international union of crystallography

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Report of the Executive Committee for 2001

1. Meetings

The IUCr sponsored the following meetings held during 2001:

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

International School on Crystal Growth: Crystal Growth of Materials for Energy Production and Energy-Saving Applications, Trieste, Italy, 5–10 March (change of venue and date; originally to be held in Monastir, Tunisia, 19–26 November 2000).

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

AsCA '01, Bangalore, India, 18–21 November.

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

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

The Executive Committee met in Los Angeles, USA, in July. The Finance Committee met once, in Copenhagen, Denmark, in March, 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:

editorial policy, pricing policy and subscription rates, approval of appointments of new Editors for *Acta Crystallographica* Sections A, B and D and for *Journal of Synchrotron Radiation*, approval of appointments of Co-editors, electronic publishing, archival policy, Special Issues, and other matters concerning the IUCr journals;

Acta Crystallographica Section E;

review of *Journal of Synchrotron Radiation*;

review of contract with Munksgaard;

approval of the audited accounts for the previous year;

the General Fund estimates and the level of the unit contribution;

the status of membership subscriptions;

investment policy;

funding and uses of the Publications and Journals Development Fund and the Research and Education Fund, establishment of the Journal Grants Fund;

cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and the Fachinformationszentrum Karlsruhe and National Institute for Standards and Technology;

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

the *IUCr Newsletter*;

the *World Directory of Crystallographers*;

promotional activities;

the Ewald Prize;

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

discussion of the arrangements for the 2002 General Assembly and Congress;

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

Other items dealt with in this way were:

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;

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

crystallography in Africa;

use of financial support through ICSU;

the Inter-Union Bioinformatics Group;

review of the activities of the Commissions;

review of the activities of Regional Associates;

review of the reports of IUCr Representatives on other bodies.

Items concerning the Chester office were:

staffing requirements, upgrading of office technology, provision of internet services, upgrading of internet connection, establishment of mirror sites.

2. Publications

Volume 57 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. The year saw the publication of a total of 9,215 pages and 2,464 articles compared with 7,565 pages and 1,825 articles in 2000.

Milestones accomplished in the year were the launch of *Acta Crystallographica* Section E in January 2001 and the completion of the 50 year digitization project in November 2001. In both these projects we witness again the electronic revolution. With *Acta Cryst*. Section E, we have a very fast mechanism for chemical crystal structure publication in e-form. With the full archive of papers now digitized, we have complete access at the click of a mouse to all articles for our subscribers back to 1948. In the accompanying reports, there are very buoyant trends in numbers of articles for *Acta Cryst*. Sections D and E, and a level number for *Acta Cryst*. Sections B, C and *Journal of Applied Crystallography*. The *Journal of Synchrotron Radiation* (*JSR*) has been subject again to considerable variations in published pages between Conference Proceedings and issues containing regular articles. The number of regular articles in *JSR* is causing concern and discussions have started to evaluate what benchmarks represent a 'minimum viability' and of ideas for broadening its scope.

Journal article highlighting has continued and been well received. The close collaboration with the *IUCr Newsletter* and its Editor W. L. Duax is gratefully acknowledged. The Working Group on Journals has produced a general promotional leaflet for the journals and also a joint marketing leaflet for *Acta Cryst*. Section D and Volume F of *International Tables for Crystallography*. This involved working closely with the Promotion Committee (Chair A. M. Glazer, whose collaboration is also gratefully acknowledged). Preparations are under way for a CD-ROM on Diffraction Physics (edited by A. Authier, B. Batterman and M. Hart).

A survey of the contents of the IUCr journals is given in Table 1. Details of each journal can be found in the reports below.

Finally, let me especially thank the following retiring Section and Main Editors for their major commitment to serving the IUCr journals these past years, namely Professor A. Authier (Section Editor of *Acta Cryst*. Section A), Dr F. H. Allen (Section Editor of *Acta Cryst.* Section B), Professor S. S. Hasnain and Dr H. Kamitsubo (two of the Main Editors of *JSR*). Their successors will be formally appointed at the upcoming Geneva Congress and General Assembly.

J. R. Helliwell, Chair

4.1.2. *Acta Crystallographica* Section A. Section A published 803 pages in 2001, comprising 75 full Research Papers and 12 Short Communications. These numbers represent a sharp increase with respect to the corresponding figures for 2000 and are back to the same level as in 1997; the numbers in 1998 and 1999 were higher because there was a Special Issue in each of these two years. Special Issues have been very successful and it would be good to have another dedicated to 'Crystallography Across the Sciences' (CATS2). Several Lead Articles are also in preparation.

The average handling time of manuscripts by Co-editors is now stable at around 2.8 months. Systematic use of electronic submission would help the Co-editors to reduce handling times further.

A. Authier, Editor of Section A

4.1.3. *Acta Crystallographica* Section B. Section B published 877 pages in 2001, its content comprising 98 full Research Papers, two Short Communications, one Lead Article and one Topical Review. The reduced number of printed pages, lower by 250 than the figure for 2000, is partly due to the removal of printed atomic coordinate tables. However, the total of 101 articles published during the year is comparable to 1998 and 1999 data, but lower than the 121 papers published in 2000. This apparent shortfall is accounted for by the clearance of a small backlog of papers during 2000, as the improved in-house typesetting procedures became the norm at Chester. During 2001, Co-editorial turnaround times have maintained the improvements seen in 2000, while further efficiencies have been introduced at the Editorial Office.

The chemical focus of full Research Papers during 2001 was divided almost equally between inorganic and metal–organic systems (51%) and organic systems (49%). These data are almost identical to those for 2000, and maintain the increased focus on organic systems, up from a figure of 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, computational modelling and the prediction of crystal structures, powder diffraction methodologies, studies of phase transitions *etc.*

The international nature of the journal is reflected in contributions from 343 individual authors from 28 countries, figures that are very similar to data for 2000. It is also encouraging to record that the impact factor of Section B for 2000 (made available during 2001) was 1.734, its fourth annual rise from the 1.463 of 1997.

The principal changes during 2001 have been that (*a*) coordinate lists are no longer printed in the journal, except in very special circumstances, and (*b*) all papers are now typeset in-house from electronic files of finalized manuscripts supplied by authors. Further developments in electronic processing of manuscripts are being planned.

It is a pleasure to record thanks to the IUCr editorial staff in Chester, for the high quality of their work for the journal, and for the continuing technical innovations that improve their service to authors, editors and readers.

F. H. Allen, Editor of Section B

4.1.4. Acta Crystallographica Section C. Section C published 1,504 pages in 2001 comprising 541 Full Papers. With the advent of the electronic journal, *Acta Crystallographica* Section E, in January 2001, all electronic (CIF-access) papers that had previously appeared in Section C are now published in Section E. Section E published 799 electronic papers in 2001. It is gratifying to note that the overall total of C+E papers is considerably increased over the totals for previous years when we only had Section C available for publication.

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

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	
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	492	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	
A57	2001	803	7162	103	1948	78	527	8.9	6.4	25	85	5.6	1.7
B57		877		110		100		8.6		10		1.6	
C57		1504		545		541		2.7		4		2.8	
D57		1980		390		349		5.2		41		3.3	
E57	1998			800		795		2.5		5		1.7	

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
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
34	2001	798	140	93	7.1	21	3.5	26	1.5

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
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
8	2001	1255	376	70	5.4	280	2.9	26	1.1

§ Numbered pages excluding contents pages. † 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, Current Events and Editorials. †† 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).

appearance of the published paper. When the proofs are ready, the submitting author and the Section Editor are informed simultaneously by e-mail that proofs are available for downloading from the Section C web site. The Section Editor reviews all proofs and reserves the right to make minor changes for consistency and conformity to Section C standards.

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

The data-validation suite of programs, which is used by authors to pre-check their submissions, has been revised and updated as the need arose and as required by changes in the Notes for Authors. Explanatory notes to the pre-check output have been introduced and

Table 2
Some of the macromolecular crystal structures reported in 2001 in Section D

Structure	Resolution
1.0 Å and better	
Fusarium oxysporum trypsin	0.81 Å at 100 K
Bovine pancreatic trypsin inhibitor	0.86 Å
Hen egg-white lysozyme	0.94 Å
Trypsin and radiation damage	0.95, 1.00 Å
DNA oligomer	0.95–1.50 Å
Bovine pancreatic phospholipase A_2	0.97 Å
Endothelin-1-inhibitor BQ123	1.0 Å
Vancomycin aglycon with anomalous scattering of chlorine	1.0–1.9 Å
1.0–1.5 Å	
Endoglucanase Cel5A/methyltetrathiocellopentoside	1.1 Å
Bacillus agaradhaerens Xyn11 with xylotriose	1.1, 1.9 Å
Spectrin SH3 domain	1.12 Å
Thermoascus aurantiacus xylanase I refinement	1.14 Å
Deacetoxycephalosporin C synthase merohedral twins	1.3 Å
Cupredoxin amicyanin direct-method *ab initio* phasing	1.31 Å
Streptococcus pneumonia YlxR	1.35 Å
Vipera ammodytes meridionalis (snake) vipoxin	1.4 Å
Lobster apocrustacyanin A_1	1.4 Å
Hen egg-white lysozyme – supersaturation/crystal quality	1.4–1.6 Å
Escherichia coli dUTPase	1.45 Å
Pectate lyase of polysaccharide lyase family 3	1.5 Å
Rusticyanin mutant	1.5 Å
Fluorouracil destabilization of an RNA duplex	1.5–1.8 Å
DNA dodecamer containing deoxyformyluridine	1.5–1.8 Å
Desulfovibrio vulgaris flavodoxin	1.5, 2.0 Å
1.5–2.0 Å	
RNA duplex with unusual GC pair	1.6 Å
Coprinus cinereus laccase	1.6 Å
Plastocyanin with an engineered disulfide bond	1.6 Å
Porcine β-trypsin–detergent complexes	1.6–1.9 Å
GM1 receptor of heat-labile enterotoxin and cholera toxin	1.6–2.0 Å
Mouse L-chain ferritin	1.6, 2.1 Å
Grifola frondosa 'aspzincin' metalloendopeptidase	1.6–2.8 Å
Escherichia coli calmodulin fragment	1.7 Å
Rhodospirillum centenum cytochrome c_2	1.7 Å
Peptostreptococcus magnus protein L – B1 domain	1.7, 1.8 Å
Human grancalcin with calcium	1.7, 1.9 Å
HIV integrase ligand site	1.7, 2.3 Å
Tryptophanyl-tRNA synthetase with tryptophanyl-5′AMP	1.72 Å
Major urinary protein – X-ray *versus* NMR structures	1.75 Å
Thermomonospora fusca β-mannanase	1.8 Å
Lysozyme and stabilizing additives	1.8–1.9 Å
SH3 domains of chicken src tyrosine kinase	1.8–1.95 Å
Urtica dioica agglutinin isolectin I	1.9 Å
Daboia russelli pulchella phospholipase A_2	1.9 Å
Hemophilus influenzae HsIV protein	1.9 Å
Human RNase 1ΔN7	1.9 Å
Desulfuromonas acetoxidans cytochrome c_7	1.9 Å
Blue copper nitrite reductase – high pH and copper-free	1.9 Å
Bacillus subtilis NH_3-dependent NAD^+ synthetase	1.9–2.3 Å
Human replication protein A14/32	1.9–2.4 Å
Human peroxiredoxin 5 twin	1.9–2.8 Å
Human S100A12 (EF-hand calcium binding)	1.95 Å
Human mitochondrial branched-chain aminotransferase	1.95–2.5 Å
Yersinia pestis YopH	2.0 Å
Streptomyces sp. 538 11 endo-β-1,4-xylanase Xyl1	2.0 Å
Moloney murine leukemia virus reverse transcriptase + 16-mer DNA	2.0–2.1 Å
Staphylococcal enterotoxin C2	2.0–2.3 Å
Pyrobaculum aerophilum imidazole glycerol phosphate synthase	2.0, 3.1 Å
2.0–2.5 Å	
Interleukin 4	2.05 Å
Escherichia coli isocitrate lyase	2.1 Å
Aspergillus phoenicis aspergillopepsin I	2.18 Å
Calf spleen purine nucleoside phosphorylase	2.2 Å
Gracilaria chilensis R-phycoerythrin	2.2 Å
Manihot esculenta hydroxynitrile lyase	2.2 Å
Spirulina platensis C-phycocyanin	2.2 Å
Haementeria officinalis (leech) anti-platelet protein	2.2 Å
L-Asparaginase (two of them) – packing	2.2–2.5 Å
Leuconostoc mesenteroides glucose 6-phosphate dehydrogenase	2.2–2.8 Å
Thermus thermophilus 3-isopropylmalate dehydrogenase	2.2–2.5 Å
Cytosolic bovine retinal creatine kinase	2.3 Å
Haemophilus influenzae heat-shock locus U protein	2.3 Å
Anser indicus bar-headed goose aquomet haemoglobin	2.3 Å
Thermus thermophilus ribosomal protein TL5 + *Escherichia coli* rRNA	2.3 Å
Corynebacterium diphtheriae diphtheria toxin repressor	2.3–2.8 Å
Bacillus thuringiensis bacterial δ-endotoxin Cry3Bb1	2.4 Å
Human erythrocyte catalase	2.4 Å
Desulfovibrio desulfuricans bacterioferritin	2.4–2.9 Å
Human uropepsin	2.45 Å
Acyl-homoserinelactone synthase Esa1	2.5 Å
Topical Review – rat transthyretin with thyroxine	2.5 Å
Clostridium botulinum neurotoxin B-doxorubicin binding	2.5 Å
Murine Tcl1 (T-cell prolymphocytic leukemia)	2.5 Å
2.5–3.0 Å	
C-terminal sterile α-motif domain of human p73α	2.54 Å
Phenylalanyl-tRNA synthetase + phenylalanyl-adenylate	2.6 Å
Glycosylated fibroblast growth factor 9	2.6 Å
Rhodobacter sphaeroides membrane protein interactions	2.6–3.5 Å
Tetraubiquitin	2.7 Å
Chicken egg-white lysozyme – powder diffraction study	2.8–3.0 Å
Human liver fructose-1,6-bisphosphate aldolase	2.82 Å
N-Methyltransferase with iodinated myristoyl-CoA	2.9 Å
Head–tail connector of bacteriophage φ29	2.9–3.5 Å
Human transthyretin	3.0 Å
Orotidine-5′-monophosphate decarboxylase SeMet	3.0 Å
Human vascular cell adhesion molecule-1 integrin-binding	3.0 Å
Lower than 3.0 Å	
Greylag goose hemoglobin – compare bar-headed goose	3.09 Å
HIV-1 protease with hydroxyethylamine isostere	3.1 Å
Human muscle creatine kinase	3.5 Å

these give concise details of problems that have been detected; these notes have been much appreciated by authors. I am indebted to Professor A. L. Spek for his invaluable work on the *PLATON* checking suite of programs.

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, devoted to biological crystallography, published 390 articles in 2001. These included Research Papers (142), Short Communications (30), a Topical Review, a Scientific Comment and Crystallization Papers (207). The three Co-editors N. Chayen, A. Zagari and M. Pusey handle most of the Crystallization Papers. They deserve our thanks for streamlining this procedure. The proceedings of the Collaborative Computational Project CCP4 Study Weekend on Molecular Replacement and its Relatives, held 3–9 January 2001 at York University, UK, and organized by K. Cowtan, J. Naismith, A. Ashton, I. D. Brown, P. Broadhurst and M. H. Eales, was published in Section D in October 2001. K. Cowtan and J. Naismith were the guest editors for this issue. It includes an introduction to the method by P. R. Evans, a historical account by M. G. Rossmann and 17 other articles. Therefore, it should be very useful for all, and extra copies can be purchased of this one issue. The extra thickness of the November issue of Section D (the issue after the CCP4 issue) indicates the good general influx of manuscripts.

The year saw several papers on crystal stabilization by additives, effects of microgravity, behaviour on flash cooling and on synchrotron-radiation damage to macromolecular crystals. Neutron diffraction, atomic force microscopy, small-angle scattering and powder diffraction were topics discussed. The addition of anions, cations and noble gases to assist in phasing, and some methods for dealing with crystal twinning were also presented. Printed articles reflect the increasingly high resolution at which diffraction patterns of macro-

molecular crystals can now be analysed and their structures ultimately refined. Statistics on resolution illustrate this; 8 structures are reported with a resolution of 1.0 Å or better, with an additional 15 up to 1.5 Å resolution (see Table 2). These make up approximately 24% of the total number of structures reported, compared with 14% at these resolutions published in 2000.

Another area of advance involves the use of anomalous scatterers and MAD phasing, the subject of 11 articles. There were also 9 articles on phase angle determination (in addition to the 19 CCP4 articles on molecular replacement). There were 6 articles on *ab initio* structure determination and those on structure refinement showed the increased sophistication of the macromolecular crystallographer (involving the use of **TLS** parameters, for example). Finally, several analyses of molecular geometry, intermolecular interactions and the binding of ligands extended our structural information and provided further data for the structural databases.

Now that we are entering the area of 'high throughput' macromolecular crystallography, it is necessary to consider the impact of such results on published journals, such as *Acta D*. Crystallization papers may eventually be published in an electronic subsection of *Acta D* and we are considering an electronic-only Structural Genomics subsection. We welcome Mitchell Guss as a Co-editor helping with this. The journal continues to have excellent illustrations (colour in these is free) and authors are generally delighted when their work is chosen for the monthly cover.

The high-quality appearance of the journal and the excellent rapport set up with most authors is made possible by our excellent Co-editors, reviewers and the staff at Chester. They are all thanked for their efforts.

A table of articles published in 2001 is available as an Appendix *via* **Crystallography Journals Online** and Table 2 lists structure determinations (with resolution).

J. P. Glusker, Editor of Section D

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

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

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

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

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

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

All published articles are available in HTML and PDF formats, and free reprints are made available electronically to authors. A range of supplementary material is provided. This includes the output of the checkcif process and any associated responses from authors. Throughout the year, there has been a steady increase in the number of submissions and it will probably not be long before we have 100 articles in a single monthly issue. In anticipation of this, another five Co-editors have been appointed and another three to four may be needed by mid-2002.

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

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

4.1.7. Journal of Applied Crystallography. *JAC* published 798 pages in 2001 (down from 1,020 in 2000, not including 448 pages of the Small-Angle Scattering Conference Proceedings, and 1,208 in 1999). This included 93 full Research Papers and 21 shorter papers. In late 2001, a promotion leaflet was prepared in cooperation with the IUCr Promotions Officer and the Working Group on Journals. The leaflet will be available in 2002, and it aims at convincing biologists, chemists, physicists and materials scientists to place their crystallography-based work in *JAC*.

G. Kostorz, Editor of JAC

4.1.8. Journal of Synchrotron Radiation. *JSR* published over 1,250 pages of articles during the 2001 calendar year, including the Proceedings of the Eleventh International Conference on X-ray Absorption Fine Structure (XAFS XI) held in Ako, Japan, 26–31 July 2000. Guest Editors for this 968-page proceedings were Professors T. Ohta and M. Nomura. A succession planning exercise is underway for the replacement of several Co-editors and two of the founding *JSR* Main Editors, namely S. S. Hasnain and H. Kamitsubo. Both have served as *JSR* Main Editors for nine years and we thank each of them for their hard work and dedication in getting *JSR* off the ground. The new Main Editors will be appointed during the 2002 IUCr Congress.

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

4.2. Commission on International Tables

The main activity during the year 2001 consisted of proof-reading and printing several volumes of *International Tables*. Two volumes, B and F, have appeared in 2001, whereas volumes A, D and E, as well as the Brief Teaching Edition of Volume A, are scheduled for publication in 2002. For the two 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.

4.2.1. Volume A. Space-Group Symmetry; Editor Th. Hahn. Proof-reading of the text sections and the space-group tables for the Fifth Edition of Volume A was completed. Publication of the volume is envisaged for spring 2002. Shortly afterwards, the Fifth Edition of the Brief Teaching Edition of Volume A will appear.

4.2.2. Volume B. Reciprocal Space; Editor U. Shmueli. The first few months of 2001 were devoted to final correspondence with authors and the Technical Editor, regarding minor corrections of the page proofs. The second edition of Volume B was then sent to press and was published in April 2001. The description of the second edition of Volume B, and a table of its contents are available at the following addresses: http://crystal.tau.ac.il/xtal/comit/promot.html and http://www.iucr.org/iucr-top/it/index.html.

4.2.3. Volume C. Mathematical, Physical and Chemical Tables; Editor E. Prince. The stock of the second edition of Volume C is projected to run out early in 2003. Because the entire contents of the volume are in machine-readable files, it is possible to make fairly extensive modifications with little effort, so a memorandum was sent to all authors in August 2001, asking if any revisions or corrections were needed. A deadline of 31 July 2002 has been established for submission of revisions, and about ten of the authors have indicated that they would submit revisions by that time.

4.2.4. Volume D. Physical Properties of Crystals; Editor A. Authier. Parts 1 and 2 of the volume were complete in 2000 and Part 3 is now also complete. It is expected that the volume will be printed in 2002.

4.2.5. Volume E. Subperiodic Groups; Editors V. Kopsky and D. B. Litvin. Volume E is being readied for publication which is anticipated to be in 2002.

4.2.6. Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. A. Arnold. Volume F was published in July 2001. It comprises 26 chapters and a total of 72 articles written by 156 authors. 450 copies of Volume F have been sold as of mid-January 2002. The contents and further description of the volume can be found at the IUCr web site: http://www.iucr.org/iucr-top/it/itf.html. Now that Volume F has been published in print version, it is important to consider different possible modes of electronic access. We suggest that the IUCr might consider making a version available on the internet, accessible to those who have either purchased the volume or who have paid for a password. A CD-ROM version of Volume F would also be a valuable and readily portable resource. A CD-ROM version could be sold separately, perhaps at a very substantial discount for owners or new buyers of the volume.

4.2.7. Volume G. Crystallographic Information; Editors B. McMahon and S. R. Hall. The plan for the first edition of this volume remains: to describe the crystallographic information file (CIF) format and the data dictionaries maintained by COMCIFS, within four parts: (1) Concepts and specification; (2) CIF data definition and classification; (3) Data dictionaries; and (4) Applications. Parts (1) and (3) are essentially complete in draft, while the most substantial contributions to Part (2) are also in hand in first draft. Some revision to chapters contributed to Part (4) will be necessary to reflect changes in available software since they were first drafted. Publication in late 2002 or early 2003 is now envisaged. At the request of the Executive Committee, a change of title is under consideration to reflect the specialized emphasis of this edition.

4.2.8. Volume A1. Maximal Subgroups of Space and Plane Groups; Editors H. Wondratschek and U. Müller. Volume A1, first under the editorship of H. Wondratschek and for some time called Volume H, has been reorganized. It has been decided to combine the data on 'Maximal subgroups of space and plane groups' by M. Aroyo, Y. Billiet and H. Wondratschek with the data on 'Wyckoff positions of group–subgroup related space groups' by U. Müller. The volume now has two editors and three parts, the title has not been changed. The three parts are: Part 1: Introduction, containing the chapters: Historical introduction; Introduction to the topic of the volume. Part 2: Maximal subgroups of space groups, containing the chapters: Guide to the tables and diagrams; Tables of maximal subgroups of space and plane groups; Subgroup diagrams; Mathematical background of the subgroup tables. Part 3: Splitting of Wyckoff positions, containing the chapters: Remarks on Wyckoff positions; Guide to the tables and tables of the relations between the Wyckoff positions of the space groups and their maximal subgroups. The completion of Volume A1 has been delayed because of illness; work has now resumed.

Th. Hahn, Chair

4.3. Commission on Aperiodic Crystals

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

The Commission has asked Professor N. Speziali to organize Aperiodic 2003. This meeting will take place in Belo Horizonte (Brazil) in September 2003. Information can be found at the Commission's web pages or at http://www.fisica.ufmg.br/~ap2003/.

The Commission continued to promote activities on the crystallography of aperiodic crystals at national and international meetings. Members of the Commission were actively involved in the organization of microsymposia at the European Crystallographic Meeting ECM-20 in August 2001 in Krakow (Poland), and the meeting of the Asian Crystallographic Association AsCA '01 in November 2001 in Bangalore (India).

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

The Commission maintains internet pages at the web site of the IUCr at http://www.iucr.org/iucr-top/comm/capd/index.html. A web site on all aspects of the crystallography of aperiodic crystals is maintained by the special interest group (SIG) on aperiodic crystals of the European Crystallographic Association. It is maintained by M. Dusek (Prague, Czech Republic) and may be found at http://www-xray.fzu.cz/sgip/aphome.html.

S. van Smaalen, Chair

4.4. Commission on Biological Macromolecules

The Commission covers what is arguably the most active and vigorous scientific community within the IUCr. It may therefore seem incongruous that the Commission undertakes relatively few independent activities. This may be explained by noting that the scientific outlets for the macromolecular community are so diverse and numerous and relatively well supported by other bodies including industry that little call is placed by this community on this Commission of the IUCr. Macromolecular crystallography is strongly represented at meetings of the Regional Associates of the IUCr, namely the American Crystallographic Association, the Asian Crystallographic Association and the European Crystallographic Association, as well as at meetings of national crystallographic societies. Vigorous representation at these meetings is sometimes even mistaken for dominance by other members of the crystallographic community. In addition there are many specialized workshops and schools held regularly that cater for the macromolecular crystallographic community, including those at Cold Spring Harbor (USA), Erice (Italy), Uppsala (Sweden) and the CCP4 study weekends (UK).

The Commission supported an International Symposium on Crystallography and Bioinformatics held in November 2001 in Bangalore, India. The Symposium immediately followed an extremely successful meeting of AsCA held in the same location. The meetings incorporated wonderful felicitations for Professor S. Ramaseshan and for Professor M. Vijayan in honour of his birthday. The Symposium showcased the range and depth of biomolecular crystallography in India as well as keynote talks from both Indian and foreign attendees. The enthusiastic participation by so many students was extremely pleasing.

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

J. M. Guss, Chair

4.5. Commission on Charge, Spin and Momentum Densities

The Commission held no formal meetings in 2001, although Commission members were active in the organization of relevant international conferences. The Gordon Research Conference on Electron Distributions and Chemical Bonding was held at Mount Holyoke College, USA, 8–13 July 2001 (Chair C. Lecomte, Vice Chair J. C. H. Spence). The number of attendees was a considerable increase on previous meetings, and most pleasingly 52% of attendees were under 40 years of age. The scientific programme was designed to bring together experimentalists and theoreticians, X-ray and electron diffraction experts, crystallographers, physicists, materials scientists and chemists, and resulted in very stimulating and interesting discussions. The conference was a success owing to the quality of lecturers, discussion leaders and poster sessions (which always lasted very late into the night). Support from the Gordon Research Conferences, IUCr, NSF, Oxford Cryosystems, Bruker Nonius, Molecular Structure Corporation and JEOL allowed 65 conferees to be partly or fully sponsored. The meeting demonstrated that charge-density-related research is entering a new and very alive period, attracting more and more new communities of physicists, chemists and materials scientists. As always, the conference was evaluated, and a future meeting has been approved for 2004.

The International Conference on Inelastic X-ray Scattering, IXS2001, was organized under the auspices of the Commission, chaired by K. Hämäläinen, S. Manninen and P. A Suortti, and held in Haikko, Finland, 22–26 August 2001. This was the fourth conference in the series (previous meetings being in Montauk, USA, in 1998, Tokyo, Japan, in 1995 and Krakow, Poland, in 1993). The main emphasis of the meeting was on the application of inelastic X-ray scattering in the study of electronic structure and dynamics, as well as in many-body phenomena. The purpose of the meeting was to bring together specialists to discuss both the experimental advances accomplished at various synchrotron-radiation sources, and the theoretical and computational challenges that have been overcome, and that are to be met. The scientific programme was designed to encourage dialogue between theorists and experimentalists. Participants numbered 70, and the conference was truly international, with the greatest representation coming from outside Europe.

Inelastic X-ray scattering has recently demonstrated tremendous breakthroughs owing to the advent of third-generation synchrotron sources. Besides very strong fundamental research, real applications in materials science, chemistry and even in biology have started to appear. Highlights included work on high-resolution X-ray spectroscopy on biomaterials, especially on photosynthesis, several resonant scattering studies on high-T_c cuprates, studies under high pressure, and impressive theoretical progress on understanding the electron–hole interaction. The conference was funded mainly through registration fees, with some sponsorship received from the IUCr, the University of Helsinki, the Academy of Finland, and private foundations and companies. The next meeting will be organized by APS 'somewhere close to Chicago' (to be chaired by E. Alp) in 2004. This is very timely because at that time several IXS-capable beamlines under construction at APS will have begun to produce new results. Planning for Sagamore XIV, the next triennial conference on charge, spin and momentum densities, is well under way. The meeting is being organized by M. A. Spackman, and will be held 14–18 August 2003 in Broome, Western Australia, following a joint meeting of the Society of Crystallographers in Australia & New Zealand and the Asian Crystallographic Association. Preliminary details may be found at http://www.crystal.uwa.edu.au/CrystalsDownUnder.

M. A. Spackman, Chair

4.6. Commission on Crystal Growth and Characterization of Materials

The Commission focused its activity on four events during 2001. All four events, listed below, received IUCr sponsorship.

(1) International School on Crystal Growth of Materials for Energy Production and Energy-Saving Applications, Trieste, Italy, 5–10 March 2001. This school was organized by the Commission under the auspices of the International Organization for Crystal Growth (IOCG) and directed by R. Fornari. Three more members from the Commission were involved as lecturers.

The school was held at the Abdus Salam International Centre for Theoretical Physics (ICTP). It was specifically aimed at young researchers, PhD and Masters students working in materials science. The main objective was to provide an overview of classical and modern growth technologies along with a series of lectures focused on the crystal growth of energy-related materials. Three main classes of materials were considered: materials for energy conversion (terrestrial and space solar cells, thermo–photovoltaic

converters), for energy storage (carbon nanotubes and superconductors) and for energy saving (superconductors, soft magnets for low-loss transformers, nitrides for visible and white light LEDs). Some lectures on structural and electrical characterization were also included, bearing in mind the important role that extended and point defects play in material characteristics and device performance. The school was attended by 40 participants (15 from Italy, 15 from Eastern and Western Europe, 4 from Northern Africa and the others from South America and Asia). In addition to registered participants, several ICTP guests were able to follow the lectures. The truly international character of the ICTP and the friendly behaviour of participants and lecturers provided a pleasant and stimulating atmosphere for scientific (and non-scientific) discussions. The interest of the participants for the subjects of the school is witnessed by the high level of attendance at each lecture. In addition to the official school programme, two afternoon sessions were devoted to short presentations by students: 24 young participants enthusiastically talked about their current research interests. These informal presentations were highly appreciated as they proved to be useful in order to promote new contacts and strengthen relations among participants.

(2) International Workshop on Preparation and Characterization of Technologically Important Single Crystals, New Delhi, India, 26–28 February 2001. This meeting was held at the National Physical Laboratory. Four members of the Commission were involved in the organization of this meeting either as a member of the International Advisory Committee or as lecturers.

The Workshop dealt with growth and characterization of single crystals (in particular oxides) but also served to celebrate the 60th birthday of K. Lal, an eminent scientist who has contributed for more than three decades to the development of new crystallographic methods for the characterization of defects in crystalline materials. He was also a member of this Commission for three triennia between 1987 and 1996. Nearly 150 abstracts of contributed papers were accepted. Proceedings of the workshop consisting of 727 pages containing 17 invited papers and 119 contributing papers were released at the Inaugural Function of the workshop. These were distributed to over 180 delegates, including 20 from outside India representing, for example, countries such as the USA, UK, Germany, Japan, Russia, Bangladesh *etc.*

(3) 11th International Summer School on Crystal Growth, Doshisha, Japan, 24–29 July 2001. This school is held every three years and it is certainly the most important school organized by the IOCG. The Commission contributed to the Japanese venue with many suggestions and by supporting the sponsorship application presented by the Chair, K. Sato. 25 lectures were presented, ranging from theory of crystal pattern formation to nanocrystal formation. The level of the lectures was in most cases tutorial but some high-level seminars regarding advanced fields were also included (blue light emitters, high-efficiency solar cells, quantum structures, superlattices *etc.*). The school was successful and attracted a large number of students, particularly from the crystal growth community of Japan.

(4) International Conference on Crystallogenesis and Mineralogy, St Petersburg State University, Russia, 17–21 September 2001. This Conference focused on the development of fundamental crystallogenesis in mineralogy: modelling of mineral formation processes; analysis of genetic character of crystal morphology and crystal chemistry of minerals; studies of aggregate structures. These subjects also included some applied aspects of crystallogenesis in multicomponent media: synthesis of minerals and other crystalline materials; crystallization in glasses and adhesive crystalline materials; treatment of mineral resources.

The Conference was timed to coincide with a centenary celebration of the birthday of Professor G. G. Laemmlein (23 August 1901–15 November 1962), who was an outstanding crystallographer and mineralogist and one of the founders of modern crystallogenesis and of crystallogenic modelling of mineral formation. The conference was chaired by A. E. Glikin and two members of the Commission served on the Programme Committee.

The Commission discussed and decided to support the Latin-American Summer School on Crystal Growth, chaired by E. Dieguez, which will be held 3–7 July 2002 at the Universidad Autonoma de Madrid, Spain. Two members of the Commission are already enrolled as lecturers at the school.

R. Fornari, Chair

4.7. Commission on Crystallographic Computing

During 2001, the Commission has been almost solely involved in affairs in Europe. As last year, we have received no leads to enable us to become involved as a Commission in the USA, Asia or Australasia.

I was unable to generate any enthusiasm for a Computing School to be run in conjunction with the Geneva Congress. This, together with the uncertainty of the final location for the meeting, led me to abandon the idea. At the Congress itself, there will be a single session on 'Validation', chaired by A. L. Spek and C. Haltiwanger. The Open Meeting of the Commission will be used to discuss software issues.

D. J. Watkin, Chair

4.8. Commission on Crystallographic Nomenclature

The principal concerns of the Commission in 2001 continued to be the nomenclature of phase transitions and of crystallography in n dimensions, as it has been over the last several years. A new nomenclature concern over the possibility of assigning crystalline phase identifiers for use in databases arose at the end of the year.

Following publication of the first Report of the Working Group on Phase Transition Nomenclature in *Acta Cryst*. (1998), A**54**, 1028–1033, the renewed Working Group, with J.-C. Tolédano as Chair, was charged with extending the nomenclature recommendations for structural phase transitions to other classes of phase transition. The six-field notation of the first Report was found fully applicable to the more complex nomenclature of transitions involving magnetic phases, incommensurate phases and transitions that occur as a function of composition change. The notation also proved readily applicable to a series of other types of phase, including polytype, radiation-induced, other transient and quasicrystalline phases and their transitions. The conditions for phase stability in this series of phases are ill-defined, hence their recommended nomenclature is necessarily tentative. A uniform notation for translational periodicity, propagation vector or wavevector was prescribed for magnetic and/or incommensurate substances. The notation adopted for incommensurate phases that rely in part on the existence of an average structure also proved to be consistent with that for commensurate phases in a sequence. The sixth field of the nomenclature is used to emphasize the special features of polytypes and transient phases. Illustrative examples are provided for each category of phase sequence. The second Report, as accepted by the Commission, appeared in *Acta Cryst.* (2001), A**57**, 614–626 with six minor printing errors corrected in *Acta Cryst*. (2002), A**58**, 79.

The first Report of the Sub-committee on the Nomenclature of n-Dimensional Crystallography, entitled I. Symbols for Point Group Transformations, Families, Systems and Geometric Classes, appeared

in *Acta Cryst.* (1999), A**55**, 761–782. The renewed Sub-committee with T. Janssen as Chair [see *Acta Cryst.* (2000), A**56**, 616 for membership] was charged by the Commission with supplementing the recommendations in the first Report by the provision of a complete nomenclature and symbolism for use in *n*-dimensional crystallography. Following discussion throughout the year, the Sub-committee produced the zeroth draft of a final Report with recommended symbols for arithmetic crystal classes, Bravais classes and space groups in four, five and six dimensions in the second week of 2002. The final version is expected to be ready for review by the Commission before the Geneva Congress.

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

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. For instance, the msCIF dictionary of data names for the description of modulated incommensurate structures and the dictionary of symmetry data names, cif_sym.dic, have been developed and are now approved. Work is also in progress in other fields such as diffuse scattering.

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

S. C. Abrahams, Chair

4.9. Commission on Crystallographic Teaching

The main concern of the present Commission is to design a powerful teaching web site that can be used in a very informative way by a wide spectrum of users: crystallographers, school teachers and children, the general public and industrialists. The Commission discussions for the last two years mainly centred on how to implement the strategies previously discussed in our reports.

During ECM-20 at Krakow, Poland, an informal meeting was held with the Commission members attending the meeting. The discussion centred mainly on three items: (1) The development of the teaching web site, which still needs great effort and non-conventional steps in developing it. The results of the discussion were promising and not in favour of the present way of handling the teaching web site. (2) The Ismailia workshop; the outcome of the discussion agreed on the revised date of 2 February 2002 instead of 3 November 2001. (3) The Geneva Congress and this was our main concern during that meeting. The Commission agreed on an Open Meeting specializing in teaching of macromolecular crystallography. After the Krakow meeting, K. Crennel agreed to cooperate with D. S. Moss, the Commission web master, on work on the web site.

The Ismailia workshop remains the most important outcome of the Commission during 2001. All the topics mentioned in the circular were covered (teaching by the internet, teaching by interactive CD-ROM, teaching by simulation, teaching by transparencies, teaching school children by video games).

The most interesting session was that for school children. Three Egyptian lecturers ran this session and about 20 children from different schools in the age range 10–14 years attended; they enjoyed making models by themselves and playing games to learn about symmetry. A complete report on the workshop will be given in the triennial report.

K. El-Sayed, Chair

4.10. Commission on Electron Diffraction

No report has been received from the Chair.

4.11. Commission on High Pressure

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

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

The workshop included a special session to celebrate the life and work of J. M. Besson, whose untimely death in early 2001 robbed the high-pressure community of one of its great pioneers and leaders. Most of his working life had been spent in Paris and at LURE near the conference site. Four of his close colleagues gave talks on his seminal contributions to high-pressure science. The session was

introduced and chaired by the Commission Chair, who had been a close collaborator of Michel Besson's over the past decade.

This workshop was also the occasion of the main meeting of Commission members and consultants during the triennium. Ten members and consultants were present. The principal items of business were future membership of the Commission, plans for sessions at the Geneva Congress, the general issue of how the Commission should best participate in Congresses for the benefit of its very wide and to some extent 'non-crystallographic' community, and other future plans and activities. Leading up to this meeting, Commission members had already put considerable effort into devising the Commission's programme for the Geneva Congress, particularly W. F. Kuhs acting as a member of the Programme Committee. Several other members and consultants had agreed to act as Chairs or Co-chairs of the planned four microsymposia, two Open Commission Meetings, and three keynote lectures, which together were designed to form a focused 'workshop' over three days of the Congress. Concerning future plans and activities, it was agreed to organize workshops in 2003 and 2004, at venues yet to be finally agreed – but most probably at the Canadian Light Source in 2004. Already well advanced plans for the International School on High Pressure Crystallography to be held in Erice, Italy, 4–15 June 2003, were discussed. Commission member A. Katrusiak is to be a Director of the School. This will be a major and important first venture of its kind for the Commission, and is planned as a substantial contribution to the dissemination of high-pressure methods and science to which the Commission is committed, particularly for the benefit of younger scientists.

R. J. Nelmes, Chair

4.12. Commission on Neutron Scattering

Following the change of venue for the XIX IUCr General Assembly and Congress from Jerusalem, Israel, to Geneva, Switzerland, the ILL and ESRF scientists including our Commission member welcomed an IUCr satellite meeting at Grenoble, France, on neutron scattering and synchrotron radiation to be linked to the Geneva Congress. By taking such scientific and geographical advantages of Grenoble, where the world top-class neutron and synchrotron facilities are located only 150 km from Geneva, this Commission decided to co-host this satellite with the Commission on Synchrotron Radiation with generous support from ILL and ESRF. The satellite meeting is now entitled 'Crystal Chemistry of New Materials and Soft Matter – Studied by Synchrotron and Neutron Diffraction' and will be held 1–4 August 2002; this complements another satellite meeting 'Neutron and Synchrotron X-ray Scattering in Condensed Matter Research' to be held 4–6 August 2002 at Villigen, Switzerland, to celebrate the new neutron source (PSI) and Swiss synchrotron source, and several microsymposia on neutron and synchrotron science at the main Congress in Geneva.

The Commission business meeting was held 11 September 2001 at Munich, Germany, where the International Conference on Neutron Scattering (ICNS-2001) was held, the quadrennial international festival for neutron scattering. Topics of the microsymposia programmed for the Geneva Congress, based on our previously submitted request, and the procedures for forming Programme and Local Committees of the Satellite Meeting at Grenoble were discussed. Both Commission Chairs have served as Programme Chairs and all Commission members as Programme Committee members. Also discussed was the continuous work on our project to compile a 'Catalogue of Neutron Sources', to pursue carefully the future of neutron sources and to update the current status of existing and planned neutron sources all over the world. This contains specifications of source and instruments as well as users programmes of nearly 100 sources. However, this project will be carried over to the next triennium to enable it to be completed fully. The first two years of the present triennium carried bad news about the permanent shut-down of two major neutron sources, *i.e.* the High Flux Beam Reactor at Brookhaven National Laboratory (USA) in 1999 and the DR-3 reactor of Risø National Laboratory (Denmark) in 2001, both of which were always in the forefront of neutron science, of course, including crystallography, for more than three decades. In 2001, on the other hand, the 1 MW Japanese Spallation Neutron Source Project was funded after the construction of the American 2 MW Spallation Neutron Source started in the previous year. In view of the present situation on neutron sources worldwide, the Commission Chair (Y. Fujii) was invited to the Workshop 'Large Facilities for Studying Structure and Dynamics of Matter' organized by the OECD Global Science Forum, transformed from the former Mega Science Forum, at Copenhagen, Denmark. About half of the 75 participants were scientific experts while others were policy makers of OECD countries responsible for funding scientific programmes. The large facilities chosen for this workshop were neutron sources, photon sources (SR, FEL) and NMR. Its charge was to discuss scientific priorities and promising future lines of research, as well as to obtain information on the utility, feasibility, time-scale and cost of various types of research facilities and related infrastructures. The need for international cooperation was also discussed. The Commission Chair gave a keynote lecture on the future of reactor-based neutron scattering (not explicitly in his capacity as Chair of this Commission, but as a large-facility representative). Both Representatives from IUPAP and IUPAC (not from IUCr) gave an invited talk on their Union's view on these issues. Thus both academic and governmental organizations have paid their strong attention to neutron sources. The European Spallation Source (ESS, now 10 MW planned) project has been well matured so that it should be started as soon as possible to minimize the 'neutron drought'. However, it must be emphasized that both reactor- and accelerator-based neutron sources must be well balanced because of their complementary role as mentioned in my lecture. The Report by this OECD–GSF is now available.

Some Commission members met briefly to exchange their opinion on the progress of the Commission's activities at the 4th AsCA (Asian Crystallographic Association) Meeting at Bangalore, India, 18–21 November 2001. The Commission has been involved in making preparations for forming the Asia–Oceania Neutron Scattering Association (tentatively named) which was initiated by the former Chair, J. W. White, to complement the ENSA (European Neutron Scattering Association) and NSSA (The Neutron Scattering Society of America) for overarching the globe. By taking several opportunities, the present Chair (Y. Fujii) has contacted key persons in each country/region who would recommend both user representatives and facility representatives. It has been agreed that both Japan and Australia, having already established strong users societies, would take an initiative in progressing the process toward its formation in the next few years.

The Commission has been expected to play a more important role not only for promoting purely academic research/education but also for taking an initiative in global scientific programmes, particularly because it is the only standing committee overarching the globe in the research field of neutron scattering.

Y. Fujii, Chair

4.13. Commission on Powder Diffraction

The Commission (CPD) was particularly active during 2001, with support to congresses, schools, round robins and considerable improvements to the CPD *Newsletter*. The number of contacts with scientists from many countries is increasing steadily, especially considering the third world and less favoured countries, for which the *Newsletter* and the internet are a major support to access vital information on new results, events, methodologies, publications and any possible activities related to powder diffraction. This is an important point and should be considered as a main objective for the future: to improve connections and involvement of scientists from less favoured countries. CPD round robins and the *Newsletter* are the forte of the CPD activity. The latter has now a recognized authority, and is currently cited in the scientific literature. For this reason, an ISSN number was acquired so that the publication is also officially registered. Round robins are followed with interest by the PD community. The positive effects are manifold: experts can debate the state-of-the-art and novices can learn important methodological bases. The collaboration with the IUCr editorial office was essential for providing free reprints of scientific publications related to the round robin activity.

4.13.1. Meetings/workshops/schools. Important events of 2001 were Accuracy in Powder Diffraction III (APD3), held at Gaithersburg, MD, USA, in April 2001, and the Third Size–Strain Conference (SS-III), held in Trento, Italy, in December. APD is a historical conference in the PD field. Started in the late 1970s, it was repeated after nearly ten years, always with considerable success. APD3 was also the site of the CPD meeting for 2001. Several CPD members were involved in the programmes of both events and/or participated as speakers and session Chairs. The SS-III conference was endorsed by the CPD and supported by the IUCr. The CPD also took part in the planning activity for the next EPDIC conference (EPDIC8, Uppsala, Sweden, 23–26 May 2002), also through the CPD Chair, *ex officio* a member of the EPDIC Committee and related ECA-SIG.

The CPD also gave support to the II International School on Powder Diffraction, organized by the Indian Association for the Cultivation of Science (Jadavpur, Calcutta, India). The school was scheduled for 2001, but for political reasons was moved to January 2002.

4.13.2. Projects. During 2001, the two main projects run by the CPD or in collaboration with the CPD were the round robins on quantitative phase analysis (QPA) and on size–strain (SS) determination. Details and extensive reports can be found on the web pages.

(i) *Quantitative phase analysis*

During 2001, the results obtained during the previous year were published by I. C. Madsen and co-workers in an important publication appearing in *Journal of Applied Crystallography (JAC)*. Free reprints of this paper were distributed as an annex to *Newsletter* No. 25. A special budget was allocated thanks to the generous contribution of the commercial sponsors advertising in the *Newsletter*. Copies of the article can also be freely downloaded from the *JAC* web site and are also available through the CPD web site. The activity continues with the preparation of a second part of the round robin results, currently under refereeing for publication in *Journal of Applied Crystallography*.

(ii) *Size–strain analysis*

This project was mostly carried out in 2000. During 2001, the promoter and CPD member D. Balzar produced a detailed report on the results which should also appear soon as a publication in an IUCr journal. All the data are still available *via* the internet for free download. Several scientists have made use of the data sets provided by the round robin and results are now appearing in several publications. Specific presentations were given at the SS-III conference on this subject.

4.13.3. Web site. The CPD web site is still the reference point for powder diffractionists around the world. Besides links and information on events related to PD (including the CPD round robins) the web site gives free access to the CPD *Newsletter* archive, from which recent and past issues can be downloaded in pdf (Acrobat) and in doc (Word) formats. This initiative was extremely successful and greatly expanded the number of readers.

4.13.4. Newsletters. During 2001, two issues of the CPD *Newsletter* were published (see also the URL http://www.iucr.org/iucr-top/comm/cpd/index.html for downloading). The summer issue (No. 24) was edited by W. I. F. David and was entitled 'Structure Determination from Powder Diffraction Data', whereas the following fall issue (No. 25) was edited by R. Dinnebier and focused on 'Rietveld Refinement from Powder Diffraction Data'. These two issues can really be considered as important references for the state-of-the-art in PD. Newsletter No. 25 also included as an annex the paper on the QPA round robin: 'Outcomes of the International Union of Crystallography Commission on Powder Diffraction Round Robin on Quantitative Phase Analysis: Samples 1a to 1h' by I. C. Madsen, N. V. Y. Scarlett, L. M. D. Cranswick & T. Lwin [*J. Appl. Cryst.* (2001), **34**, 409–426]. The popularity of the computer software pages by L. M. D. Cranswick is still very high. These pages are highly appreciated by readers for their quick and effective presentation. News from ICDD and from the IXAS are also present in all issues, together with news on forthcoming events. Starting with summer 2001, the CPD *Newsletter* was assigned an ISSN number (1591-9552).

P. Scardi, Chair

4.14. Commission on Small-Angle Scattering

4.14.1. Commission Meetings. During July and August 2001, various members of the Commission were able to get together face-to-face in conjunction with the Los Angeles, USA, meeting of the ACA and the ICDD's Denver X-ray Conference in Steamboat Springs, Colorado, USA. The opportunity for extended interaction and discussions among this subset of the group proved to be very valuable. In the course of these meetings, the Commission dealt with the following topics.

(1) Commemoration of the passing of H. Brumberger. G. Kostorz delivered a very moving tribute at a session of the ACA Small-Angle Scattering Special Interest Group.

(2) Nominees to replace J. D. Barnes and G. Kostorz, who will be retiring from the Commission at the Geneva Congress. In renewing its membership, the Commission seeks to balance the need for 'institutional memory' with the need for new ideas.

(3) Plans for the Commission's activities at the Geneva Congress. These include two sessions and a workshop on 'Scattering Methods for Nanoscale Structure Characterization'.

(4) Means of establishing 'satellite' status for SAS 2002, Venice, Italy, 26–29 August 2002. The Commission was unanimous in its support of this idea. The idea had been considered in 1999, but a meeting in Venice did not meet the specifications for a proper satellite meeting. With the change of the IUCr Congress venue to Geneva, Switzerland, this idea was reopened and the necessary arrangements have been successfully concluded. Inasmuch as the SAS 2002 organizers were not fully familiar with IUCr procedures, issues regarding the financing of the support and the publication of the SAS 2002 proceedings needed to be worked out explicitly.

(5) Guidelines for the Commission's oversight role with regard to future triennial SAS Congresses. Prior to 1996, there was very little concern about efficient coordination between the SAS community and the IUCr with regard to Congress arrangements. Both events seemed to fall in the same part of the year, often on different continents. The Commission was established partly as a reaction to this situation. It was thought that the SAS community's Congresses would benefit from closer interaction with a larger body and that the SAS community as a whole would benefit from the technical experience of the IUCr in many areas.

The SAS Congresses had been organized since 1965 on a rotating basis with the major responsibility being passed from one member to another among a coterie of senior scientists. As the SAS Congresses become larger and as the informal organizing group loses members by attrition, it is apparent that a more formal approach must be taken. The members of the Commission have determined that its best role is as an advisory body to groups of researchers who seek to organize the Congresses in venues that are close at hand.

The Commission has posted a 'Call for Proposals' for the next Congress in the series ('SAS 2002+'). There has been no response as of April 2002, but the Commission expects to assist one or more groups of organizers in preparing a formal proposal that can be presented to the attendees at SAS 2002 and posted to the IUCr web space for an e-mail ballot by the entire community before the close of 2002.

(6) Technical issues. There has been considerable concern about poor practices for publishing experimental errors and error estimates for derived parameters from SAS experiments. Very few laboratories use the best available practices for estimating the precision and accuracy of SAS results. The Commission's efforts to come to grips with these matters have not been very fruitful.

4.14.2. Education. (1) J. S. Pedersen presented (i) Small-Angle Neutron Scattering as part of a NorFa course on The Use of Neutrons in Structural Studies of Crystalline and Disordered Materials, Uppsala, Sweden, 13–24 August 2001 and (ii) Instrumentation and Resolution Effects as part of a tutorial workshop on Small-Angle Scattering at the 50th Annual Denver X-ray Conference, Steamboat Springs, Colorado, USA, 30 July–3 August 2001.

(2) An EMBO Practical Course on Solution Scattering from Biological Macromolecules was held at EMBL Hamburg Outstation, 5–14 September 2001. The organizers were D. Svergun of the European Molecular Biology Laboratory, Hamburg Outstation, and R. Willumeit, GKSS Research Center, Geesthacht.

4.14.3. Other activities. (1) canSAS. J. D. Barnes represented the Commission at the canSAS III meeting in Grenoble, France, in May 2001. Efforts to make progress on standardization of data formats and analytical tools seem to be mired down in inertia and technical uncertainties regarding the NeXuS scheme for employing Hierarchical Data Format as a means of creating portable self-describing data sets. In the absence of analytical tools that actually work with the metadata from experiments, it is unlikely that anyone will alter their current practices.

The Commission's sasCIF format for 1D SAS data has been published [*J. Appl. Cryst.* (2000), **33**, 812–816], but has not yet seen widespread implementation.

The canSAS activity has been provided space on the SAS 2002 agenda in an effort to inform the wider community regarding these data standardization issues.

(2) Round Zero Round-Robin. This effort to establish the degree of agreement that exists among SAS laboratories is proceeding very slowly. Some of the original participants have dropped out, some have reported data that could not be interpreted for lack of supporting details, others have failed to follow the request to submit in the sasCIF format *etc*. This effort was directed at X-ray laboratories because there are many more of these. This is to be expected in a measurement system that is not based on the use of standards.

The results of this activity may serve to motivate the community towards a better appreciation of the needs for standardization and proper techniques for empirically characterizing precision and accuracy. Slow progress in such areas is not unusual.

(3) Other software development activities. CCP13 and NOBUGS are two noteworthy activities aimed at improving life for users of scattering methods by improving the software that is available to them. The 4th edition of NOBUGS will be held at NIST in November 2002. Retiring Commission Chair J. D. Barnes is a co-organizer. The CCP13 community, which has mainly been active in the UK, has begun to recognize the need for 'open source' software development as opposed to the distribution of precompiled binaries. It is hoped that other members of the Commission can become involved in these activities.

4.14.4. Communication. The Commission's web pages have been relocated to IUCr web space so that they can be more easily maintained after J. D. Barnes completes his retirement. A new mailing list/bulletin board system is expected to replace the existing NIST-operated listserver in the near future.

J. D. Barnes, Chair

4.15. Commission on Structural Chemistry

2001 was a busy year for the Commission. Most Commission activities centred on assisting in programme preparations for the Geneva Congress. The Commission collected suggestions for microsymposia topics, potential session organizers and plenary lectures that were then submitted to the programme Chair for consideration. The Commission Chair (J. Flippen-Anderson) served as a member of the International Programme Committee. In addition, two Commission members (G. Punte and L. Brammer) served as microsymposia organizers and four others (V. Belsky, J. Flippen-Anderson, T. W. Hambley and D. C. Levendis) served as co-organizers for microsymposia. As a result of the Commission's input and involvement, there will be a very strong structural chemistry presence in Geneva. Overall there will be more than 20 microsymposia and a number of plenary lectures on topics related to structural chemistry, including such diverse topics as small-molecule drug design, nanomaterials, coordination chemistry, twins, disorders, solid-state reactions, zeolites, crystal growth, recent advances in supramolecular chemistry, molecular recognition and enantioselectivity, self-organization and self-assembly of biomaterials and biomimetics.

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

A structural chemistry discussion group was started, on the IUCr web site, for the purposes of exchanging ideas and information within the community. The discussion group was established on an 'open' basis so that membership is not limited solely to members of the Commission. There has yet to be a large amount of 'discussion' among the members of the group and the Commission is exploring ways to make its existence more well known.

The Cambridge Structural Database passed 250,000 entries in 2001 and the rate of new entries continues to grow at a rapid pace. The Commission encouraged the Cambridge Crystallographic Data Centre to make incremental updates to the database available to be downloaded over the internet to registered users. This process went into β test late in 2001 and will become available to all users with the April 2002 release of the database. As the database continues to grow at an ever increasing rate, it becomes more and more important for coordinates to be deposited 'automatically' by journals. Discussions were held with Cambridge personnel on ways the Commission members might help convince more journals to send CIF files directly to Cambridge when papers containing X-ray structures are accepted for publication. The Commission also initiated a discussion on adding more terms to the small-molecule CIF dictionary to describe twinning and disorder so that information on these facets of a structure analysis could be easily captured by the database in a way that would facilitate searching.

A number of these issues, such as expansion of the CIF dictionary and automatic deposition of coordinates by the journals, are topics that will remain on the Commission's agenda as it moves forward into 2002.

J. Flippen-Anderson, Chair

4.16. Commission on Synchrotron Radiation

The Commission has been active in participating in the organization of various satellite-related conferences in connection with the Geneva Congress, and other meetings. In particular, it has been involved in the organization of the following two satellite meetings: (1) Crystal Chemistry of Materials and Soft Matter studied by Neutron Diffraction, 1–3 August 2002 at the ESRF–ILL site in Grenoble, France. This is a joint Neutron Scattering/Synchrotron Radiation Commission activity and the joint Commissions constitute the Programme Committee. (2) Neutron and Synchrotron X-ray Scattering in Condensed Matter Research, 4–6 August 2002 to be held at the Paul Scherrer Institute, Villigen, Switzerland. In this case, C. Vettier is representing this Commission on the International Advisory Committee.

Commission members have also been significantly involved in the work of the Programme Committee for the Geneva Congress and in the chairing (2) and co-chairing (1) of microsymposia. In addition, S. W. Wilkins was a member of the Programme Committee for the Third International Conference on Synchrotron Radiation in Materials Science (SRMS-3), 21–24 January 2002, Singapore. This meeting helped celebrate the recent commencement of operation of the Singapore Synchrotron Light Source (SSLS).

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

S. W. Wilkins, Chair

4.17. Commission on XAFS

No report 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 2001 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 2001 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2002, but approved in 2001, are listed below:

International School on Powder Diffraction, Calcutta, India, 20–23 January 2002.

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

School on Computer-Based Crystallographic Teaching Materials, Ismailia, Egypt, 2–7 February 2002.

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

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

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. A new Chair will be appointed in Geneva. For up-to-date contact information, see http://www.iucr.org/iucr-top/iucr/calendar.html.

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

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.

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

Following the unanimous proposition of the CEP, the IUCr's Executive Committee appointed S. Parsons of the University of Edinburgh, UK, to the CEP on 9 May 2001. S. Parsons has accepted the responsibility of the day-to-day running of **Crystallography Online**, the IUCr's information service.

6.1. Meeting attendance

Members of the CEP attended the following meetings.

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

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

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

H. D. Flack visited the IUCr editorial offices, Chester, UK, in early November 2001.

B. McMahon attended a meeting on XML Use in Chemistry in Cambridge, UK, January 2002.

Y. Epelboin attended a seminar on Digital Preservation of the Record of Science – State of the Art, UNESCO, Paris, France, 14–15 February 2002. H. D. Flack also attended as ICSTI Representative.

P. R. Strickland gave a short presentation on the IUCr's experience in selling journals to library consortia at a meeting of the Association of Learned and Professional Society Publishers in London, UK, on 19 February 2002.

The meeting attendances of B. McMahon as CODATA Representative and H. D. Flack as ICSTI Representative are recorded in their individual reports.

6.2. Information services

The CEP has continued its task as editorial body for the online information services of the IUCr. In May 2001, the task of day-to-day maintenance of **Crystallography Online** passed from H. D. Flack to S. Parsons. The former wishes to thank the IUCr for its active and continuing support for this project which saw the light of day during 1992 as part of the European Union's CONCISE project (see http://www.iucr.org/cww-top/crystal.mar95.html for details). As part of the changeover, a set of detailed maintenance instructions was prepared for the incoming editor. Discussions on the restyling of **Crystallography Online** took place during the CEP Chair's annual visit to Chester. A questionnaire was subsequently sent to those responsible for maintaining the mirror sites of **Crystallography Online** to obtain information and sound out opinion on matters such as advertising, perceived necessity of continuing with mirrors, and infrastructure at mirror sites.

6.3. *World Directory of Crystallographers* (WDC)

The new online interface of WDC 11 was launched in mid-December 2001. This enables individual crystallographers to update their own entry as and when necessary. New entries are checked by the Regional Editors before being accepted. The immediate result was a heavy overload on the equipment serving the database resulting in very slow response as many crystallographers simultaneously attempted to update their entries. The system had to be extensively reconfigured on the eve of a holiday period but was soon functioning correctly. At present there is still a steady stream of new entries and over 5,000 people have logged in or created new entries. A printed version of the directory of those who have logged in at least once is planned to be produced in late 2002.

6.4. NeXus CD-ROM

Under the continued leadership of L. M. D. Cranswick, 1,000 copies of a new version of the Xtal NeXus: Virtual Crystallographic Internet on CD-ROM version 8.32 were produced in October 2001. 400 of these were distributed free of charge at the AsCA meeting in Bangalore, India, and the rest through our usual channels of distribution. All of these CD-ROMs have now been distributed and at present individual CD-ROMs are being made on request. The CD-ROM is made available to laboratories and scientists with an interest in crystallography lacking adequate connection to the internet. The CD-ROMs contain public domain software and copies of web sites of interest to crystallographers. The CD-ROMs were publicized through many channels in such a way that scientists have to apply to receive a copy. We propose to continue this project and make further batches of CD-ROMs. The European Crystallographic Meeting in South Africa in August 2003 will be an ideal opportunity to find further markets for this popular product.

6.5. Crystallography Journals Online

It was possible in November 2001 to complete the project to make available online all back copies of IUCr journals six weeks ahead of schedule. By this action, the IUCr confirms itself as a prime publisher in the field of crystallography committed to providing online services. On 18 July 2001, the Executive Committee approved the document Archive Policy of the IUCr submitted by the CEP on which it had been working. Attention has been given to ways of improving the sale of the IUCr journals to consortia of libraries.

At the UNESCO meeting on electronic publishing, there were recurring calls for more openness in the refereeing process of journal articles. As a result, a discussion document IUCr Publishing Policy was prepared detailing developments in the definition of scientific publications (preprint *versus* final publication), comparing the characteristics of preprints and final publications, the acceptability of preprint manuscripts for journal publication, peer review (its operation and confidentiality), and the usefulness of a preprint service for crystallography. A part of this document, reformulated, was circulated to the Commission on Journals for consideration. It appears that there is only very modest interest in the establishment of a preprint server in crystallography.

6.6. Miscellanea

The IUCr's participation in an Ingenta study and developments in the field of crystalline phase descriptors are treated in the report of the Representative to ICSTI.

The CEP has participated in testing both the CD-ROM to accompany *International Tables* Volume D and the new templates for authoring journal articles.

The CEP maintains a watch on electronic publishing activities and initiatives of interest to crystallography. In particular, there are the IUPAC projects concerning chemical identifiers and the use of XML/CML and the Open Archive Initiative (OAI) with its metadata harvesting protocol, which is of interest in linking together information found in heterogeneous databases.

H. D. Flack, Chair

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

7.1. Introduction

COMCIFS is the Committee appointed by the Executive Committee to oversee the Crystallographic Information File project (CIF) on behalf of the Union. It is composed of six voting members appointed by the Executive Committee on the recommendation of COMCIFS following each General Assembly. In addition, the Chair of COMCIFS appoints others to the COMCIFS discussion list, all of whom can participate in the work of COMCIFS. Only the voting members make decisions on CIF policy.

7.2. Membership

The voting members during 2001 were I. D. Brown (Chair), B. McMahon (Secretary), H. M. Berman, H. J. Bernstein, S. R. Hall and G. Madariaga.

7.3. Current status of CIF

It is now over a decade since the Crystallographic Information File (CIF) was adopted by *Acta Crystallographica* for the submission and archiving of crystal structures. When it was first adopted, CIF was intended to provide a common format for electronic submission of crystal structure reports to the Union journals, which would then archive them and make them available to their subscribers in computer-readable form. Since these modest expectations were first adopted, CIF has evolved from a simple file structure towards a crystallographic language in which the knowledge of the discipline is contained in computer-readable dictionaries. We anticipate that in a few years all crystallographic information will be handled by generic programs using CIF as the underlying language, with the dictionaries providing the necessary base of crystallographic knowledge.

A review of the 12 year CIF archive accumulated by *Acta Crystallographica* has revealed that many of the CIFs do not strictly conform to the standard. While this does not cause serious problems with the limited way in which CIFs are currently used, it will present difficulties for the advanced CIF applications that are currently being developed. The review has also revealed a number of improvements needed in the core dictionary. The Protein Data Bank (PDB) has addressed similar problems by developing an extension to the mmCIF dictionary to address issues of data exchange and the conversion of the historical PDB format to CIF.

7.4. Status of CIF dictionaries

The current strength of CIF lies in the extensive suite of dictionaries that have been developed. These dictionaries, and their underlying structure, put CIF at the leading edge of information technology. No other discipline is as well equipped with such a computer-based language. Currently there are six approved dictionaries and advanced drafts are available for three more. Each of the approved dictionaries has a Dictionary Maintenance Group composed of members of its respective community. Their job is to monitor the use of the dictionary and propose any needed revisions.

No changes have been made during 2001 in the macromolecular, powder and image dictionaries. Minor additions were approved in the core dictionary in January 2001 but a major review of this dictionary is planned for the coming year in order to address the problems raised by *Acta Crystallographica* and the Cambridge Crystallographic Data Centre. Two new dictionaries have been approved. The first defines items needed to describe modulated structures (msCIF.dic approved in July 2001) and will be used, *inter alia*, for reporting incommensurate and modulated structures to *Acta Crystallographica*. The second, symCIF.dic (approved in December 2001), provides an extensive and coherent list of items needed to describe crystal symmetry. These will replace and extend the symmetry items currently included in the core and mmCIF dictionaries. Advanced drafts exist for three further dictionaries, namely magnetic structures, electron densities and small-angle scattering, the last two sponsored by IUCr Commissions.

7.5. Software

While the extensive suite of approved dictionaries places the crystallographic community among the leaders in advanced information technology, there has not been a commensurate development of software to make use of the knowledge they contain. Many existing crystallographic programs are being modified to read and write CIFs, but so far there are few programs that extract their knowledge directly from the dictionaries rather than having this knowledge built into the program code. The notable exception is the PDB which has developed an extensive collection of software tools that make use of data dictionaries. These include editing tools, validation tools and format conversion tools, all of which are dictionary driven. General purpose software tools in C/C++/JAVA/Perl are also distributed by PDB to access mmCIF and mmCIF dictionaries. Other dictionaries are currently less well supplied with dictionary-driven software and represent a challenge to the programming community.

A possible short-term solution is to interface CIF to XML (extensible markup language), the standard developed by the information technology community. XML is a widely supported syntax and the existence of CIF to XML conversion routines opens the door to a broader range of applications and users.

7.6. Interoperability

It is important that CIF be compatible with other developments occurring in information technology. A chemical markup language (CML) is being developed within XML and the ability to convert CIF to XML is one way in which the chemical community will be able to access crystallographic information. The Research Collaboratory for Structural Bioinformation has encouraged related disciplines to develop dictionaries that are fully compatible with CIF, and standards based on CIF have been adopted for the interchange of structural information between molecular biology databases (http://deposit.pdb.org/mmcif/).

7.7. Intellectual property rights

The CIF standard is owned by the IUCr in order to prevent the development of CIF dialects. We encourage the widespread use of CIF for both crystallographic archives and software and do our best to help those who have difficulties in following the standard.

7.8. Advanced concepts in CIF

Currently under development is an advanced dictionary language that will both simplify and extend CIF and should, in the longer term, remove the incompatibilities between existing dictionaries. Chief among the new features is the inclusion of computer-readable definitions in the form of algorithms that will allow an application to calculate any item of crystallographic information from the basic experimental information contained in a CIF. This will revolutionize crystallographic computing since testing a new algorithm will be as simple as adding a new item to the dictionary. Strict compliance with the standard is needed for these advanced applications, and educating the user community about this need is one of the tasks of COMCIFS.

7.9. Publicity

All CIF dictionaries and the discussions of COMCIFS and many of its committees are accessible on the IUCr web site. In addition, reports from COMCIFS appear in the *IUCr Newsletter*. Our best publicity comes from the interaction of the user community with *Acta Crystallographica* and the Protein Data Bank which use CIF as their preferred or required mode of submission. Other databases and many crystallographic programs provide CIF outputs, all of which help to spread the knowledge of the standard throughout the community. An open COMCIFS meeting is planned at the Geneva Congress to draw attention to new CIF developments.

I would like to thank the large number of people who have volunteered their time and expertise in order to develop the CIF dictionaries and software. The cooperation and collaboration of the IUCr staff has been particularly important to the success of the project.

I. D. Brown, Chair

8. Committee on Crystallographic Databases

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

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

F. H. Allen, Chair

9. Promotion Committee

The year witnessed two milestones for the IUCr journals: the launch of *Acta Crystallographica* Section E: *Structure Reports Online* in January (and its subsequent selection for inclusion in the ISI Web of Science®)] and the completion of the back-issue digitization project in November. The Promotion Committee's Working Group on Journals, enthusiastically and effectively chaired by J. R. Helliwell, has been instrumental in publicizing these events throughout the crystallographic community through the journals themselves, the *IUCr Newsletter* and web site, promotional leaflets and exhibition posters, e-mail announcements, direct mail and press releases. The digitization of all back issues to 1948 has opened up the exciting prospect of 'themed CD-ROMs'; the Promotion Committee considered a long list of suggestions at ECM-20, and the first of these collections will be available at the Geneva Congress.

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

2001 also saw the publication of the second edition of *International Tables for Crystallography* Volume B and the first edition of *International Tables for Crystallography* Volume F, and work began on inviting non-IUCr journals to review these books. As a new publication, Volume F was extensively advertised in *Acta Crystallographica* Section D and the *IUCr Newsletter*, and promoted to the structural biology community through the above-mentioned leaflet. An *International Tables* order form downloadable from the IUCr web site has proved effective.

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

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

A. M. Glazer, Chair

10. *IUCr Newsletter*

Four issues of the *IUCr Newsletter* were printed in 2001. Each contained 32 pages. 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.

Each issue devoted two or three pages to brief summaries of selected articles recently published in IUCr journals. Articles of particular interest in Volume 9 (2001) were the Call for Papers for the Geneva Congress, a report of the activities of the Commission on High Pressure, the Protein Data Bank, and the Cambridge Structural Database. 34 meeting reports from 20 different countries, announcements of 22 future meetings in 14 countries, and 10 obituaries of prominent crystallographers in 8 countries were published. The letter column featured an exchange of opinions concerning electron and X-ray diffraction measurements of charge density in a metal complex.

The mailing list was maintained with little change in total circulation. 18 countries continue to assist in the effective and economic distribution of the *Newsletter*. Sustained advertising volume coupled with efficient production has kept the cost to the IUCr below USD 35,000 for the year.

W. L. Duax, Editor

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

The following books were published in 2001: (i) *The Basics of Crystallography and Diffraction*, 2nd edition, by C. Hammond; (ii) *Dynamical Theory of X-ray Diffraction*, by A. Authier; (iii) *The Chemical Bond in Inorganic Chemistry*, by I. D. Brown.

12. Regional Associates and Scientific Associates

12.1. American Crystallographic Association (ACA)

The ACA annual meeting for 2001 held in Los Angeles, California, was scientifically and financially successful. The meeting was attended by 931 crystallographers. The programme included 476 abstracts, 33 half-day oral sessions and four workshops. The workshops were on the topics of Interactive Single-Wavelength Anomalous Scattering Methods, Real-Space Pair Distribution Function Methods, Atomic Force Microscopy of Crystal Surfaces, and Neutron Diffraction. The Transactions Symposium was on High Throughput Crystallography. The Fankuchen Award was presented to J. M. Stewart, the ACA's Public Service Award was presented to C. Cole, Science Editor of the *Los Angeles Times*, and the ACA Service Award was presented to J. R. Deschamps. A Memorial Session was held for H. Brumberger.

Student travel awards totalling USD 23,900 were presented to 55 participants.

The ACA contributed financial support to the 2001 Summer Crystallography School in Athens, Georgia, and the 2001 Physics Olympiad. Four issues of the *ACA Newsletter* were published. Volume 35 of the *ACA Transactions*, Using Crystallography to Understand Enzyme Mechanism, edited by D. H. Ohlendorf and D. Ringe is now in print. The final total membership for 2000 was 1,860 (1,461 regular, 159 student, 211 retired and 29 corporate).

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

W. L. Duax, IUCr Representative

12.2. Asian Crystallographic Association (AsCA)

The 4th AsCA Meeting was held at the Indian Institute of Science in Bangalore, India, 18–21 November 2001. The IUCr President, Professor H. Schenk, and General Secretary and Treasurer, Professor S. Larsen, attended the meeting. A Keynote Lecture was given by Professor Schenk; four plenary lectures, 10 microsymposia and 290 posters were presented.

The Council meeting was held on the afternoon of 19 November. The members of 11 among 17 countries attended the meeting. Professor M. Vijayan, the Chair of the Local Organizing Committee, reported that full participants from foreign countries and India numbered 160 and 260, respectively. He pointed out that, owing to the events of 11 September, a significant number (>50) of participants from countries outside India had cancelled their registrations. The scientific programme was affected by the withdrawal of a number of scheduled speakers, resulting in some alterations to the programmes for oral presentations. In this context, he also reported on the cancellation of the satellite meeting on powder diffraction, which had been scheduled to be held in Calcutta prior to AsCA '01. The meeting on Crystallography and Bioinformatics in Structural Biology was to take place as scheduled in Bangalore following the main conference, with more than 370 registered participants.

The following items were discussed, though the final decisions will be made at the ninth Council meeting during the IUCr Geneva Congress.

(1) *Future AsCA meetings*. The council discussed the proposal by the President, Professor Y. Ohashi, that, in addition to the normal AsCA meetings, AsCA meetings should also be held in conjunction with the meetings of the Society of Crystallographers in Australia and New Zealand (SCANZ) and the Crystallographic Society of Japan (CrSJ), so that AsCA members would have the opportunity to confer as a body twice in three years. Professor S. R. Hall spoke in favour of the proposal and suggested that the upcoming Crystal-23 meeting of SCANZ, to be held in Broome, Western Australia, in August 2003, be the first such meeting to be jointly hosted by AsCA. It was noted that SCANZ meetings normally attract around 100 participants. A workshop on Biological Structure and a Sagamore Meeting, run by the IUCr Commission on Charge, Spin and Momentum Densities, would be associated with Crystal-23 and would provide additional opportunities for participation of AsCA members.

In discussion, it was stressed that it would be important not to lose the unique quality of the triennial AsCA meetings and that this could be achieved by flexibility in the timing of both the meetings and by maintaining the excellent rates of student participation.

(2) *Timing of AsCA elections*. A second proposal from the President's report concerned the timing of the election of officers and selection of venues for forthcoming AsCA meetings. Traditionally, both had been done at the triennial IUCr Congress, a situation that arose from the fact that, when the Association was inaugurated, there were no AsCA conferences. There was general agreement that such important decisions would be more appropriately made in Council meetings held at AsCA conferences. In particular, this would ensure more inclusive representation of Councillors throughout the region. It was also noted that it may be necessary to make minor changes to the Constitution of the Association to incorporate this process. Proposals for such a change would be brought to the next Council meeting.

(3) *Location of AsCA '04*. It was proposed that the next AsCA meeting, AsCA '04, be held in Hong Kong, People's Republic of China. The representative from Hong Kong, Professor I. D. Williams, indicated that Hong Kong was still anxious to hold the meeting but that there would be logistical problems if the meeting were to be held at the traditional time of October/November. In discussion, it was agreed that the Association needed to be flexible over the meeting time as it was clearly impossible to pick an ideal time that suited all participants. It was proposed that representatives from Hong Kong provide Councillors with a detailed proposal with dates and a venue for the conference before the next Council meeting. A final decision would then be taken in Geneva.

(4) *New AsCA Council member*. The application from crystallographers in Mongolia for their country to join the Association was approved unanimously.

M. Tanaka, IUCr Representative

12.3. European Crystallographic Association (ECA)

The main ECA meeting, ECM-20, took place in Krakow, Poland, 25–31 August 2001, and was organized by crystallographers from the Jagiellonian University in collaboration with scientists from Stanislaw Staszic University of Mining and Metallurgy. The scientific programme comprised 15 plenary lectures, 59 microsymposia and 400 posters. 720 participants registered and 24 exhibitors were present. Six satellite meetings were also organized: (i) International Symposium on Organic Crystal Chemistry, 20–24 August, with 70 participants; (ii) International Symposium on Synchrotron Crystallography, 31 August–4 September, with 60 participants; (iii) International Seminar on Inclusion Compounds, 1–5 September, with 80 participants; (iv) International Conference on Liquid Crystals, 3–7 September, with about 60 participants; (v) Protein Crystallography beyond 2000, 1–2 September, with about 60 participants; and (vi) Aperiodic Structures, 1–6 September, with about 60 participants.

The second ECA Prize was awarded to Professor J. R. Schneider of HASYLAB at DESY, Hamburg, Germany, during the opening ceremony of the ECM. Greece and Turkey applied for ECA membership, increasing the number of National Members to a total of 30. Contacts for possible membership of African countries – Tunisia, Algeria, Morocco, Cameroon, Senegal and Kenya – are in progress. Osmic and Macromolecular Simulations were also approved as new Corporate Affiliate Members adding up to a total of 8 such members. 10 Special Interest Groups (SIGs) are formally constituted and reported their operation. The possibility of forming a new SIG on Crystallography under Extreme Conditions was discussed and progress outlined.

The news and information Newsletter from the Executive Committee, *ECANEWS*, was assigned an Editorial Committee.

ECM-21, to be held in Durban, South Africa, in 2003, is being prepared and will be coordinated by Professors A. Roodt and D. C.

Levendis. ECM-22 will be held in Budapest, Hungary, in August 2004. For ECM-23, a choice between two proposals, Darmstadt, Germany, and Leuven, Belgium, will be made during the ECA Council meeting at the IUCr Geneva Congress.

M. A. Carrondo, IUCr Representative

12.4. International Organization of Crystal Growth (IOCG)

The International Conference on Crystal Growth (ICCG-13) took 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) took place 24–29 July 2001. These are certainly the two events that more deeply characterized the life of the IOCG and were both very successful. It is worth mentioning that ICCG-13 attracted over 1,200 delegates, which is approximately twice the number of participants at the previous meetings of the IOCG.

Following tradition, during the conference two scientists who gave outstanding contributions to either fundamental (Frank Prize) or technological (Laudise Prize) aspects of crystal growth were honoured. The Frank Prize was jointly assigned to Professor D. Hurle and Dr S. Coriell for their great contribution to 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 was awarded to Professor G. Mueller for his contributions to the development of technological aspects and computer modelling of crystal growth processes.

The IOCG Council Meeting was held 1 August 2001 and discussion led to the following conclusions: (i) a short discussion identified the need for an IOCG Representative to IUPAP; (ii) ICCG-14/ICVGE-12 will be held in Grenoble, France, and ISSCG-12 will be held in Berlin, Germany, in summer 2004; (iii) possible hosts of ICCG-15 (in 2007) were discussed – a vote was taken to accept the US proposal and G. Stringfellow (proposed Chair of the conference) presented a brief description of plans to the Council; and (iv) there have been two proposals for hosting ICCG-16 (2010) – one formal inquiry was from the Polish Association of Crystal Growth while the second was an informal e-mail inquiry from China.

The Officers and Executive Committee for the triennium 2001–2004 are as follows: President: R. F. Sekerka (USA); Vice Presidents: K. W. Benz (Germany), J. P. Van der Eerden (The Netherlands); Secretary: T. F. Kuech (USA); Treasurer: T. Ohachi (Japan); Past President: T. Nishinaga (Japan); Honorary Principal Founder IOCG: M. Schieber (Israel). Executive Committee: T. Duffar (France), R. Fornari (Italy), Jiang Min-Hua (China), G. Mueller (Germany), V. V. Osiko (Russia), M. Roth (Israel), K. Sato (Japan), J. N. Sherwood (UK).

Among the future activities of the IOCG, R. F. Sekerka, the new President of IOCG, mentioned: (i) maintain continuity in ICCG and ISSCG organization and execution; (ii) create an IOCG web site for a 'continuous existence in cyberspace'; (iii) consider IOCG funding of expenses associated with Laudise and Frank Prizes, specifically the paying of travel expenses for winners; and (iv) consider expanding finances of IOCG by some type of membership tax on national organizations. During 2001, the President and Executive Committee of IOCG have also started exploring the possibility for IOCG to become an International Union to be affiliated to ICSU.

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

R. Fornari, IUCr Representative

12.5. International Centre for Diffraction Data

As for the previous year, R. L. Snyder represented the ICDD at the CPD meetings, and now also the International X-ray Analysis Society (IXAS). During the 2001 CPD meeting, R. L. Snyder reported on the many PD related activities carried out by the two organizations (information is available *via* the ICDD web site http://www.icdd.com/ and the IXAS web site http://www.ixas.org/). It is still a main target of the CPD to maintain active collaborations and positive relationships with these organizations.

P. Scardi, IUCr Representative

13. Representatives on Other Bodies

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

The IUCr, together with the Bureau International des Poids et Mesures (BIPM), the International Organization for Standardization (ISO) and four other International Unions [of Biochemistry and Molecular Biology (IUBMB), Nutritional Sciences (IUNS), Pure and Applied Physics (IUPAP), and Pharmacology (IUPHAR)] are represented on IDCNS as the body charged by the International Union of Pure and Applied Chemistry (IUPAC) with responsibility for ensuring that all recommendations concerned with terminology, nomenclature and symbols made in its name are consistent with its own and other international standards. IUPAC recommendations are published in *Pure and Applied Chemistry* following revision and final acceptance. A total of 65 such documents passed through IDCNS hands in the year 2001. The annual IDCNS meeting was held in Brisbane, Australia, in association with the 41st IUPAC General Assembly. In the interests of economy, Professor D. C. Creagh, University of Canberra, Australia, kindly stood in for the Representative at Brisbane.

Among matters of interest to crystallographers discussed in Brisbane were several additions to the recommended use of italic and roman fonts for symbols in scientific text; an earlier version of the rules may be found in http://www.iupac.org/standing/idcns/fonts_for_symbols.html. A draft quick-reference table to determine which fonts, for a wide range of symbols, should be used in a document was returned for improvement. Correct font usage in inorganic, organic, macromolecular and biochemical nomenclature will be presented later, in a single page. Proposed IDCNS guidelines on quantity calculus, the printing of numbers and the use of terms such as % and p.p.m. that are consistent with *Quantities, Units and Symbols in Physical Chemistry*, 3rd edition, were presented. It was reaffirmed that dates should follow the standard ISO 8601, in which the order is yyyy/mm/dd. A Working Party has made substantial progress on a 'Glossary of Terms in Pharmaceutical Process Chemistry', another on a 'Handbook on Pharmaceutically Acceptable Salts'. BIPM had proposed the use of 'uno' for denoting the unit of one, when used in relation to dimensionless quantities, to its Council but this was returned for further consideration. It was agreed that the 'Gold Book' (*Compendium of Chemical Technology*) should be modified for web delivery.

IUPAC has now restructured IDCNS to become the Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS). The change recognizes 'terminology' as part of the charge and the restructuring has added titular and associate members and provided a clear connection between the Committee and each Division Committee to ensure that all documents for publication are adequately reviewed.

S. C. Abrahams, IUCr Representative

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

The IUCr Representative attended the following ICSTI meetings.

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

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

Seminar on Digital Preservation of the Record of Science – State of the Art, UNESCO, Paris, France, 14–15 February 2002. (Y. Epelboin also in attendance.)

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

From the presentation of the planning of the Ingenta study on Research into the Relationship between Journal Subscriptions and Document Delivery and the Impact of Online Delivery on Article Distribution, it turned out that the IUCr would be able to contribute to this study by providing data on some of its own journals. The detailed results on these were made available at the conclusion of the study. The IUCr's Managing Editor, P. R. Strickland, attended the public presentation of the whole study in London on 25 September 2001.

Progress on the IUPAC–CODATA–ICSTI project on the Standardization of Physico-Chemical Property Electronic Datafiles (IUCODIX), which seeks to bring to the world of physical chemistry the advantages that CIF has brought to crystallography, has shown up a problem in the nomenclature of phase identifiers for crystals. An existing nomenclature proposal entitled Structural Phase Transition Nomenclature produced by an IUCr working group [Tolédano *et al.* (1998). *Acta Cryst.* A**54**, 1028–1033] is not of a nature nor in a form to generate unique identifiers suitable for use in the constitution of crystalline-phase property databases. Following communication of these comments to the IUCr's Commission on Crystallographic Nomenclature and a subsequent preliminary and thoughtful exchange of views amongst interested parties, a working group has been constituted under the auspices of the IUCr's Commission on Crystallographic Nomenclature to study this matter in detail and to come forward with concrete proposals to resolve the problem. It is of interest to report that within the IUCODIX project an attempt was made to establish identifiers for physico-chemical properties associated with an appropriate resolving mechanism in the way that CrossRef (http://www.crossref.org) coupled to DOIs (digital object identifiers) operates for locating electronic journal articles. There was insufficient interest from commercial partners to proceed with the establishment of physico-chemical property identifiers for the moment. Moreover, two current IUPAC projects in the field of electronic publishing and databases have relevance to crystallography. The first is the Chemical Identifier project (IChI), which seeks to develop a public-domain inversible identifier for molecules. In its current stage of development, the identifier is coded in XML and is claimed to work for a large proportion of molecules. The use of XML allows a clear syntax and structuring of the identifier enabling efficient searching. Other typographic formats of the identifier may be developed subsequently. The other IUPAC project concerns the development of chemical markup language (CML). These projects are closely monitored by the IUCr's Representatives to ICSTI and CODATA, and by the IUCr's Sub-Committee on Electronic Publishing, Dissemination and Storage of Information.

Within ICSTI, there have been exchanges of views concerning the EU copyright directive which gives much power and freedom to database generators. As reported elsewhere, this topic was the subject of a one-day workshop preceding the CODATA annual meeting. Moreover, ICSU itself is concerned about the implications of the EU directive on copyright and ICSTI has received correspondence from ICSU's President on this matter. The topic will be followed closely within ICSTI.

The ICSU Navigator for Primary Scientific Publications has been prepared by ICSU's Committee on Dissemination of Scientific Information (ICSU Press). The main goal of this project is to create a representative source of information on the primary scientific publications in all disciplines covered by the International Council for Science (ICSU). In fact, **Crystallography Online** already provides such a service for crystallography and it was not felt useful to make use of the ICSU Navigator.

The preservation of the world's cultural heritage in digital form is becoming a subject of concern in many quarters. Thus UNESCO has announced its own programme, the current (Spanish) Presidency of the EU is using its power to propose resolutions to the EU ministers of culture, a CODATA data archiving working group has been established, and position papers have been drafted by UKOLN, CIMI and Resource group in the United Kingdom. ICSTI has decided to take action in the advocacy of the digital preservation of the record of science. A consultant (an ICSTI former President) has been appointed to draft a white paper for discussion at the meeting in Stockholm, Sweden. The intention is that, in its final form, this position paper will be of use in convincing those holding political power of the necessity of digital preservation and the need for resources to achieve it. Another aspect of preservation will come up at the IUCr's Geneva Congress where the Commission on Crystallographic Computing is devoting a session to software archiving and preservation.

13.2.1. Publications. ICSTI maintains a public web site at http://www.icsti.org/, where the newsletter *ICSTI Forum*, published three times in 2001, 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 Sub-Committee on Electronic Publishing, Dissemination and Storage of Information (CEP). Of particular interest to the IUCr, *Forum* No. 38 (June) presented articles on digital generation and preservation and a compendium of some of the acronyms used in the STM industry. No. 37 (March) contained an enlightening article on the interplay between primary scientific and patent literature and No. 39 (September) contained the text and slides of some of the presentations at the annual meeting in Munich, Germany. A distribution list operates where the ICSTI Executive Director distributes news clips and other information.

In 2002, the ICSTI annual meeting will take place in Stockholm, Sweden, 15–19 June, organized and sponsored by the Royal Institute of Technology Library. The IUCr will be represented by its Managing Editor, P. R. Strickland. As part of the ICSTI effort, the meeting includes a one-day public conference entitled Scientific Information: the Challenges of Creating and Maintaining Access. In 2003, the winter meeting will probably take place in Paris, France, and the

annual meeting will be in Ottawa, Canada, organized and sponsored by CISTI (Canadian Institute of Scientific and Technical Information). ICSTI is composed of a large spectrum of professionals from the STM and library sectors but with few scientists present. IUCr membership of ICSTI continues to fulfil its expectations by providing a source of current documentation and personal contacts in the field of scientific and technical information (electronic publishing).

H. D. Flack, IUCr Representative

13.3. International Council for Science (ICSU)

A meeting of International Union Presidents took place in Paris, France, in February 2001. An outcome of this meeting was the decision of ICSU to play an increased role in scientific debate on issues of significant scientific and public interest. During the past year, some 20 topics have been chosen for the preparation of position statements. These range from issues of great public interest, such as GM foods, human cloning and gene therapies, to others such as gene patenting, access to data and databases, and the value of basic sciences. Unions are invited to contribute on these topics, and it is hoped that some can be prepared before the ICSU General Assembly in Rio de Janeiro, Brazil, in September 2002. One that is of immediate interest to IUCr members is the topic of access to data and databases.

E. N. Baker, IUCr Representative

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

A compendium on ICSU activities in capacity building is being prepared by the ICSU secretariat. The IUCr Representative received no communications in 2001.

K. El-Sayed, IUCr Representative

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

CODATA hosted or sponsored the following meetings during 2001:

– A joint workshop with the Taxonomic Database Working Group of the International Union of Biological Sciences at Santa Barbara, California, USA, 11–13 June 2001, on Biological Collection Data Access. The focus of the working group is the development of an XML schema for biological collection units, embodying tagging of semantic content (*cf.* CIF dictionaries in crystallography or the CML chemical markup language). Development of a common software architecture to support distributed queries across collection databases is another goal, also of interest in the context of interdisciplinary distributed database searches.

– A European Science Foundation course in Functional Genomics: Curation of Databases in Molecular Biology, Paris, France, 11–14 October 2001. Proper annotation of the first-class primary data from structural genomics and other biomedical projects is often perceived as a weak point in the long-term archiving of information, and a number of strategies and commentaries to counter this were presented. Among the presentations was an account of the mmCIF format for macromolecular crystal structures.

– An international workshop on Information and Infrastructure for Science and Technology in Zurich, Switzerland, 12–13 October 2001. Participants from eight countries emphasized the interest in CODATA of promoting knowledge infrastructure (reliability of data, documentation, function, services *etc.*) as a key to effective international use of data collections.

Three Task Groups met formally.

– The Task Group on Fundamental Constants continues to work on revisions to the CODATA recommended values of the fundamental physical constants.

– An inaugural meeting of the Task Group on Data on Natural Gas Hydrates took place in Paris, France, to determine how to establish a comprehensive information system of all aspects of natural gas hydrates.

– The Task Group on Data Sources in Asian and Oceanic Countries held a joint forum on Taxonomy Initiatives for Biodiversity Conservation in an IT Era with Species 2000 in Tokyo.

The IUCr Representative to ICSTI introduced by e-mail a discussion between H. Kehiaian, the project leader of the IUPAC–CODATA Task Group on Standardization of Physicochemical Property Datafiles, and several members of the IUCr Commission on Crystallographic Nomenclature. The discussion concerned the need for a nomenclature of phases suitable for identification of the same phase across heterogeneous databases, and has prompted the appointment of a working group within the Commission to revisit the topic of phase nomenclature.

The *Ad Hoc* Working Group on Archiving Scientific Data, established during the CODATA 2000 General Assembly, has established a web site at http://www.nrf.ac.za/codata/ with a substantial list of resources relating to digital archiving.

The IUCr Representative's description of the Union's web services as presented to the CODATA 2000 conference was published in the online Proceedings at http://www.codata.org, and an expanded version was invited for the inaugural issue of the CODATA journal *Data Science*.

While the alternate years in the CODATA Schedule between General Assemblies are often less active, it is clear that as a body it continues to reflect the current major interdisciplinary issues of archiving, interoperability, portable tagging of data semantics, maintenance of data quality, and legal issues of access to and ownership of data. As such, it is an important body for the IUCr to be involved with at this time of rapid technological development.

B. McMahon, IUCr Representative

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

COSTED-IBN is an advisory body to ICSU, with a primary focus on the needs of developing countries. A review of COSTED is currently in progress. No further communications concerning COSTED were received during the past year.

E. N. Baker, IUCr Representative

13.7. ICSU Committee on Space Research (COSPAR)

As reported by its Chair, Professor G. Haerendel, 2001 was a quiet year from both administrative and scientific points of view. In the administration, the major change was in January 2001 when a new Executive Director was appointed by COSPAR. The new Director is Dr I. Revah, formerly at the French Centre National d'Etudes Spatiales.

Regarding space science, there were few major launch events but nevertheless the harvest of new scientific insights was rich: the discovery of what lies beneath a sunspot and the new information on the Earth's magnetosphere, for example.

A meeting of the COSPAR Bureau was held in Paris, France, in April 2001. In addition to a number of items strictly related to COSPAR life (budgets, categories of membership, administrative questions), the discussion focused on the next COSPAR Scientific Assembly, which will be held in conjunction with the 2nd World Space Congress, Houston, USA, 10–19 October 2002.

The preliminary programme of the Congress and all relevant information (deadlines, applications for travel support *etc*.) may be found in *COSPAR Bulletin* Nos. 151 (August 2001) and 152 (December 2001).

R. Fornari, IUCr Representative

14. Finances

The audited accounts of the year 2001 are given at the end of this Report. For comparison, the figures for 2000 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 2001 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, an apparent loss has arisen on the assets of the Union, in terms of CHF, amounting to CHF 380,429. The loss attributable to investment activities has been assigned to the General Fund and the loss attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2001. It should be noted that this loss in CHF is not a real loss of money, but rather a loss on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2001.

The balance sheet shows that the assets of the Union, including the loss of CHF 380,429 resulting from fluctuations in rates of exchange, have decreased during the year, from CHF 6,763,941 to CHF 5,553,575. The decrease in assets is largely attributable to the poor performance of the stock markets in 2001 and to the investments made in developing **Crystallography Journals Online**, the digitization of all back issues of the journals and in producing the new and revised volumes of *International Tables for Crystallography*. The movement in market value of the investments was CHF −563,263 in 2001 (CHF −863,121 in 2000).

A transfer of CHF 200,000 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 100,000 was made to the Research and Education Fund from the *Acta Crystallographica* Fund. Transfers of CHF 25,000 and CHF 25,000 were made to the *Newsletter* Fund from the General Fund and the *Journal of Applied Crystallography* Fund. A transfer of CHF 75,000 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 deficit of CHF 329,961 before the transfers totalling CHF 25,000, as compared with a surplus in 2000 of CHF 23,868 before transfers totalling CHF 25,000. The administrative expenses were CHF 405,597 in 2001 as compared with CHF 433,818 in 2000. Of this amount, CHF 177,884 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 3,840. The cost of the Finance Committee meeting held in 2001 was CHF 12,854, while the Executive Committee meeting cost CHF 54,892. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 8,353. The Union received CHF 8,656 from the UNESCO subvention to ICSU. The subscriptions from Adhering Bodies were CHF 164,998. Interest on bank accounts and investments credited to the General Fund was CHF 141,183.

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 3,207. Grants totalling CHF 5,196 were paid from the fund.

The *Acta Crystallographica* account for 2001 shows a surplus of CHF 420,646 before the transfer of CHF 575,000 to other fund accounts, as compared with a surplus of CHF 246,067 in 2000 before transfers of CHF 740,000.

The subscription rates were increased for 2001. In 2001, the number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 43 (43) personal subscriptions, was 497 (525) (values for 2000 are given in parentheses). The number of paid subscriptions to *Sections A+B+C*, including 17 (12) personal subscriptions, was 127 (120). The number of paid subscriptions to the separate sections of the journal were: *Section A* 232 (236 for 2000), *Section B* 170 (186), *Section C* 144 (150) and *Section D* 254 (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*, the *International Tables* and the Book Fund accounts in percentages based on the staff time spent on each publication. The technical editing costs for *Acta Crystallographica* were CHF 1,013,651 (for 7,162 published pages) as compared with CHF 1,172,552 in 2000 (5,678 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 91,148, as compared with a surplus of CHF 28,885 in 2000. In 2001, the number of paid subscriptions, including 114 (100 in 2000) personal subscriptions, was 708 (715 in 2000).

The *Journal of Synchrotron Radiation* account shows a surplus of CHF 9,977 before receiving a transfer of CHF 75,000 from the *Acta Crystallographica* Fund, as compared with a deficit of CHF 85,270 in 2000 before receiving a transfer of CHF 150,000. In 2001, the number of paid subscriptions, including 108 (104 in 2000) personal subscriptions, was 259 (252 in 2000).

The *International Tables* account shows a deficit of CHF 271,046, as compared with a deficit of CHF 319,096 in 2000. The net sales income was CHF 167,706 in 2001 as compared with CHF 82,608 in 2000. The deficits in 2000 and 2001 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.

The Book Fund is credited with the sales of the remaining publications of the Union. The deficit of CHF 72,875 is attributable to the significant amount of programming time involved in the restructuring and updating of the *World Database of Crystallographers*, which is used to produce the *World Directory of Crystallographers*.

The *Newsletter* Fund account received transfers of CHF 25,000 from the General Fund and CHF 25,000 from the *Journal of Applied Crystallography* Fund in 2001 (CHF 25,000 from the General Fund and CHF 50,000 from the *Acta Crystallographica* Fund in 2000). The cost to the Union of producing the *Newsletter* in 2001 was CHF 36,429 (CHF 53,561 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 includes interest as well as transfers from other fund accounts. In the Publications and Journals Development Fund account, the computer and promotion expenses are divided between the General Fund, the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Journal of Synchrotron Radiation* Fund and the *International Tables* Fund. STAR/CIF costs, Special Issue costs and web input costs are also charged to the Publication and Journals Development account. From 2000, costs associated with the Crystallographic neXus Project to provide CD-ROMs (containing crystallographic software and web material) free of charge to developing countries has been charged to this Fund. CHF 127,092 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union and CHF 6,937 for the Visiting Professorship Programme were charged to the Research and Education Fund.

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

We have audited the financial statements of the International Union of Crystallography for the year ended 31 December 2001 which comprise the income and expenditure account, the balance sheet, the cash flow statement and the related notes 16.1 to 16.15. These financial statements have been prepared under the accounting policies set out therein.

Respective responsibilities of Executive Committee and Auditors

As described in the statement of the Executive Committee's responsibilities, the Executive Committee is responsible for the preparation of the financial statements in accordance with applicable law and accounting standards.

Our responsibility is to audit the financial statements in accordance with relevant legal and regulatory requirements and United Kingdom auditing standards.

We report to you our opinion as to whether the financial statements give a true and fair view.

Basis of opinion

We conducted our audit in accordance with United Kingdom 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 2001 and of the result for the year then ended.

Deloitte & Touche
Chartered Accountants and Registered Auditors
28 June 2002

16. Notes to the Accounts

The Income and Expenditure Account, the Balance sheet and the Cash Flow statement for the year ended 31 December 2001 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.

Transactions denominated in foreign currencies are translated into Swiss Francs at the rates ruling at the dates of the transactions. Monetary assets and liabilities denominated in foreign currencies at the balance sheet date are retranslated at the rates ruling at that date.

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 the lower of cost and net realizable value. Stocks of all other publications, including back issues of journals, are not valued for accounts purposes as sales are uncertain.

(*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 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 over the term of the lease. 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.

(*j*) *Pension costs*

The Union operates a defined contribution pension scheme for its employees. The assets of the scheme are held separately from those of the Union. The amount charged to income and expenditure in the year in respect of pensions represents employer's contributions payable in the year. No amounts were due to or from the pension scheme at 31 December 2001 (the same was true in 2000).

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:

	2001	*2000*
Netherland Guilders (NLG)	1.4970	*1.4489*
Danish Crowns (DKK)	5.0606	*4.9148*
Pounds Sterling (GBP)	0.4242	*0.3977*
US Dollars (USD)	0.6061	*0.5682*

The net assets of the Union at 1 January 2001 (CHF 6,763,941) would have had the value of USD 3,843,271 or GBP 2,690,019 if expressed in those currencies.

At 31 December 2001, the net assets (CHF 5,553,575) would have had the value of USD 3,366,022 or GBP 2,355,826, respectively, being a decrease of USD 477,249 or a decrease of GBP 334,193 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 2001.

16.6. Creditors

Table 8 lists the creditors, with the amounts falling due within one year for 2000 and 2001.

16.7. Investment income

Table 9 lists the income from investments for 2000 and 2001.

16.8. Bank interest

Table 10 lists the bank interest for 2000 and 2001.

16.9. Loss/profit on disposal/redemption of investments

Table 11 lists the loss or profit on disposal/redemption of investments for 2000 and 2001.

16.10. Information regarding employees

Staff costs during the years 2000 and 2001 are given in Table 12.

16.11. Operating lease commitments

At 31 December 2001, the Union was committed to making the payments listed in Table 13 during the next year in respect of operating leases.

16.12. Sponsorship commitments

At 31 December 2001, the Union had authorized, but not contracted for, sponsorship grants of CHF 88,275 (2000: CHF 72,160).

16.13. Exchange rate fluctuations

Table 14 lists exchange rate fluctuations attributable to operating activities for 2000 and 2001.

16.14. Changes in cash during the year

Table 15 is an analysis of cash changes during 2000 and 2001.

16.15. Balances of cash as shown in the balance sheet

Table 16 is an analysis of cash balances as shown in the balance sheet.

Tables 17–28 give the accounts for the year ended 31 December 2001 for the various fund accounts.

Table 3
Income and Expenditure Account for the year ended 31 December 2001.

	Note	2001	Swiss Francs	*2000*	
Income					
Membership subscriptions			164,998		*152,316*
Sales					
Journals		3,409,139		*3.327,321*	
Books		256,969		*129,538*	
Back numbers and single issues		28,264	3,694,372	*35,125*	*3,491,984*
Investment income					
Income from investments	16.7	212,929		*294,981*	
Bank interest	16.8	28,029		*27,817*	
(Loss)/profit on sale of investments	16.9	(215,339)	25,619	(*7,197*)	*315,601*
Other income					
Grants		38,213		*12,492*	
Royalties and copyright fees		6,112		*6,685*	
Advertising income		198,038		*189,468*	
Donations		–	242,363	*14,806*	*223,451*
Total Income			4,127,352		*4,183,352*
Expenditure					
Journals					
Publication costs		929,800		*1,360,238*	
Editorial expenses		187,717		*160,047*	
Technical editing		1,309,644		*1,278,679*	
Subscription administration		44,956	2,472,117	–	*2,798,964*
Books					
Publication costs		95,756		*94,176*	
Editorial expenses		66,417		*55,704*	
Technical editing		192,874	355,047	*233,480*	*383,360*
Newsletter					
Publication costs		152,277		*167,759*	
Editorial expenses		73,175	225,452	*81,782*	*249,541*
President's Fund Grants and Young Scientists' support			132,288		*116,263*
General Assembly costs			41,397		*1,315*
Committee meetings and expenses			67,746		*36,601*
Publications and journals development					
General		460,387		*413,212*	
Electronic Publishing Committee/Section Editors meeting expenses		10,676		*2,765*	
STAR/CIF		556		*1,319*	
Promotions Officer		126,560	598,179	*137,922*	*555,218*
Subscriptions paid			10,568		*9,707*
Visiting Professorship Programme			6,937		*10,700*
Administration expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		12,090		*12,378*	
Audit and accountancy charges		48,794		*33,885*	
Legal and professional fees		20,259		*43,836*	
Travelling expenses		8,423		*11,583*	
Bank charges		2,744	92,310	*2,451*	*104,133*
Executive Secretary's office:					
Salaries and expenses		290,346		*308,506*	
Travel expenses of IUCr Representatives on other bodies		3,840		*6,276*	
Commission expenses		10,315		–	
Sponsorship of meetings		1,824		*4,426*	
President's secretary		10,000		*10,000*	
IUCr/FIZ agreement		(8,353)		(*7,960*)	
Bad debts – subscriptions		8,000	315,972	*4,000*	*325,248*
Depreciation			76,013		*54,243*
Total Expenditure			4,394,026		*4,645,293*

Table 3 (continued)

	Note		2001		*2000*
			Swiss Francs		
Deficit of income over expenditure			(266,674)		(*461,941*)
Movement in market value of investments in year	16.5		(563,263)		(*863,121*)
			(829,937)		(*1,325,062*)
Fluctuation in rates of exchange					
Trading activities	16.2	15,489		*45,686*	
Investment activities	16.2	(395,918)	(380,429)	*382,398*	*428,084*
Total recognized gains and losses relating to the year			(1,210,366)		(*896,978*)
Opening fund accounts at 1 January			6,763,941		*7,660,919*
Closing fund accounts at 31 December			5,553,575		*6,763,941*

All the income and expenditure related to continuing activities. Historic cost results would only differ from above by the loss 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 2001.

	Note		2001		*2000*
			Swiss Francs		
Fixed Assets					
Tangible fixed assets	16.4		97,216		*78,168*
Current Assets					
Stock			77,359		*19,219*
Cash at bank and in hand					
Current accounts		62,708		*14,388*	
Deposit and savings accounts		244,167		*147,934*	
Cash with Union officials		29,466	336,341	*31,704*	*194,026*
Investments at market value	16.5		4,772,261		*6,349,963*
Debtors, accrued income and payments in advance			450,736		*317,407*
Subscriptions due from Adhering Bodies			23,874		*10,698*
Total Current Assets			5,660,571		*6,891,313*
Creditors: amounts falling due within one year	16.6		(204,212)		(*205,540*)
Net Current Assets			5,456,359		*6,685,773*
Total Funds			5,553,575		*6,763,941*

Table 5
Cash Flow statement for the year ended 31 December 2001.

	Note	2001	Swiss Francs	*2000*
Net cash outflow from operating activities (see below)			(409,322)	(*701,763*)
Returns on investments				
Interest received		28,029		*27,817*
Investment income (net of notional dividends)		78,209		*106,374*
Net cash inflow from returns on investments			106,238	*134,191*
Investing activities				
Purchase of fixed assets	16.4	(95,061)		(*38,475*)
Purchase of investments	16.5	(1,374,937)		(*1,902,055*)
Disposal of investments	16.9	1,912,839		*2,468,708*
Net cash inflow from investing activities			442,841	*528,178*
Increase/(decrease) in cash	16.14		139,757	(*39,394*)
Reconciliation of Deficit of Income over Expenditure to Net Cash Outflow from Operating Activities				
Deficit of income over expenditure			(266,674)	(*461,941*)
Exchange rate fluctuations attributable to operating activities	16.13		12,931	(*2,838*)
Interest received	16.8		(28,029)	(*27,817*)
Investment income	16.7		(212,929)	(*294,981*)
Loss/(profit) on disposal of investments	16.9		215,339	*7,197*
Depreciation charges			76,013	*52,243*
(Increase)/decrease in stock			(58,140)	*15,843*
(Increase)/decrease in debtors			(146,505)	*2,548*
Increase/(decrease) in creditors			(1,328)	*5,983*
Net cash outflow from operating activities (see above)			(409,322)	(*701,763*)

Table 6
Tangible fixed assets.

	Leasehold property improve-ments CHF	Office equipment CHF	Computer equipment CHF	Total CHF
Cost				
As at				
1 January 2001	102,987	73,192	208,323	384,502
Additions	–	13,345	81,716	95,061
As at				
31 December 2001	102,987	86,537	290,039	479,563
Accumulated depreciation				
As at				
1 January 2001	53,833	65,371	187,130	306,334
Charge for the year	10,299	7,728	57,986	76,013
As at				
31 December 2001	64,132	73,0991	245,116	382,347
Net book value				
31 December 2001	38,855	13,438	44,923	97,216
31 December 2000	49,154	7,821	21,193	78,168

Table 7
Investments.

	Swiss Francs								
	Holding at market value 1 January 2001	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 2001	Holding at revalued cost 31 December 2001	Holding at revalued cost 31 December 2000
Held by Merrill Lynch									
GNM P169332-2016 (USD)									
3,969 Units	10,477	–	–	(3,002)	(566)	239	7,148	6,325	9,592
Haussmann Holdings (USD)									
82 Units	210,561	–	–	–	(13,160)	(1,429)	195,972	64,495	70,928
Global Allocation Portfolio Class O									
(USD) 2,700 Units	101,028	–	–	–	(6,314)	1,515	96,229	47,000	50,134
MLBS SP PF EU EQ (US) B									
3,292 Units	194,480	–	–	–	(12,155)	(34,907)	147,418	165,922	176,984
Sector SPDR Energy 2075 Units	121,201	–	–	–	(7,575)	(22,212)	91,414	79,773	85,091
Banco Bilbao	67,155	–	–	(61,813)	(5,342)	–	–	–	73,545
Seligman Japan FD CL B	92,615	–	–	(88,405)	(4,210)	–	–	–	113,256
Mercury Selected Trust USD Global									
Bond Fund B 6,790 Units	186,903	–	–	–	(11,681)	4,257	179,479	165,285	176,304
ML Internet Strategies Portfolio Fund									
CLA	73,061	–	–	(69,740)	(3,321)	–	–	–	99,000
Janus Global Life Sciences Fund									
4,700 Units	96,534	–	–	–	(6,033)	(19,465)	71,036	78,203	83,417
Janus US Venture Fund									
4,800 Units	64,120	–	–	–	(4,008)	(8,950)	51,162	82,084	87,556
Seligman US Comm + Info Fund									
1,750 Units	52,144	–	–	–	(3,259)	578	49,463	81,894	87,354
Seligman Horizon Global Tech									
Fund 1,500 Units	56,892	–	–	–	(3,555)	(11,212)	42,125	81,386	86,812
B2B Internet	3,135	–	–	(2,992)	(143)	–	–	–	6,992
Broadband	8,019	–	–	(7,654)	(365)	–	–	–	14,392
Cisco Systems Inc. 1,700 Units	33,660	41,842	–	–	(5,159)	(19,544)	50,799	92,032	56,795
Internet Infrastructure	3,893	–	–	(3,716)	(177)	–	–	–	9,620
Internet Archecture	10,131	–	–	(9,670)	(461)	–	–	–	14,999
Pharmaceutical 200 Units	20,108	18,532	–	–	(2,609)	(3,524)	32,507	33,229	17,121
Telecom	9,393	–	–	(8,966)	(427)	–	–	–	13,856
Global SR (DE) 600 Units	47,788	–	–	–	(2,987)	(13,598)	31,203	99,518	106,153
Consults Portfolios									
No.17P-07M16	267,841	441,224	–	(504,993)	(15,913)	25,086	213,245	206,021	286,893
No.17P-07M17	189,396	183,968	–	(219,787)	(11,179)	(4,704)	137,694	141,635	188,582
No.17P-07P52	146,089	210,875	–	(232,153)	(8,839)	7,036	123,008	132,723	163,956
No.17P-07P53	172,626	115,496	–	(141,843)	(9,934)	(1,205)	135,140	130,504	166,396
Held by Foreign & Colonial									
Reserve Asset Fund Class L (GBP)									
25,538 Units	1,848,522	–	74,131	–	(110,469)	(331,544)	1,480,640	1,205,221	1,202,980
Reserve Asset Fund Class X (GBP)									
2,566 Units	125,535	–	6,177	–	(7,502)	(595)	123,615	130,299	132,011
Reserve Asset Fund Class M (USD)									
5,144 Units	467,203	363,000	25,618	–	(44,494)	(103,308)	708,019	520,815	157,323
Reserve Asset Fund Class E (GBP)									
11,556 Units	801,578	–	28,794	(368,897)	(38,758)	(20,990)	401,727	408,451	772,546
	5,482,088	1,374,937	134,720	(1,723,631)	(340,595)	(558,476)	4,369,043	3,954,815	4,510,588
Treasury Stock									
7.75% UK Treasury Stock 2006									
150,000 Units	867,875	–	–	(404,547)	(55,323)	(4,787)	403,218	374,992	797,652
	6,349,963	1,374,937	134,720	(2,128,178)	(395,918)	(563,263)	4,772,261	4,329,807	5,308,240

Table 8
Creditors: amounts falling due within one year.

	Swiss Francs 2001	*2000*
Accruals	161,708	*140.882*
Payroll creditor including tax and social security	42,504	*59,638*
Operating lease creditor relating to property	–	*5,020*
	204,212	*205,540*

Table 9
Investment income.

	Swiss Francs 2001	*2000*
GNM P169332 - 2016	767	*1,004*
Haussmann Holdings	274	*284*
Foreign and Colonial – Reserve Asset Fund Class L	74,132	*112,816*
Foreign and Colonial – Reserve Asset Fund Class X	6,177	*7,531*
Foreign and Colonial – Reserve Asset Fund Class M	25,617	*29,102*
Foreign and Colonial – Reserve Asset Fund Class E	28,794	*39,157*
UK Treasury 7.75% 22.9.2006	56,381	*74,836*
Repsol International Capital Ltd	–	*4,712*
Santander Finance Ltd	–	*6,938*
Banco Bilbao	6,993	*4,625*
ML Debt Strategy	48	–
Sector SPDR Strategy	1,432	*1,384*
Pharmaceutical	266	*181*
Telecom	30	*75*
Internet Archecture	2	*137*
B2B Internet	–	*28*
Broadband	1	*11*
Internet Infrastructure	–	*74*
Consults Portfolios		
No. 17P-07M16	3,508	*2,282*
No. 17P-07M17	3,092	*4,227*
No. 17P-07P52	3,341	*4,373*
No. 17P-07P53	2,074	*2,452*
Reversal of opening US tax debtor	–	(*1,248*)
	212,929	*294,981*
Allocated to:		
President's Fund	3,207	*2,164*
Publication and Journals Development Fund	20,714	*11,916*
Research and Education Fund	48,532	*47,366*
Ewald Fund	27,322	*25,591*
Balance left in General Fund	113,154	*207,944*
	212,929	*294,981*

Table 10
Bank interest.

	Swiss Francs 2001		*2000*	
National Westminster Bank Plc				
Manchester Business Reserve Account	5,544		*7,880*	
Manchester Capital Reserve Account	4,160	9.704	*10*	*7.890*
Merrill Lynch CMA Account		2.557		*4,016*
Foreign & Colonial Cash balance		325		*435*
Interest from Munksgaard		15,443		*15,476*
Allocated to General Fund		28,029		*27,817*

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

	Swiss Francs 2001	*2000*
Proceeds	1,912,839	*2,468,708*
Book value	2,128,178	*2,475,905*
(Loss)/Profit allocated to General Fund	(215,339)	(*7,197*)

Book value represents market value at 1 January 2001. The loss on disposal based on historic cost was CHF 244,220 (2000: loss of CHF 2,125). Therefore historic cost results would be as follows:

	Swiss Francs 2001	*2000*
Deficit of income over expenditure	(295,555)	(*456,869*)

Table 12
Information regarding employees.

	2001	*2000*
Average number of persons employed during the year	22	*23*

	Pounds Sterling 2001	*2000*
Staff costs incurred during the year in respect of these employees:		
Salaries	629,846	*628,965*
Social security	62,809	*64,477*
Pension	113,497	*105,497*
Total staff costs	806,152	*798,030*

	Swiss Francs 2001	*2000*
Total staff costs	1,958,439	*2,061,008*

Table 13
Operating lease commitments.

	Swiss Francs			
	Land and Buildings 2001	Other 2001	*Land and Buildings 2000*	*Other 2000*
Leases which expire:				
within one year	–	41,961	–	*41,164*
within two to five years	61,360	–	–	*3,464*
after five years	27,140	–	*94,125*	–
	88,500	41,961	*94,125*	*44,628*

Table 14
Exchange rate fluctuations attributable to operating activities.

	Swiss Francs	
	2001	*2000*
Total fluctuations in exchange rates dealt with in fund accounts	(380,429)	*428,084*
Adjustments for exchange differences attributable to:		
Investments (Note 16.5)	395,918	(*382,398*)
Cash and bank balances	(2,558)	*48,524*
	12,931	(*2,838*)

Table 15
Analysis of changes in cash during the year.

	Swiss Francs			
	2001		*2000*	
Balance at 1 January 2001		194,026		*184,896*
Net cash inflow/(outflow)	139,757		(*39,394*)	
Fluctuations in rates of exchange on cash and bank balances	(2,558)	142,315	*48,524*	*9,130*
Balance at 31 December 2001		336,341		*194,026*

Table 16
Analysis of cash balances as shown in the Balance sheet.

	Swiss Francs			
	2001	*2000*	Change 2001	*Change 2000*
Cash at bank and in hand	336,341	*194,026*	142,315	*9,130*

Table 17
Fund Accounts as at 31 December 2001.

	Swiss Francs						
	As at 1 January 2001	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Loss on market value of investments	Fluctuations in exchange rates (Note 16.2) Trading	Fluctuations in exchange rates (Note 16.2) Investments	Balance at 31 December 2001
Fund Accounts							
General Fund	3,560,747	(25,000)	(329,961)	(563,263)	6,898	(395,918)	2,253,503
President's Fund	58,644	–	(1,989)	–	148	–	56,803
Acta Crystallographica	962,804	(575,000)	420,646	–	2,110	–	810,560
Journal of Applied Crystallography	136,139	(25,000)	91,148	–	528	–	202,815
International Tables	69,026	200,000	(271,046)	–	(5)	–	(2,025)
Book Fund	41,468	–	(72,875)	–	(82)	–	(31,489)
Publications and Journals Development Fund	413,468	200,000	(47,526)	–	1,477	–	567,419
Research and Education Fund	913,346	100,000	(55,941)	–	2,499	–	959,904
Ewald Fund	455,363	–	27,322	–	1,260	–	483,945
Newsletter Fund	134,306	50,000	(36,429)	–	386	–	148,263
Journal of Synchrotron Radiation	18,630	75,000	9,977	–	270	–	103,877
	6,763,941	–	(266,674)	(563,263)	15,489	(395,918)	5,553,575

Table 18
General Fund Account for the year ended 31 December 2001.

	Note	2001	Swiss Francs	*2000*	
Income					
Grant received from UNESCO subvention to ICSU			8,656		*12,493*
Subscriptions from Adhering Bodies			164,998		*152,316*
Income from investments	16.7		113,154		*207,944*
Interest on bank accounts	16.8		28,029		*27,817*
Profit/(loss) on disposal/redemption of investments	16.9		(215,339)		(*7,197*)
Amounts charged to the following journals and publications:					
Acta Crystallographica		127,294		*139,793*	
Journal of Applied Crystallography		19,727		*38,831*	
Journal of Synchrotron Radiation		30,863	177,884	*11,549*	*190,173*
Total Income			277,382		*583,546*
Expenditure					
Subscriptions to ICSU and ICSU bodies			10,568		*9,707*
Administrative expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		12,090		*12,378*	
Audit and accountancy charges		48,794		*33,885*	
Legal and professional fees		20,259		*43,836*	
Travelling expenses		8,423		*11,583*	
Bank charges		2,744		*2,451*	
Executive Secretary's office:					
Salaries and expenses		290,346		*308,506*	
Depreciation of office equipment		12,642		*10,880*	
Depreciation of freehold property		10,299	405,597	*10,299*	*433,818*
Nineteenth General Assembly and Congress					
Expenses		6,620		*1,315*	
Programme Committee		34,777		–	
Meeting of the Executive Committee		54,8924		*18,084*	
Finance Committee expenses		12,854		*18,518*	
Programming and development costs		42,361		*61,494*	
Promotion		14,048		–	
Travel expenses of IUCr Representatives on other bodies		3,840		*6,276*	
Commission expenses		10,315		–	
Sponsorship of meetings		1,824		*4,426*	
President's secretary		10,000		*10,000*	
IUCr/FIZ agreement		(8,353)		(*7,960*)	
Bad debts – subscriptions		8,000	191,178	*4,000*	*116,153*
Total Expenditure			607,343		*559,678*
(Deficit)/surplus of income over expenditure			(329,961)		*23,868*
Reconciliation of movements					
Balance at 1 January			3,560,747		*4,019,849*
Transfers to other funds					
Newsletter Fund			(25,000)		(*25,000*)
(Deficit)/surplus of income over expenditure		(329,961)		*23,868*	
Movement in market value of investments in the year	16.5	(563,263)	(893,224)	(*863,121*)	(*839,253*)
Fluctuations in rates of exchange			(389,020)		*405,151*
Balance at 31 December			2,253,503		*3,560,747*

Table 19
Acta Crystallographica Account for the year ended 31 December 2001.

	Note	2001		*2000*	
		Swiss Francs			
Income					
Subscriptions to Volume 57 (*2000 Volume 56*)		2,580,225		*2,591,111*	
Sale of back numbers and single copies		18,612		*26,122*	
Distribution costs charged to subscribers		105,510		*109,046*	
Royalties and copyright fees		11,164		*9,018*	
Special Issue income		30,316		*30,761*	
Pay per view and secondary services (net)		4,803		–	
		2,750,630		*2,766,058*	
Less Publisher's commission on sales		185,612	2,565,018	*183,888*	*2,582,170*
Income from advertisements (net)			3,214		*4,735*
(Recredit)/recharge for Special Issue			(11,943)		*28,585*
Total Income			2,556,289		*2,615,490*
Expenditure					
Publication expenses:					
Production Volume 57 (*2000 Volume 56*)		507,782		*523,715*	
Distribution costs		86,147		*119,722*	
		593,929		*643,437*	
Net (profit)/loss on reprints		(28,732)		(*2,751*)	
Special Issue costs		18,373	583,570	*59,346*	*700,032*
Editorial expenses:					
Editorial honoraria		116,035		*105,034*	
Secretarial assistance		8,019		*7,822*	
Postage, travel and sundries		24,796		*19,777*	
Technical editing:					
Salaries and expenses		946,969		*1,070,894*	
Computer expenses		55,591		*86,279*	
Subscription administration		36,255		–	
Promotion		56,574		–	
Depreciation of office equipment		11,091	1,255,330	*15,379*	*1,305,185*
Programming and development costs			169,449		*224,413*
Administration expenses recharged from General Fund			127,294		*139,793*
Total Expenditure			2,369,423		*2,177,396*
Surplus of income over expenditure			420,646		*246,067*
Reconciliation of movements					
Balance at 1 January			962,804		*1,449,844*
Transfers to other funds					
International Tables		200,000		*250,000*	
Publications and Journals Development Fund		200,000		*200,000*	
Research and Education Fund		100,000		*70,000*	
Newsletter Fund		–		*50,000*	
Journal of Synchrotron Radiation		75,000		*150,000*	
President's Fund		–	(575,000)	*20,000*	(*740,000*)
Surplus of income over expenditure			420,646		*246,067*
Fluctuations in rates of exchange			2,110		*6,893*
Balance at 31 December			810,560		*962,804*

Table 20
Journal of Applied Crystallography Account for the year ended 31 December 2001.

	Note	2001		*2000*	
		Swiss Francs			
Income					
Subscriptions to Volume 34 (*2000 Volume 33*)		384,698		*391,819*	
Sale of back numbers and single copies		4,852		*3,556*	
Distribution costs charged to subscribers		28,889		*30,165*	
Royalties and copyright fees		2,120		*2,368*	
Advertising income		702		*3,388*	
Special Issue income		–		56,606	
		421,261		*487,902*	
Less Publisher's commission on sales		27,703		*28,184*	
Total Income			393,558		*459,718*
Expenditure					
Publication expenses:					
Production Volume 34 (*2000 Volume 33*)		68,595		*114,624*	
Distribution costs		11,726		*30,927*	
		80,321		*145,551*	
Special Issue costs		–		*50,590*	
Net profit on reprints		(4,563)	75,758	(*2,605*)	*193,536*
Editorial expenses:					
Editorial honoraria		4,006		*9,995*	
Secretarial assistance		8,785		*6,873*	
Postage, travel and sundries		1,074		*950*	
Technical editing:					
Salaries and expenses		134,867		*113,627*	
Computer expenses		8,615		*24,219*	
Subscription administration		7,251		–	
Promotion		13,921		–	
Depreciation of office equipment		1,718	180,237	*4,317*	*159,981*
Programming and development costs			26,688		*32,059*
Administration expenses recharged from General Fund			19,727		*39,241*
Recredit for Special Issue			–		6,016
Total Expenditure			302,410		*430,833*
Surplus of income over expenditure			91,148		*28,885*
Reconciliation of movements					
Balance at 1 January			136,139		*106,279*
Transfers to other funds					
Newsletter Fund			(25,000)		–
Surplus of income over expenditure			91,148		*28,885*
Fluctuations in rates of exchange			528		*975*
Balance at 31 December			202,815		*136,139*

Table 21
Journal of Synchrotron Radiation Account for the year ended 31 December 2001.

	Note	2001		*2000*	
		Swiss Francs			
Income					
Subscriptions to Volume 8 (*2000 Volume 7*)		163,649		*134,396*	
Sales of back numbers and single issues		4,407		*1,442*	
Distribution costs charged to subscribers		5,143		*5,160*	
Special Issue income		125,058		*3,081*	
		298,257		*144,079*	
Less Publisher's commission on sales		12,528	285,729	*10,723*	*133,356*
Income from advertisements			5,099		*7,365*
Income from copyright fees			1,397		*724*
(Recredit)/recharge for Special Issue			(5,389)		*17,216*
Total Income			286,838		*158,661*
Expenditure					
Publication expenses:					
Special Issue costs		119,669		*20,297*	
Production Volume 8 (*2000 Volume 7*)		44,276		*43,679*	
Distribution costs		4,560		*5,452*	
		168,505		*69,428*	
Net (profit)/loss on reprints		(8,771)	159,734	*4,052*	*73,480*
Editorial expenses:					
Editorial honoraria		9,348		*9,792*	
Secretarial assistance		4,770		*5,604*	
Postage, travel and sundries		408		*1,223*	
Technical editing:					
Salaries and expenses		30,455		*84,053*	
Computer expenses		13,478		*7,128*	
Subscription administration		1,449		–	
Promotion		13,921		–	
Depreciation of office equipment		2,690	76,519	*1,271*	*109,071*
Programming and development costs			9,743		*49,831*
Administration expenses recharged from General Fund			30,863		*11,549*
Total Expenditure			276,859		*243,931*
Surplus of income over expenditure			9,977		(*85,270*)
Reconciliation of movements					
Balance at 1 January			18,630		(*46,233*)
Transfers from other funds					
Acta Crystallographica			75,000		*150,000*
Surplus of income over expenditure			9,977		(*85,270*)
Fluctuations in rates of exchange			270		*133*
Balance at 31 December			103,877		*18,630*

Table 22
President's Fund Account for the year ended 31 December 2001.

	Note	Swiss Francs 2001	*2000*
Income			
Investment income	16.7	3,207	*2,164*
Expenditure			
Grants		5,196	*4,063*
Deficit of income over expenditure		(1,989)	(*1,899*)
Reconciliation of movements			
Balance at 1 January		58,644	*40,123*
Transfers from other funds			
Acta Crystallographica		–	*20,000*
Deficit of income over expenditure		(1,989)	(*1,899*)
Fluctuations in rates of exchange		148	*420*
Balance at 31 December		56,803	*58,644*

Table 23
International Tables Account for the year ended 31 December 2001.

	Note	Swiss Francs 2001		*2000*	
Income					
Sales of copies					
Volume A		811		(*503*)	
Teaching Edition of Volume A		116		*3,671*	
Volume B		67,989		*22,250*	
Volume C		45,091		*68,056*	
Volume F		112,122		–	
Volumes II, III and IV		–		*96*	
		226,129		*93,570*	
Less Publisher's commission on sales		58,423	167,706	*25,768*	*67,802*
Donation			–		*14,806*
Total Income			167,706		*82,608*
Expenditure					
Publication expenses:					
Production Volume A		–		*30,287*	
Production Volume B		30,036		*33,027*	
Production Volume C		5,569		*10,830*	
Production Volume D		1,507		*1,536*	
Production Volume E		–		*3,651*	
Production Volume F		57,307		*7,874*	
Production Teaching Edition of Volume A		–	94,419	*4,811*	*92,016*
Editorial expenses:					
Editorial honoraria		15,039		*4,108*	
Secretarial assistance, postage and office equipment		7,994		*29,936*	
Technical editing		192,874	215,907	*233,480*	*267,524*
Programming and development			114,378		*42,164*
Promotion			14,048		–
Total Expenditure			438,752		*401,704*
Deficit of income over expenditure			(271,046)		(*319,096*)
Reconciliation of movements					
Balance at 1 January			69,026		*137,628*
Transfers from other funds					
Acta Crystallographica			200,000		*250,000*
Deficit of income over expenditure			(271,046)		(*319,096*)
Fluctuations in rates of exchange			(5)		*494*
Balance at 31 December			(2,025)		*69,026*

Table 24
Book Fund Account for the year ended 31 December 2001.

	Note	Swiss Francs 2001	*2000*
Income			
Sales of copies, net of Publisher's commission on sales			
Historical Atlas of Crystallography		140	*296*
World Directory of Crystallographers 10th edition		900	*1,830*
Escher *Kaleidozyklen*		127	–
Structure Reports		393	*4,005*
Royalties			
IUCr/OUP Book Series		2,595	*3,593*
Total Income		4,155	*9,724*
Expenditure			
Publication expenses			
World Directory of Crystallographers 10th edition		1,980	*2,160*
Programming and development		61,002	–
Promotion		14,048	–
Total Expenditure		77,030	*2,160*
(Deficit)/surplus of income over expenditure		(72,875)	*7,564*
Reconciliation of movements			
Balance at 1 January		41,468	*33,607*
(Deficit)/surplus of income over expenditure		(72,875)	*7,564*
Fluctuations in rates of exchange		(82)	*297*
Balance at 31 December		(31,489)	*41,468*

Table 25
Publications and Journals Development Fund Account for the year ended 31 December 2001.

	Note	Swiss Francs 2001		*2000*	
Income					
Investment income	16.7		20,714		*11,916*
Expenses					
Computer expenses:					
Purchase of computer equipment and software		9,207		*50,308*	
Programming and development		414,414		*409,961*	
Recharged to other funds		(423,621)	–	(*409,961*)	*50,308*
Electronic Publishing Committee/ Section Editors' Meeting			10,676		*2,765*
Special Issue (surplus)/deficit (recredited)/recharged (from)/to other funds			(17,331)		*39,785*
NeXus			2,244		*2,774*
STAR/CIF			556		*1,319*
Promotion			126,560		*137,922*
Promotion recharged to other funds			(126,560)		–
Web input			626		*1,502*
Journal subscription subsidies			968		–
Digitisation project			32,928		–
Depreciation of computer equipment			37,573		*12,097*
Total Expenditure			68,240		*248,472*
Deficit of income over expenditure			(47,526)		*(236,556)*
Reconciliation of movements					
Balance at 1 January			413,468		*447,064*
Transfers from other funds					
Acta Crystallographica			200,000		*200,000*
Deficit of income over expenditure			(47,526)		*(236,556)*
Fluctuations in rates of exchange			1,477		*2,960*
Balance at 31 December			567,419		*413,468*

Table 26
Research and Education Fund Account for the year ended 2001.

	Note	Swiss Francs 2001		*2000*	
Income					
Investment income	16.7		48,532		*47,366*
Refund of Congress income			29,556		–
Total Income			78,088		*47,366*
Expenditure					
Young Scientists' Support		127,092		*112,200*	
Visiting Professorship Programme		6,937		*10,700*	
Total Expenditure			134,029		*122,900*
Deficit of income over expenditure			(55,941)		(*75,534*)
Reconciliation of movements					
Balance at 1 January			913,346		*912,341*
Transfers from other funds					
Acta Crystallographica			100,000		*70,000*
Deficit of income over expenditure			(55,941)		(*75,534*)
Fluctuations in rates of exchange			2,499		*6,539*
Balance at 31 December			959,904		*913,346*

Table 27
Ewald Fund Account for the year ended 31 December 2001.

	Note	Swiss Francs 2001	*2000*
Income			
Investment income	16.7	27,322	*25,591*
Expenditure			
Prize/Selection Committee and expenses		–	–
Surplus of income over expenditure		27,322	*25,591*
Reconciliation of movements			
Balance at 1 January		455,363	*426,512*
Excess/(deficit) of income over expenditure		27,322	*25,591*
Fluctuations in rates of exchange		1,260	*3,260*
Balance at 31 December		483,945	*455,363*

Table 28
Newsletter Fund Account for the year ended 2001.

	Note	Swiss Francs 2001		*2000*	
Income					
Income from advertisements			174,692		*173,980*
Reimbursement of 19GAC circular			14,331		–
Total Income			189,023		*173,980*
Expenditure					
Editorial honoraria			7,260		*7,920*
Editorial expenses			65,915		*51,862*
Newsletter printing and distribution			108,604		*124,264*
Advertising costs			43,673		*43,495*
Total Expenditure			225,452		*227,541*
Deficit of income over expenditure			(36,429)		(*53,561*)
Reconciliation of movements					
Balance at 1 January			134,306		*133,905*
Transfers from other funds					
General Fund		25,000		*25,000*	
Acta Crystallographica		–		*50,000*	
Journal of Applied Crystallography		25,000	50,000	–	*75,000*
Deficit of income over expenditure					
Current year (above)		(36,429)		(*53,561*)	
Accumulated underspend in prior years not previously recognized		–	(36,429)	(*22,000*)	(*75,561*)
Fluctuations in rates of exchange			386		*962*
Balance at 31 December			148,263		*134,306*