

IUCr membership of ICSTI continues to fulfil its expectations by providing a current source of documentation and personal contacts in the field of scientific and technical information (electronic publishing).

H. D. Flack, IUCr Representative

13.3. International Council for Science (ICSU)

Since the ICSU General Assembly in Cairo, Egypt, in September 1999, ICSU has had a new Executive Board and a new Executive Director, L. Kohler. This has signalled a period of review of all ICSU activities. Of particular note is that the ICSU Executive feels that it has too long taken for granted its links to its foundation, *i.e.* its Scientific Unions and its National Scientific Members. We can expect greater interaction between ICSU and the IUCr over the next few years. As part of this a meeting of all the Scientific Union Presidents is planned for February 2001.

ICSU has a number of important current initiatives, some of them coordinated by Scientific Unions and others coordinated by some of the ICSU Committees. As one example, the ICSU Steering Committee on Genetics and Biotechnology has been reconstituted as an *ad hoc* Advisory Committee on Genetic Experimentation and Biotechnology (ACOGEB) and is now assessing the available scientific data on genetically modified plants. Another organization established by ICSU, the International Network for the Availability of Scientific Publications (INASP), seeks to address the concern that in developing countries the gap between those who have access to information and those who do not may actually be widening with advances in technology. Other issues of major interest to the IUCr concern policies on free and unrestricted access to data and information, at a time when intellectual property rules are changing. This falls within the province of CODATA.

E. N. Baker, IUCr Representative

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

The IUCr Representative received no communications in 2000.

K. El-Sayed, IUCr Representative

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

13.5.1. Overview. CODATA (http://www.codata.org) is an interdisciplinary Scientific Committee of the International Council for Science (ICSU), which focuses on the quality, reliability, management and accessibility of data in all fields of science and technology. Currently 23 countries are members, and 14 International Scientific Unions have assigned liaison delegates. Its general objectives are: improvement of the quality and accessibility of data, and methods of data acquisition, management, analysis and evaluation; facilitation of international cooperation; promotion of an increased awareness within the scientific and technical community of the importance of these activities; and consideration of data access and intellectual property issues.

It addresses these objectives through four primary activities:

(1) Sponsorship of a biennial international interdisciplinary conference. During 2000, one such was held at Lake Maggiore, Italy, 15–19 October. A report on this meeting is given below.

(2) Specialist meetings of scientific data experts, which address issues specific to one discipline or topic. Among such meetings in 2000 were: Workshop on Building Information on Molten Salts, Marseilles/Corsica, 18–20 September; CODATA Korea 2000 Symposium on Biodiversity Information Network, 1 December; Workshop on the European Directive on the Legal Protection of Databases, Baveno, Italy, 14 October; and a noteworthy regional conference, the First International CODATA Africa Workshop, Dakar, Senegal, 19–21 July.

(3) Publications on data handling, data compilation, surveys of data activities and conference proceedings.

(4) Sponsorship of Task Groups, Working Groups, Commissions and other groups addressing specific data issues. The Task Groups approved for the period 2000–2002 are as follows:

Fundamental Constants;

Data Information and Visualization;

IUPAC–CODATA Task Group on Standardization of Physicochemical Property Electronic Datafiles (IUCOSPED), in association with ICSTI;

Comparative Mathematical Methodologies for Data Handling and Knowledge Interpretation;

Survey of Data Sources in Asian–Oceanic Countries;

Information System on Natural Gas Hydrates;

Reliable Scientific Data Sources in Africa;

Global Species Databases Task Group.

13.5.2. CODATA 2000. The CODATA 2000 Conference, subtitled Data and Information for the Coming Knowledge Millennium, brought together about 250 scientists. Despite adverse weather and local flooding which forced a change of venue during the meeting, over 240 oral presentations and 20 posters in four parallel sessions were presented, with a dozen plenary lectures.

Among the highlights of the plenary sessions a few should be noted. An opening address by D. Snowden of IBM (UK) criticized the linear data → information → knowledge → wisdom paradigm, and emphasized the complexity and subtlety of the educational process. J. Enderby of the Royal Society, UK, discussed the continuing dangers to global well being of pollution, overpopulation and depletion of natural resources. The recently discovered sea-floor layer of solid gas hydrates (frozen methane–water clathrates) provides a potential alternative to fossil fuels. The properties and potential of this new material were discussed by R. Hesse of Agder College, Norway. O. Favorsky (Academy of Sciences, Russia) detailed recent research on the pollution impact of high-altitude aircraft. Techniques for analysing and understanding large volumes of data were illustrated by U. Fayyad's account of astronomical objects identified from a digitized sky survey using novel database science techniques.

The body of the conference was structured along a number of tracks and themes, covering such topics as: collection and analysis of geological and geophysical data for prospecting and natural disasters information; collection and dissemination of taxonomic and biological data to comprehend and preserve biodiversity and species distribution; genomics and the identification of biological structure, function and evolution through genetic and biomolecular studies; access to chemical and crystal structures, and to the physical structure of non-organic materials; interpretation of astronomical data and increasing the power of astronomical observation through operations within a virtual observatory; access to and validation of tables and datasets of fundamental physical properties.

Despite this great range of applications, a few common problems and interests were discernible as common to all or most disciplines.

First is interoperability. Even within well defined areas of science, experts find it difficult to communicate information and data to each other. At one level, work is needed to link different data collections, and projects such as the Global Change Master Directory (S. M. Leicester, NASA, USA) focus on the need for metadata standards to permit the location of items of mutual relevance. But there is also a need to detail the fine structure of data to allow access to specific information within a dataset. Projects such as the IUPAC–CODATA Task Group on Standardization of Physicochemical Property Electronic Datafiles (IUCOSPED: H. Kehiaian, Paris, France) and the proposed NIST repository of data on units of measurement (R. Dragoset, NIST, USA) are beginning to address this. A contribution by P. Murray-Rust (Nottingham, UK) on mark-up languages described the technical functions of document mark-up, but also emphasized the need for community cooperation in using such standards, and in populating the mark-up dictionaries needed by each discipline. Many other oral presentations described standardization efforts that used XML as a *lingua franca* of machine-driven data exchange, but there was comparatively little evidence of awareness of the need to codify the sets of concepts ('ontologies') common to practitioners within disciplines. In the field of crystallography, the CIF dictionaries have demonstrated what can be achieved.

Second is data access. In part this is technical and depends upon the development of common standards for global metadata or for the internal structure of data, as mentioned above. There is also the issue of interoperability between database management systems and other software tools. But data access also touches upon the interpretation and visualization of large or complex data sets; on the cost of access to data of interest, and the motives and practices of people who manage databases as commercial resources; on issues of privacy and confidentiality; and on the increasingly relevant and complex issues of intellectual property rights (IPR). A one-day workshop in association with the main conference addressed some relevant IPR issues.

Also related to data access is the prospect of access in perpetuity, *i.e.* the need to archive digital data in a secure and properly structured manner. A presentation by L. Reich (NASA, USA) described the Open Archival Information System (OAIS) reference model adopted by the space science data community and developed in collaboration with a number of other interested parties, including ICSTI. While the reference model provides a context and vocabulary for discussing archiving, rather than a specific implementation, it serves to raise awareness of the problem, and codifies ideas that are common across disciplines.

Another recurrent theme through the conference was the benefits of the world-wide web as a medium for accessing and visualizing data. The IUCr CODATA Representative gave a presentation in the theme session on novel web applications, describing the Union's integrated online publishing, news and communications activities. It is clear that the web is an enabling technology and a powerful method for coordinating and linking activities within and between disciplines.

13.5.3. General Assembly. The 22nd General Assembly of CODATA took place immediately following the CODATA 2000 conference at Lake Maggiore. Beyond routine administrative affairs, the main function of the General Assembly is the appointment or reconfirmation of Task Groups or Working Groups. The Task Groups approved for the period 2000–2002 are listed above.

An *ad hoc* Working Group on Data Archiving was formed to address the issues and involve CODATA at an appropriate level. This group includes the IUCr CODATA Representative whose interest in this area stems from an opportunity to review the OAIS reference model mentioned above in collaboration with the IUCr ICSTI Representative, H. D. Flack.

The General Assembly also reviewed the CODATA publications programme. Proposals were in hand to launch a CODATA journal of scholarly papers on data activities. It was anticipated that the journal would be purely electronic, and would handle about 40 papers per year. The CODATA *Newsletter* would continue as a vehicle for informing the membership, but emphasis would shift towards providing it in electronic form, with at least one hard-copy issue for distribution each year.

13.5.4. Conclusions. CODATA remains a very active body and serves the scientific community well as a cross-disciplinary forum. While the interests of the IUCr in crystallographic databases are now overseen by the Committee on Crystallographic Databases, it is valuable to meet representatives of other communities and interests. Database and electronic publishing activities are also increasingly convergent, and there is a growing synergy between CODATA and ICSTI. At this time of rapid developments in both fields, it is helpful that the IUCr Representatives on both CODATA and ICSTI are able to collaborate under the umbrella of the Unions's Committee for Electronic Publishing, Dissemination and Storage of Information.

B. McMahon, IUCr Representative

13.6. ICSU Committee on Science and Technology in Developing Countries – International Biosciences Network (COSTED–IBN)

COSTED–IBN is concerned with strengthening science in small states and developing countries. Its focus has largely been on capacity building. Recently COSTED–IBN has begun a new study, sponsored by UNESCO and centred on six Asian countries, to analyse the relationships between development and the mobility of science and technology professionals. The intention is to find ways to reverse the 'brain drain' from such countries. At the ICSU Executive Board meeting, there was a feeling that the activities of COSTED–IBN should be better coordinated with those of ICSU Scientific Unions and other bodies (for example the Union Teaching Commissions). A major review of COSTED–IBN is planned.

E. N. Baker, IUCr Representative

13.7. ICSU Committee on Space Research (COSPAR)

A meeting of the COSPAR Bureau was held in Paris, France, in March 2000. In addition to a number of items strictly related to COSPAR life (budgets, categories of membership, administrative questions), the discussion included the list of meetings sponsored/organized by COSPAR during 2000:

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

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

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

First International Solar Cycle Symposium, Tatranska Lomnica, Slovakia, July 2000;

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

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

First S-RAMP Conference, Sapporo, Japan, October 2000;

MARISY, Rabat, Morocco, November 2000;

Second SPARC General Assembly, Mar del Plata, Argentina, November 2000.

The 33rd COSPAR Scientific Assembly and Associated Events took place in Warsaw, Poland, 16–23 July 2000. This meeting included a plenary session entitled Space 2000 and another main session on Back to the Moon. During the meeting some distinguished scientists were presented with the Space Science Award (R. Bonnet, ESA), the International Cooperation Medal (J. H. Carver, Australia) and the William Nordberg Medal (K. Ljiri, Japan). It was decided that the 34th COSPAR Assembly will jointly be held with the 2nd World Space Congress in Houston, Texas, USA, in October 2002.

A survey of the most important space missions and relevant results may be found in *COSPAR Bulletin* Nos. 147, 148 and 149, published by Elsevier in April, August and December 2000, respectively. Other important information is available at the COSPAR web site: http://cospar.itodys.jussieu.fr.

R. Fornari, IUCr Representative

14. Finances

The audited accounts of the year 2000 are given at the end of this Report. For comparison, the figures for 1999 are provided in italics. The accounts are presented in CHF.

The UNESCO rates of exchange, as issued by the ICSU Secretariat, have been used in the preparation of these accounts. As a

consequence of the many fluctuations in exchange rates during the year, the following procedure has been adopted for the accounts. Assets and liabilities in currencies other than CHF at 31 December 2000 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions.

Investments are noted in the balance sheet at their market value at 31 December 2000. The Union's investments are managed by F&C based in London, UK, and Merrill Lynch in New York, USA. During 2000, all the major markets experienced a sharp drop in value, especially those related to growth stocks, *e.g.* new technology. This negative development of the stock market has also affected the investments of the Union. The balance sheet shows that, even including the gain of CHF 428,084 resulting from fluctuations in rates of exchange, the assets of the Union decreased during the year from CHF 7,660,919 to CHF 6,763,941.

The income and expenditure account shows a deficit of income over expenditure of CHF 461,941, slightly higher than the deficit in 1999 of CHF 319,530. These annual deficits can be related to a number of factors: the expenses in terms of staff and hardware associated with making the journals available online, digitization of back issues of all the journals and the production of revised editions and new volumes of *International Tables for Crystallography*. The economical benefit from these major efforts should emerge in the coming years.

A transfer of CHF 250,000 was made to the *International Tables* Fund from the *Acta Crystallographica* Fund. A transfer of CHF 200,000 was made to the Publication and Journals Development Fund from the *Acta Crystallographica* Fund. A transfer of CHF 70,000 was made to the Research and Education Fund from the *Acta Crystallographica* Fund. A transfer of CHF 20,000 was made to the President's Fund from the *Acta Crystallographica* Fund. Transfers of CHF 25,000 and CHF 50,000 were made to the *Newsletter* Fund from the General Fund and the *Acta Crystallographica* Fund, respectively. A transfer of CHF 150 000 was made to the *Journal of Synchrotron Radiation* Fund from the *Acta Crystallographica* Fund.

Beneath the detailed figures of the expenditure and income for each fund account, the balance at 1 January, transfers to and from other funds, the difference between income and expenditure for the year and the fluctuations in rates of exchange during the year are given, showing how the balance at 31 December is obtained. Note that for the General Fund there is an additional entry for 'Movement in market value of investments in the year'.

The General Fund account shows a surplus of CHF 23,868 before the transfers totalling CHF 25,000, as compared with a deficit in 1999 of CHF 11,249 before transfers totalling CHF 50,000. The administrative expenses were CHF 433,818 in 2000 as compared with CHF 380,136 in 1999. Of this amount, CHF 190,173 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 6,276. The cost of the Finance Committee meetings held in 2000 was CHF 18,518, while the Executive Committee meeting cost CHF 18,084. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 7,960. The Union received CHF 12,493 from the UNESCO subvention to ICSU. The subscriptions from Adhering Bodies were CHF 152,316. Interest on bank accounts and investments credited to the General Fund was CHF 235,761

The President's Fund, the Publication and Journals Development Fund, the Research and Education Fund and the Ewald Fund received interest, at a nominal rate of 6% per annum, on the balances in the funds.

The President's Fund therefore received interest of CHF 2,164. Grants totalling CHF 4,063 were paid from the fund.

The *Acta Crystallographica* account for 2000 shows a surplus of CHF 246,067 before the transfer of CHF 740,000 to other fund accounts, as compared with a surplus of CHF 469,453 in 1999 before transfers of CHF 620,000.

The subscription rates were increased for 2000. In 2000, the number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 43 (47) personal subscriptions, was 525 (563) (values for 1999 are given in parentheses). The number of paid subscriptions to *Sections A+B+C*, including 12 (12) personal subscriptions, was 120 (124). The number of paid subscriptions to the separate sections of the journal were: *Section A* 236 (250 for 1999), *Section B* 186 (199), *Section C* 150 (154) and *Section D* 217 (217). The cost of the technical editing office has been divided between the *Acta Crystallographica*, the *Journal of Applied Crystallography*, the *Journal of Synchrotron Radiation* and the *International Tables* accounts in percentages based on the staff time spent on each publication. The technical editing costs for *Acta Crystallographica* were CHF 1,172,552 (for 5,678 published pages) as compared with CHF 812,952 in 1999 (6,472 pages published). The journal's accounts have also been charged with administration expenses as in previous years as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a surplus of CHF 28,885, as compared with a deficit of CHF 47,010 in 1999. In 2000, the number of paid subscriptions, including 100 (105 in 1999) personal subscriptions, was 715 (753 in 1999).

The *Journal of Synchrotron Radiation* account shows a deficit of CHF 85,270 before receiving a transfer of CHF 150 000 from the *Acta Crystallographica* Fund, as compared with a deficit of CHF 165,077 in 1999 before receiving a transfer of CHF 100,000. In 2000, the number of paid subscriptions, including 104 (119 in 1999) personal subscriptions, was 252 (279 in 1999).

The *International Tables* account shows a deficit of CHF 319,096, as compared with a deficit of CHF 259,269 in 1999. The net sales income was CHF 82,608 in 2000 as compared with CHF 132,408 in 1999. The deficits in 1999 and 2000 are a result of significant expenses being incurred in connection with production of revised editions of the four existing volumes and production costs for the five new volumes. These production costs will continue in 2001.

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

The *Newsletter* Fund Account received transfers of CHF 25,000 from the General Fund and CHF 50,000 from the *Acta Crystallographica* Fund in both 1999 and 2000. The cost to the Union of producing the *Newsletter* in 2000 was CHF 53,561 (CHF 86,232 in 1999).

As mentioned earlier, the income for the President's Fund account, the Publications and Journals Development Fund account, the Research and Education Fund account and the Ewald Fund account include interest as well as transfers from other fund accounts. In the Publications and Journals Development Fund account, the computer expenses of CHF 460,269 relate to the technical editing of the journals and software. The programming and development costs are now divided between the General Fund, the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Journal of Synchrotron Radiation* Fund and the *International Tables* Fund. Promotional costs, STAR/CIF costs, Special Issue costs and web input costs are also charged to the Publication and Journals Development account. From 2000, costs associated with the Crystallographic

NeXus Project to provide CD-ROMs (containing crystallographic software and web material) free of charge to developing countries is charged to this Fund. CHF 112,200 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union, and CHF 10,700 for the Visiting Professorship Programme were charged to the Research and Education Fund. Part of the costs of these activities is met by funds received under the ICSU/UNESCO grants programme.

15. Auditor's Report to the International Union of Crystallography

We have audited the financial statements on pages 105 to 116 which have been prepared under the accounting policies set out on page 104.

Respective responsibilities of Executive Committee and Auditors

In accordance with the Statutes and By-laws of the International Union of Crystallography, the Executive Committee is responsible for all the financial affairs of the Union and for appointing an external auditor, on the recommendation of the Treasurer, to audit the financial statements. It is our responsibility to form an independent opinion, based on our audit, on those statements and to report our opinion to you.

Basis of opinion

We conducted our audit in accordance with Auditing Standards issued by the Auditing Practices Board. An audit includes examination, on a test basis, of evidence relevant to the amounts and disclosures in the financial statements. It also includes an assessment of the significant estimates and judgements made in the preparation of the financial statements, and of whether the accounting policies are appropriate to the Union's circumstances, consistently applied and adequately disclosed.

We planned and performed our audit so as to obtain all the information and explanations which we considered necessary in order to provide us with sufficient evidence to give reasonable assurance that the financial statements are free from material misstatement, whether caused by fraud or other irregularity or error. In forming our opinion, we also evaluated the overall adequacy of the presentation of information in the financial statements.

Opinion

In our opinion, the financial statements give a true and fair view of the state of the Union's affairs as at 31 December 2000 and of the result for the year then ended.

Deloitte & Touche
Chartered Accountants and Registered Auditors
6 June 2001

16. Notes to the Accounts

The Income and Expenditure Account, the Balance sheet and the Cash Flow statement for the year ended 31 December 2000 are given in Tables 3, 4 and 5.

16.1. Accounting policies

(*a*) *Accounting convention*

The financial statements are prepared under the historical cost convention, with the exception of investments which are stated at market value, and in accordance with applicable accounting standards. The particular accounting policies adopted are described below.

(*b*) *Rates of exchange*

UNESCO rates of exchange as issued by the ICSU Secretariat are used in the preparation of the financial statements.

Assets and liabilities held in currencies other than Swiss Francs at the balance sheet date are translated into Swiss Francs at the rates operative on that date.

In each of the income and expenditure accounts, transactions in currencies other than Swiss Francs are translated by applying the rates of exchange appropriate to the individual dates of the transactions.

Profits and losses arising on trading transactions from the fluctuations in rates of exchange during the year are divided between the fund accounts with credit balances in direct proportion to those balances at the closing balance sheet date. Profits and losses on investments are allocated to the General Fund. All profits and losses arising from exchange rate fluctuations are taken directly to reserves.

(*c*) *Publication costs*

Publication, editorial and administrative expenses of publications are charged in the appropriate income and expenditure account as and when incurred.

(*d*) *Stocks*

Stocks of *International Tables* are included at cost less provision for slow moving and obsolete items. Stocks of all other publications are not valued for accounts purposes as sales are unpredictable.

(*e*) *Expenditure on premises*

Expenditure on maintenance of leasehold premises is charged against the appropriate income and expenditure accounts in the year in which it is incurred.

(*f*) *Depreciation*

(i) Office equipment is depreciated on the straight line basis at a rate of 20% per annum.

(ii) Office computer equipment is depreciated on a straight basis at a rate of $33\frac{1}{3}$% per annum.

(iii) Leasehold property improvements related to new leases are depreciated over the term of the lease.

(*g*) *Investment income*

Notional dividend income re-invested in accumulation investment funds is treated as income when declared and added to the accumulated cost of investments. Other dividends are recognized on an accruals basis.

(*h*) *Investments*

Investments are stated at market value. Changes in market value are taken directly to reserve movements in the General Fund.

(*i*) *Lease costs*

Operating lease costs are charged to the income and expenditure account on a straight line basis. Where reduced rents are payable on property in the earlier years of the lease, the total cost for the period to the first rent review date is spread on a straight line basis, and the appropriate creditor balance is maintained.

16.2. Rates of exchange

The assets of the Union are recorded in the financial statements in Swiss Francs but are held in currencies which are considered to be appropriate to the Union's requirements. Transactions in currencies other than Swiss Francs are converted into Swiss Francs at the rate of exchange ruling on the date of the transaction.

The rates of exchange operative at the balance sheet date compared with the Swiss Franc were as follows:

	2000	*1999*
Netherland Guilders (NLG)	1.4489	*1.3774*
Danish Crowns (DKK)	4.9148	*4.6478*
Pounds Sterling (GBP)	0.3977	*0.3931*
US Dollars (USD)	0.5682	*0.6289*

The net assets of the Union at 1 January 2000 (CHF 7,660,919) would have had the value of USD 4,817,952 or GBP 3,011,507 if expressed in those currencies.

At 31 December 2000, the net assets (CHF 6,763,941) would have had the value of USD 3,843,271 or GBP 2,690,019, respectively, being a decrease of USD 972,385 or a decrease of GBP 319,881 from the previous year.

16.3. Taxation

As an association incorporated in Switzerland, the Union 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 United Kingdom under present circumstances will not be subject to United Kingdom tax.

Other investment income received from countries with which Switzerland has a Double Taxation Agreement is exempt from tax.

16.4. Tangible fixed assets

Table 6 lists the tangible fixed assets.

16.5. Investments

Table 7 lists the investments of the IUCr, their disposals and additions and the holding at 31 December 2000.

16.6. Creditors

Table 8 lists the creditors, with the amounts falling due within one year for 1999 and 2000.

16.7. Investment income

Table 9 lists the income from investments for 1999 and 2000.

16.8. Bank interest

Table 10 lists the bank interest for 1999 and 2000.

16.9. Loss/profit on disposal/redemption of investments

Table 11 lists the loss or profit on disposal/redemption of investments for 1999 and 2000.

Table 3
Income and Expenditure Account for the year ended 31 December 2000.

	Note	2000		1999	
			Swiss Francs		
Income					
Membership subscriptions			152,316		*144,930*
Sales					
Journals		3,327,321		*3,260,949*	
Books		129,538		*278,166*	
Back numbers and single issues		35,125	3,491,984	*38,263*	*3,577,378*
Investment income					
Income from investments	16.7	294,981		*305,756*	
Bank interest	16.8	27,817		*28,772*	
(Loss)/Profit on sale of investments	16.9	(7,197)	315,601	*22,967*	*357,495*
Other income					
Grants		12,492		*10,619*	
Royalties and copyright fees		6,685		*5,267*	
Advertising income		189,468		*244,640*	
Donations		14,806	223,451	–	*260,526*
Total Income			4,183,352		*4,340,329*
Expenditure					
Journals					
Publication costs		1,360,238		*1,595,918*	
Editorial expenses		160,047		*165,648*	
Technical editing		1,278,679	2,798,964	*1,022,539*	*2,784,105*
Books					
Publication costs		94,176		*93,467*	
Editorial expenses		55,704		*70,949*	
Technical editing		233,480	383,360	*230,829*	*395,245*
Newsletter					
Publication costs		167,759		*138,265*	
Editorial expenses		81,782	249,541	*87,442*	*225,707*
President's Fund Grants and Young Scientists' support			116,263		*103,699*
General Assembly costs			1,315		*47,963*
Ewald Prize			–		*45,902*
Committee meetings and expenses			36,601		*129,261*
Publications and journals development					
General		413,212		*358,842*	
Electronic Publishing Committee/Section Editors meeting expenses		2,765		*1,183*	
STAR/CIF		1,319		*7,170*	
Promotions representative		137,922	555,218	*107,416*	*474,611*
Subscriptions paid			9,707		*10,099*
Visiting Professorship Programme			10,700		*20,226*
Administration expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		12,378		*11,521*	
Secretarial assistance		–		*258*	
Audit and accountancy charges		33,885		*40,801*	
Legal and professional fees		43,836		*20,156*	
Travelling expenses		11,583		*12,634*	
Bank charges		2,451	104,133	*2,493*	*87,863*
Executive Secretary's office:					
Salaries and expenses		308,506		*270,941*	
Travel expenses of IUCr representatives on other bodies		6,276		*4,231*	
Commission expenses		–		*12,075*	
Sponsorship of meetings		4,426		(*36,692*)	
President's secretary		10,000		*7,910*	
IUCr/FIZ agreement		(7,960)		(*8,759*)	
Bad debts – subscriptions		4,000	325,248	*5,000*	*254,706*
Depreciation			54,243		*80,472*
Total Expenditure			4,645,293		*4,659,859*

Table 3 (continued)

	Note	2000	Swiss Francs	*1999*	
Deficit of income over expenditure			(461,941)		(*319,530*)
Movement in market value of investments in year	16.5		(863,121)		*182,734*
			(1,325,062)		(*136,796*)
Fluctuation in rates of exchange					
Trading activities	16.2	45,686		*81,096*	
Investment activities	16.2	382,398	428,084	*800,552*	*881,648*
Total recognized gains and losses relating to the year			(896,978)		*744,852*
Opening fund accounts at 1 January			7,660,919		*6,916,067*
Closing fund accounts at 31 December			6,763,941		*7,660,919*

All the income and expenditure related to continuing activities. Historic cost results would only differ from above by the profit on sale of investments – see Note 16.9. Separate Statements of Total Recognized Gains and Losses and Reconciliation of Movements in Fund Account are not given, as the information is incorporated in the above.

Table 4
Balance sheet as at 31 December 2000.

	Note	2000	Swiss Francs	*1999*	
Fixed Assets					
Tangible fixed assets	16.4		78,168		*93,936*
Current Assets					
Stock			19,219		*35,062*
Cash at bank					
Current accounts		14,388		*24,305*	
Deposit and savings accounts		147,934		*130,521*	
Cash with Union officials		31,704	194,026	*30,070*	*184,896*
Investments at market value	16.5		6,349,963		*7,215,929*
Debtors, accrued income and payments in advance			317,407		*324,046*
Subscriptions from Adhering Bodies			10,698		*6,607*
Total Current Assets			6,891,313		*7,766,540*
Creditors: amounts falling due within one year	16.6		(205,540)		(*199,557*)
Net Current Assets			6,685,773		*7,566,983*
Total Funds			6,763,941		*7,660,919*

16.10. Exchange rate fluctuations

Table 12 lists exchange rate fluctuations attributable to operating activities for 1999 and 2000.

16.11. Changes in cash during the year

Table 13 is an analysis of cash changes during 1999 and 2000.

16.12. Balances of cash as shown in the balance sheet

Table 14 is an analysis of cash balances as shown in the balance sheet.

16.13. Operating lease commitments

At 31 December 2000, the Union was committed to making the payments listed in Table 15 during the next year in respect of operating leases.

16.14. Sponsorship commitments

At 31 December 2000, the Union had authorized, but not contracted for, sponsorship grants of CHF 72,160 (1999: CHF 73,935).

Table 5
Cash Flow statement for the year ended 31 December 2000.

	Note	2000	Swiss Francs *1999*
Net cash outflow from operating activities (see below)		(701,763)	(*616,508*)
Returns on investments			
Interest received		27,817	*28,772*
Investment income (net of notional dividends)		106,374	*88,495*
Net cash inflow from returns on investments		134,191	*117,267*
Investing activities			
Purchase of fixed assets		(38,475)	(*43,995*)
Purchase of investments	16.5	(1,902,055)	(*1,540,118*)
Disposal of investments	16.9	2,468,708	*1,711,527*
Net cash inflow from investing activities		528,178	*127,414*
Increase/(decrease) in cash	16.11	(39,394)	(*371,827*)
Reconciliation of Deficit of Income over Expenditure to Net Cash Outflow from Operating Activities			
Deficit of income over expenditure		(461,941)	(*319,530*)
Exchange rate fluctuations attributable to operating activities	16.10	(2,838)	(*3,600*)
Interest received	16.8	(27,817)	(*28,772*)
Investment income	16.7	(294,981)	(*305,756*)
Loss/(profit) on disposal of investments	16.9	7,197	(*22,967*)
Depreciation charges		52,243	*80,472*
(Increase)/decrease in stock		15,843	(*9,001*)
Decrease in debtors		2,548	*22,837*
Increase/(decrease) in creditors		5,983	(*30,191*)
Net cash outflow from operating activities (see above)		(701,763)	(*616,508*)

Table 6
Tangible fixed assets.

	Leasehold property improvements CHF	Office equipment CHF	Computer equipment CHF	Total CHF
Cost				
As at 1 January 2000	102,987	67,613	175,427	346,027
Additions	–	5,579	32,896	38,475
As at 31 December 2000	102,987	73,192	208,323	384,502
Accumulated depreciation				
As at 1 January 2000	45,534	55,119	153,438	252,091
Charge for the year	10,299	10,252	33,692	54,243
As at 31 December 2000	53,833	65,371	187,130	306,334
Net book value 31 December 2000	49,154	7,821	21,193	78,168
31 December 1999	59,453	12,494	21,989	93,936

16.15. Contingencies

During the year, the Union continued to participate in an agreement to guarantee the sales of an organization selling a crystallographic database. The Union guarantees to underwrite sales up to CHF 190,000. For sales over this level, the Union receives a percentage of the income.

Tables 16–27 give the accounts for the year ended 31 December 2000 for the various fund accounts.

Table 7
Investments.

	Swiss Francs								
	Holding at market value 1 January 2000	Additions during the year	Notional dividends	Disposals/ redemptions during the year	Fluctuations in rates of exchange	Increase/ (decrease) in market value	Holding at market value 31 December 2000	Holding at revalued cost 31 December 2000	Holding at revalued cost 31 December 1999
Held by Merrill Lynch									
GNM P169332-2016 (USD) 5,643 Units	13,386	–	–	(4,108)	1,199	–	10,477	9,592	12,254
Haussmann Holdings (USD) 82 Units	279,579	–	–	(92,052)	23,157	(123)	210,561	70,928	91,733
Global Allocation Portfolio Class A (USD) 2,700 Units	86,075	–	–	–	9,203	5,750	101,028	50,134	45,291
Repsol International Capital Limited	65,588	–	–	(71,775)	6,187	–	–	–	81,122
Santander Finance Limited	92,300	–	–	(101,007)	8,707	–	–	–	115,121
MLBS SP PF EU EQ (US) B 5,825 Units	193,940	–	–	–	20,736	(20,196)	194,480	176,984	159,889
Sector SPDR Energy 2075 Units	89,390	–	–	–	9,557	22,254	121,201	85,091	76,872
Banco Bilbao 1,500 Units	60,221	–	–	–	6,439	495	67,155	73,545	66,441
Seligman Japan FD CL B 4,437 Units	119,320	–	–	–	12,757	(39,462)	92,615	113,256	102,317
Mercury Selected Trust USD Global Bond Fund B 6,790 Units	157,191	–	–	–	16,806	12,906	186,903	176,304	159,889
ML Internet Strategies Portfolio Fund CLA 5,625 Units	132,546	–	–	–	14,171	(73,656)	73,061	99,000	89,438
Janus Global Life Sciences Fund 4,700 Units	–	81,047	–	–	2,370	13,117	96,534	83,417	–
Janus US Venture Fund 4,800 Units	–	85,069	–	–	2,487	(23,436)	64,120	87,556	–
Seligman US Comm + Info Fund 1,750 Units	–	84,872	–	–	2,482	(35,210)	52,144	87,353	–
Seligman Henderson Global Tech Fund 1,500 Units	–	84,346	–	–	2,466	(29,920)	56,892	86,812	–
B2B Internet 100 Units	–	6,794	–	–	199	(3,858)	3,135	6,993	–
Broadband 100 Units	–	13,983	–	–	409	(6,373)	8,019	14,392	–
Cisco Systems Inc. 500 Units	–	55,182	–	–	1,614	(23,136)	33,660	56,796	–
Internet Infrastructure 100 Units	–	9,347	–	–	273	(5,727)	3,893	9,621	–
Internet Archecture 100 Units	–	14,573	–	–	426	(4,868)	10,131	14,999	–
Pharmaceutical 100 Units	–	16,634	–	–	486	2,988	20,108	17,121	–
Telecom 100 Units	–	13,462	–	–	394	(4,463)	9,393	13,856	–
Global SR (DE) 600 Units	–	98,915	–	–	7,328	(58,365)	47,788	106,153	–
Consults Portfolios									
No. 17P-07M16	185,366	453,957	–	(327,283)	27,289	(71,488)	267,841	286,893	137,995
No. 17P-07M17	206,530	214,477	–	(195,674)	23,132	(56,069)	189,396	188,582	152,432
No. 17P-07P52	150,403	305,094	–	300,787)	16,607	(25,228)	146,089	163,956	143,753
No. 17P-07P53	169,965	97,782	–	(102,380)	18,035	(10,776)	172,626	166,395	154,601
Held by Foreign & Colonial									
Reserve Asset Fund Class D (USD)	759,614	–	–	(791,426)	31,812	–	–	–	796,506
Reserve Asset Fund Class L (GBP) 25,358 Units	1,930,928	134,500	112,816	–	(34,805)	(294,917)	1,848,522	1,202,980	977,730
Reserve Asset Fund Class X (GBP) 2,566 Units	370,498	–	7,531	(255,771)	3,902	(625)	125,535	132,011	388,775
Reserve Asset Fund Class M (USD) 5,144 Units	466,414	–	29,102	–	49,918	(78,231)	467,203	157,322	115,790
Reserve Asset Fund Class E (GBP) 11,556 Units	630,156	132,021	39,158	–	(14,942)	15,185	801,578	772,546	616,124
	6,159,410	1,902,055	188,607	(2,242,263)	270,711	(796,432)	5,482,088	4,510,588	4,483,458
Treasury Stock									
7.75% UK Treasury Stock 300,000 Units	1,056,519	–	–	(233,642)	1111,687	(66,689)	867,875	797,652	1,010,571
	7,215,929	1,902,055	188,607	(2,475,905)	382,398	(863,121)	6,349,963	5,308,240	5,494,029

Table 8
Creditors: amounts falling due within one year.

	Swiss Francs 2000	*1999*
Accruals	140,882	*130,710*
Payroll creditor including tax and social security	59,638	*52,565*
Lease creditor relating to property	5,020	*16,282*
	205,540	*199,557*

Table 9
Investment income.

	Swiss Francs 2000	*1999*
GNM P169332 - 2016	1,004	*1,247*
Haussmann Holdings	284	*371*
Foreign and Colonial – Reserve Asset Fund Class D	–	*36,703*
Foreign and Colonial – Reserve Asset Fund Class L	112,816	*104,863*
Foreign and Colonial – Reserve Asset Fund Class X	7,531	*20,717*
Foreign and Colonial – Reserve Asset Fund Class M	29,102	*21,592*
Foreign and Colonial – Reserve Asset Fund Class E	39,157	*23,454*
UK Treasury 7.75% 22.9.2006	74,836	*68,770*
Repsol International Capital Ltd	4,712	*5,662*
Santander Finance Ltd	6,938	*8,336*
Banco Bilbao	4,625	*5,557*
ML Debt Strategy	–	*615*
Sector SPDR Strategy	1,384	*1,156*
Pharmaceutical	181	–
Telecom	75	–
Internet Archecture	137	–
B2B Internet	28	–
Broadband	11	–
Internet Infrastructure	74	–
Consults Portfolios		
No. 17P-07M16	2,282	*1,356*
No. 17P-07M17	4,227	*1,553*
No. 17P-07P52	4,373	*3,026*
No. 17P-07P53	2,452	*778*
Reversal of opening US tax debtor	(1,248)	–
	294,981	*305,756*
Allocated to:		
President's Fund	2,164	*2,244*
Publication and Journals Development Fund	11,916	*13,686*
Research and Education Fund	47,366	*47,069*
Ewald Fund	25,591	*22,442*
Balance left in General Fund	207,944	*220,315*
	294,981	*305,756*

Table 10
Bank interest.

	Swiss Francs 2000		*1999*	
National Westminster Bank Plc				
Manchester Business Reserve Account	7,880		*5,254*	
Manchester Capital Reserve Account	10	7,890	*1,408*	*6,662*
Merrill Lynch CMA Account		4,016		*6,686*
Foreign & Colonial				
Cash balance		435		*530*
Interest from Munksgaard		15,476		*14,894*
Allocated to General Fund		27,817		*28,772*

Table 11
Profit/(loss) on disposal/redemption of investments.

	Swiss Francs 2000	*1999*
Proceeds	2,468,708	*1,711,527*
Book value	2,475,905	*1,688,560*
(Loss)/Profit allocated to General Fund	(7,197)	*22,967*

Book value represents market value at 1 January 2000. The loss on disposal based on historic cost was CHF 2,125 (1999: CHF 108,605). Therefore historic cost results would be as follows:

	Swiss Francs 2000	*1999*
Deficit of income over expenditure	(456,869)	(*233,892*)

Table 12
Exchange rate fluctuations attributable to operating activities.

	Swiss Francs 2000	*1999*
Total fluctuations in exchange rates dealt with in fund accounts	428,084	*881,648*
Adjustments for exchange differences attributable to:		
Investments (Note 16.5)	(382,398)	*800,552*
Cash and bank balances	(48,524)	(*84,696*)
	(2,838)	(*3,600*)

Table 13
Analysis of changes in cash during the year.

	Swiss Francs			
	2000		*1999*	
Balance at 1 January 2000		184,896		*472,027*
Net cash (outflow)/inflow	(39,394)		(*371,827*)	
Fluctuations in rates of exchange on cash and bank balances	48,524	9,130	(*84,696*)	(*287,131*)
Balance at 31 December 2000		194,026		*184,896*

Table 14
Analysis of cash balances as shown in the Balance sheet.

	Swiss Francs			
	2000	*1999*	Change 2000	*Change 1999*
Cash at bank and in hand	194,026	*184,896*	9,130	(*287,131*)

Table 15
Operating lease commitments.

	Swiss Francs			
	Land and Buildings 2000	Other 2000	*Land and Buildings 1999*	*Other 1999*
Leases which expire:				
within one year	–	41,164	–	*41,722*
within two to five years	–	3,464	–	*38,946*
after five years	94,125	–	*95,400*	–
	94,125	44,628	*95,400*	*80,668*

Table 16
Fund Accounts as at 31 December 1999.

	Swiss Francs						
	As at 1 January 2000	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Gain on market value of investments	Fluctuations in exchange rates (Note 16.2)		Balance at 31 December 2000
					Trading	Investments	
Fund Accounts							
General Fund	4,019,849	(25,000)	23,868	(863,121)	22,753	382,398	3,560,747
President's Fund	40,123	20,000	(1,899)	–	420	–	58,644
Acta Crystallographica	1,449,844	(740,000)	246,067	–	6,893	–	962,804
Journal of Applied Crystallography	106,279	–	28,885	–	975	–	136,139
International Tables	137,628	250,000	(319,096)	–	494	–	69,026
Book Fund	33,607	–	7,564	–	297	–	41,468
Publications and Journals Development Fund	447,064	200,000	(236,556)	–	2,960	–	413,468
Research and Education Fund	912,341	70,000	(75,534)	–	6,539	–	913,346
Ewald Fund	426,512	–	25,591	–	3,260	–	455,363
Newsletter Fund	133,905	75,000	(75,561)	–	962	–	134,306
Journal of Synchrotron Radiation	(46,233)	150,000	(85,270)	–	133	–	18,630
	7,660,919	–	(461,941)	(863,121)	45,686	382,398	6,763,941

Table 17
General Fund Account for the year ended 31 December 2000.

	Note	2000		*1999*	
		Swiss Francs			
Income					
Grant received from UNESCO subvention to ICSU			12,493		*10,544*
Subscriptions from Adhering Bodies			152,316		*144,930*
Income from investments	16.7		207,944		*220,315*
Interest on bank accounts	16.8		27,817		*28,772*
Profit/(loss) on disposal/redemption of investments	16.9		(7,197)		*22,967*
Amounts charged to the following journals and publications:					
Acta Crystallographica		139,793		*121,491*	
Journal of Applied Crystallography		38,831		*21,635*	
Journal of Synchrotron Radiation		11,549	190,173	*23,300*	*166,426*
Total Income			583,546		*593,954*
Expenditure					
Subscriptions to ICSU and ICSU bodies			9,707		*10,098*
Administrative expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		12,378		*11,521*	
Secretarial assistance		–		*258*	
Audit and accountancy charges		33,885		*40,801*	
Legal and professional fees		43,836		*20,156*	
Travelling expenses		11,583		*12,634*	
Bank charges		2,451		*2,493*	
Executive Secretary's office:					
Salaries and expenses		308,506		*270,941*	
Depreciation of office equipment		10,880		*11,033*	
Depreciation of freehold property		10,299	433,818	*10,299*	*380,136*
Eighteenth General Assembly and Congress expenses		1,315		*47,963*	
Meeting of the Executive Committee		18,084		*103,729*	
Finance Committee expenses		18,518		*25,532*	
Travel expenses of IUCr Representatives on other bodies		6,276		*4,231*	
Commission expenses		–		*12,075*	
Sponsorship of meetings		4,426		(*36,692*)	
President's secretary		10,000		*7,910*	
IUCr/FIZ agreement		(7,960)		(*8,759*)	
Bad debts – subscriptions		4,000		*5,000*	
Programming and development costs		61,494	116,153	*53,980*	*214,969*
Total Expenditure			559,678		*605,203*
Surplus/(deficit) of income over expenditure			23,868		(*11,249*)
Reconciliation of movements					
Balance at 1 January			4,019,849		*3,059,757*
Transfers to other funds					
Ewald Fund		–		*25,000*	
Newsletter Fund		25,000	(25,000)	*25,000*	(*50,000*)
Surplus/(deficit)/excess of income over expenditure		23,868		(*11,249*)	
Movement in market value of investments in the year	16.5	(863,121)	(839,253)	*182,734*	*171,485*
Fluctuations in rates of exchange			405,151		*838,607*
Balance at 31 December			3,560,747		*4,019,849*

Table 18
Acta Crystallographica Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000		*1999*	
Income					
Subscriptions to Volume 56 (*1999 Volume 55*)		2,591,111		*2,623,639*	
Sale of back numbers and single copies		26,122		*19,594*	
Distribution costs charged to subscribers		109,046		*100,368*	
Royalties and copyright fees		9,018		*12,133*	
Special Issue income		30,761		*27,976*	
		2,783,710		*2,631,773*	
Less Publisher's commission on sales		183,888	2,582,170	*185,021*	*2,598,689*
Income from advertisements (net)			4,735		*6,820*
Recharge for Special Issue			28,585		*41,340*
Total Income			2,615,490		*2,646,849*
Expenditure					
Publication expenses:					
Printing and binding Volume 56 (*1999 Volume 55*)		523,715		*680,929*	
Distribution costs		119,722		*137,240*	
		643,437		*818,169*	
Net (profit)/loss on reprints		(2,751)		*34,581*	
Index/other incidental costs		–		*9,222*	
Special Issue costs		59,346	700,032	*69,316*	*931,288*
Editorial expenses:					
Editorial honoraria		105,034		*88,084*	
Secretarial assistance		7,822		*13,267*	
Postage, travel and sundries		19,777		*13,934*	
Technical editing:					
Salaries and expenses		1,070,894		*741,423*	
Computer expenses		86,279		*37,149*	
Depreciation of office equipment		15,379	1,305,185	*34,380*	*928,237*
Programming and development costs			224,413		*196,380*
Administration expenses recharged from General Fund			139,793		*121,491*
Total Expenditure			2,369,423		*2,177,396*
Excess of income over expenditure			246,067		*469,453*
Reconciliation of movements					
Balance at 1 January			1,449,844		*1,583,252*
Transfers to other funds					
International Tables		250,000		*200,000*	
Publications and Journals Development Fund		200,000		*200,000*	
Research and Education Fund		70,000		*70,000*	
Newsletter Fund		50,000		*50,000*	
Journal of Synchrotron Radiation		150,000	(740,000)	*100,000*	(*620,000*)
Excess of income over expenditure			246,067		*469,453*
Fluctuations in rates of exchange			6,893		*17,139*
Balance at 31 December			962,804		*1,449,844*

Table 19
Journal of Applied Crystallography Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000		*1999*	
Income					
Subscriptions to Volume 33 (*1999 Volume 32*)		391,819		*363,383*	
Sale of back numbers and single copies		3,556		*12,314*	
Distribution costs charged to subscribers		30,165		*16,052*	
Royalties and copyright fees		2,368		*3,369*	
Advertising income		3,388		*734*	
Special Issue income		56,606		–	
		487,902		*395,852*	
Less Publisher's commission on sales		28,184		*26,299*	
Total Income			459,718		*369,553*
Expenditure					
Publication expenses:					
Printing and binding Volume 33 (*1999 Volume 32*)		114,624		*124,763*	
Distribution costs		30,927		*24,303*	
		145,551		*149,066*	
Net (profit)/loss on reprints		(2,605)	151,661	*2,595*	*170,744*
Editorial expenses:					
Editorial honoraria		9,995		*12,289*	
Secretarial assistance		6,873		*7,116*	
Postage, travel and sundries		950		*2,770*	
Technical editing:					
Salaries and expenses		113,627		*174,211*	
Computer expenses		24,219		*6,616*	
Depreciation of office equipment		4,317	159,981	*6,312*	*209,314*
Programming and development costs			32,059		*33,953*
Administration expenses recharged from General Fund			39,241		*21,635*
Recredit for Special Issue			6,016		–
Total Expenditure			430,833		*416,563*
Excess/(deficit) of income over expenditure			28,885		(*47,010*)
Reconciliation of movements					
Balance at 1 January			106,279		*152,033*
Excess/(deficit) of income over expenditure			28,885		(*47,010*)
Fluctuations in rates of exchange			975		*1,256*
Balance at 31 December			136,139		*106,279*

Table 20
Journal of Synchrotron Radiation Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000		*1999*	
Income					
Subscriptions to Volume 7 (*1999 Volume 6*)		134,396		*134,075*	
Sales of back numbers and single issues		1,442		*5,050*	
Distribution costs charged to subscribers		5,160		*11,299*	
Special Issue income		3,081		*64,993*	
		144,079		*215,417*	
Less Publisher's commission on sales		10,723	133,356	*9,698*	*205,719*
Income from advertisements			7,365		*11,297*
Income from copyright fees			724		*540*
Recharge for Special Issue			17,216		*19,139*
Total Income			158,661		*236,695*
Expenditure					
Publication expenses:					
Special Issue costs		20,297		*84,132*	
Printing and binding Volume 7 (*1999 Volume 6*)		43,679		*80,115*	
Distribution costs		5,452		*19,156*	
		69,428		*183,403*	
Net loss on reprints		4,052	73,480	*478*	*183,881*
Editorial expenses:					
Editorial honoraria		9,792		*6,607*	
Secretarial assistance		5,470		*3,066*	
Postage, travel and sundries		1,223		(*161*)	
Technical editing:					
Salaries and expenses		84,053		*130,658*	
Computer expenses		7,128		*7,124*	
Depreciation of office equipment		1,271	109,071	*6,351*	*156,049*
Programming and development costs			49,831		*38,542*
Administration expenses recharged from General Fund			11,549		*23,300*
Total Expenditure			243,931		*401,772*
Deficit of income over expenditure			(85,270)		(*165,077*)
Reconciliation of movements					
Balance at 1 January			(46,233)		*19,391*
Transfers from other funds					
Acta Crystallographica			150,000		*100,000*
Deficit of income over expenditure			(85,270)		(*165,077*)
Fluctuations in rates of exchange			133		(*547*)
Balance at 31 December			18,630		(*46,233*)

Table 21
President's Fund Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000	*1999*
Income			
Investment income	16.7	2,164	*2,244*
Total Income		2,164	*2,244*
Expenditure			
Grants		4,063	*21,542*
Deficit of income over expenditure		(1,899)	(*19,298*)
Reconciliation of movements			
Balance at 1 January		40,123	*58,947*
Transfers from other funds			
Acta Crystallographica		20,000	–
Deficit of income over expenditure		(1,899)	(*19,298*)
Fluctuations in rates of exchange		420	(*474*)
Balance at 31 December		58,644	*40,123*

Table 22
International Tables Account for the year ended 31 December 2000.

	Note	2000	Swiss Francs *1999*
Income			
Sales of copies			
Volume A		(503)	*52,633*
Volume B		22,250	*23,582*
Volume C		68,056	*95,974*
Teaching Edition of Volume A		3,671	*6,200*
Volumes II, III and IV		96	*86*
		93,570	*178,475*
Less Publisher's commission on sales		25,768	*46,067*
Total Income		82,608	*132,408*
Expenditure			
Publication expenses:			
Printing and typesetting Volume A		30,287	*19,329*
Printing and typesetting Volume B		33,027	*4,952*
Printing and typesetting Volume C		10,830	*61,611*
Printing and typesetting Volume D		1,536	–
Printing and typesetting Volume E		3,651	–
Printing and typesetting Volume F		7,874	*351*
Printing and typesetting Teaching Edition of Volume A		4,811	*5,448*
		92,016	*91,691*
Editorial expenses:			
Editorial honoraria		4,108	*7,263*
Secretarial assistance, postage and office equipment		29,936	*24,882*
Technical editing		233,480	*230,829*
		267,524	*262,974*
Programming and development		42,164	*37,012*
Total Expenditure		401,704	*391,677*
Deficit of income over expenditure		(319,096)	(*259,269*)
Reconciliation of movements			
Balance at 1 January		137,628	*195,270*
Transfers from other funds			
Acta Crystallographica		250,000	*200,000*
Deficit of income over expenditure		(319,096)	(*259,269*)
Fluctuations in rates of exchange		494	*1,627*
Balance at 31 December		69,026	*137,628*

Table 23
Book Fund Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000	*1999*
Income			
Sales of copies, net of Publisher's commission on sales			
Historical Atlas of Crystallography		296	*178*
World Directory of Crystallographers 10th edition		1,830	*6,222*
Escher *Kaleidozyklen*		–	*159*
Sundry publications		–	*164*
Structure Reports		4,005	*1,305*
Royalties			
IUCr/OUP Book Series		3,593	*1,358*
Total Income		9,724	*9,386*
Expenditure			
Publication expenses			
World Directory of Crystallographers 10th edition		2,160	*1,776*
Total Expenditure		2,160	*1,776*
Excess of income over expenditure		7,564	*7,610*
Reconciliation of movements			
Balance at 1 January		33,607	*25,600*
Excess of income over expenditure		7,564	*7,610*
Fluctuations in rates of exchange		297	*397*
Balance at 31 December		41,468	*33,607*

Table 24
Publications and Journals Development Fund Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000		*1999*	
Income					
Investment income	16.7		11,916		*13,686*
Expenses					
Computer expenses:					
Purchase of computer equipment and software		50,308		*37,517*	
Programming and development		409,961		*359,857*	
Recharged to other funds		(409,961)	50,308	(*359,857*)	*37,517*
Electronic Publishing Committee/ Section Editors' Meeting			2,765		*1,183*
Special Issue costs			39,785		*60,479*
NeXus			2,774		–
STAR/CIF			1,319		*7,170*
Promotions Representative			137,922		*107,416*
Web input			1,502		*3,892*
Depreciation of computer equipment			12,097		*12,097*
Total Expenditure			248,472		*229,754*
Deficit of income over expenditure			(236,556)		*(216,068)*
Reconciliation of movements					
Balance at 1 January			447,064		*457,847*
Transfers from other funds					
Acta Crystallographica		200,000	200,000	*200,000*	*200,000*
Deficit of income over expenditure			(236,556)		*(216,068)*
Fluctuations in rates of exchange			2,960		*5,285*
Balance at 31 December			413,468		*447,064*

Table 25
Research and Education Fund Account for the year ended 2000.

	Note	Swiss Francs 2000		*1999*	
Income					
Investment income	16.7		47,366		*47,069*
Expenditure					
Young Scientists' Support		112,200		*82,157*	
Visiting Professorship Programme		10,700		*20,226*	
Total Expenditure			122,900		*102,383*
Deficit of income over expenditure			(75,534)		(*55,314*)
Reconciliation of movements					
Balance at 1 January			912,341		*886,870*
Transfers from other funds					
Acta Crystallographica		70,000	70,000	*70,000*	*70,000*
Deficit of income over expenditure			(75,534)		(*55,314*)
Fluctuations in rates of exchange			6,539		*10,785*
Balance at 31 December			913,346		*912,341*

Table 26
Ewald Fund Account for the year ended 31 December 2000.

	Note	Swiss Francs 2000	*1999*
Income			
Investment income	16.7	25,591	*22,442*
Income bequest		–	*72*
		25,591	*22,514*
Expenditure			
Prize/Selection Committee and expenses		–	*45,902*
Excess/(deficit) of income over expenditure		25,591	(*23,388*)
Reconciliation of movements			
Balance at 1 January		426,512	*419,858*
Transfers from other funds			
General Fund		–	*25,000*
Excess/(deficit) of income over expenditure		25,591	(*23,388*)
Fluctuations in rates of exchange		3,260	*5,042*
Balance at 31 December		455,363	*426,512*

Table 27
Newsletter Fund Account for the year ended 2000.

	Note	Swiss Francs 2000		*1999*	
Income					
Income from advertisements			173,980		*139,475*
Total Income			173,980		*139,475*
Expenditure					
Editorial honoraria			7,920		*6,732*
Editorial expenses			51,862		*80,710*
Newsletter printing and distribution			124,264		*103,398*
Advertising costs			43,495		*34,867*
Total Expenditure			227,541		*225,707*
Deficit of income over expenditure			(53,561)		(*86,232*)
Reconciliation of movements					
Balance at 1 January			133,905		*57,242*
Transfers from other funds					
Acta Crystallographica		50,000		*50,000*	
General Fund		25,000	75,000	*25,000*	*75,000*
Excess/(deficit) of income over expenditure					
Current year (above)		(53,561)		–	(*86,232*)
Accumulated underspend in prior years not previously recognized		(22,000)	(*75,561*)	86,312	*80*
Fluctuations in rates of exchange			962		*1,583*
Balance at 31 December			134,306		*133,905*