Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

International Union of Crystallography Report of the Executive Committee for 1998

1. Meetings

The IUCr sponsored the following meetings held during 1998:

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

2. IV Latin American Workshop on Magnetism, Magnetic Materials and their Applications, São Paolo, Brazil, 7–11 June.

3. Seventh Annual ACA Summer Course for Crystallography, Athens, Georgia, USA, 5–18 July.

4. ACA Annual Meeting, Arlington, USA, 18–23 July.

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

6. Sixth International Conference on Biophysics and Synchrotron Radiation, Argonne, Illinois, USA, 4–8 August.

7. Eighteenth European Crystallographic Meeting (ECM-18), Prague, Czech Republic, 16–20 August.

8. Sixth European Powder Diffraction Conference (EPDIC-6), Budapest, Hungary, 22–25 August.

9. Gordon Research Conference on Electron Distribution and Chemical Bonding, Oxford, UK, 30 August–4 September.

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

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

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

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

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

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

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

(1) editorial policy, pricing policy and subscription rates, approval of appointments of new Editors for *Acta Cryst.* Section C and the *Journal of Applied Crystallography*, approval of appointments of Co-editors, electronic publishing, Special Issues, and other matters concerning the IUCr journals;

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

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

(4) investment policy;

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

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

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

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

(9) the *IUCr Newsletter*;

(10) the Tenth Edition of the *World Directory of Crystallographers*;

(11) fiftieth anniversary of the IUCr;

(12) the Ewald Prize;

(13) discussion of the arrangements for the Glasgow General Assembly and Congress;

(14) the role of crystallography;

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

Other items dealt with in this way were:

(16) the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* and other uses of CIF, patent application and adoption of the STAR file and CIF by other bodies, work of the Committee for the Maintenance of the CIF Standard (COMCIFS), provision of checking services to other publishers;

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

(18) crystallography in Africa;

(19) use of financial support through ICSU;

(20) access to large-scale research facilities;

(21) review of the activities of the Commissions;

(22) review of the activities of Regional Associates;

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

Items concerning the Chester office were:

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

(25) upgrading of office technology in the IUCr office in Chester, provision of Internet services, domain site name, formation of an IUCr World-Wide Web editorial board, and establishment of mirror sites.

2. Publications

Volume 54 of *Acta Crystallographica*, Volume 31 of *Journal of Applied Crystallography* and Volume 5 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 Seventeenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (1997), A**53**, 692–748].

4. Work of the Commissions

4.1. Commission on Journals

In the last year, a number of developments for the IUCr journals should be highlighted. The 50th Anniversary of *Acta Crystallographica* and the IUCr occurred, as did the 30th Anniversary of *Journal of Applied Crystallography*. A special 50th Anniversary Issue of *Acta Cryst.* was published in Section A in November 1998, comprising specially commissioned articles. The Guest Editor was H. Schenk, whose excellent work and contribution is acknowledged here. This special issue was distributed to all subscribers of IUCr journals free of charge and is available for purchase at a very competitive price in book form as *Crystallography Across the Sciences*. The *Journal of Synchrotron Radiation* published proceedings from the SRI '97 triennial Synchrotron Radiation Instrumentation Congress held at SPring-8 in Japan; this was by far the largest single Conference Proceedings ever undertaken by the IUCr journals team and comprised over 1050 pages. The Proceedings of the XAFS X Conference held in Chicago, USA, in 1998 are about to go to press at the time of writing. For the latter, the introduction of camera-ready copy of the final, fully refereed, articles by authors is worth noting here as a radical departure from past practice, and has resulted in an important reduction in the costs of such Proceedings. The biological community expands apace and *Acta Cryst.* Section D (*Biological Crystallography*) is now published monthly; the January 1999 issue heralded the start of this monthly frequency and was introduced in a completely new format. Publication of the very popular Daresbury CCP4 Conference Proceedings series commenced as a supplement to *Acta Cryst.* Section D in 1998. The IUCr web coverage of the journals, including the services to authors and Co-editors for manuscript tracking, is now extensive. Most recently, electronically available proofs have been made available as a service to a first group of authors. Preparation for web access to the journals themselves is most advanced for *Acta Cryst.* Section D and release is imminent at the time of writing. There is a greater emphasis on the marketing of the journal titles to the crystallographic community, as well as to structural science communities in biology, chemistry, materials science and physics. Highlighting of IUCr journal articles *via* mini-reviews within the *IUCr Newsletter* is about to commence at the time of writing. This opens a channel to 15 000 readers and is clearly an exciting promotional strategy. A survey of the contents of the IUCr journals is given in Table 1. Details of each journal can be found in the accompanying reports below.

4.1.1. *Acta Crystallographica* Section A (A. Authier, Editor). In 1998, 76 Research Papers and 11 Short Communications were published in the six normal issues of the journal and 26 articles in the Special Issue dedicated to the 50th Anniversary of *Acta Crystallographica* and the IUCr. The total number of pages was 1049. It is a pleasure to note that the number of manuscripts received by Section A was back to its earlier level of 1996. This shows that the journal is very healthy and serves its purpose. The main problem is, however, the decreasing number of subscriptions, as for the other journals. The Special Issue was a real success with papers of a very high standard covering nearly every aspect of crystallography. The number of potential papers was actually much larger and a very severe selection process was operated. It is therefore possible to consider having more such Special Issues in the future. These issues could increase the attractiveness of the journal to potential subscribers.

4.1.2. *Acta Crystallographica* Section B (F. H. Allen, Editor). Section B published 943 pages in 1998, comprising 101 full Research Papers, 4 Short Communications and 1 Topical Review. These figures are slightly lower than comparable data for 1996 and 1997 owing to the changeover to in-house typesetting at the Chester office in the early part of the year. Two small issues, containing only 10 and 11 papers each, were followed by four more normal issues averaging 21 papers each, the norm for previous years. The chemical balance of papers was 51% concerned with inorganic structures and topics, 44% organics, and just 7% metal-organic. Papers in the latter category have decreased from 19% in 1997 with associated increases in the other categories.

Apart from papers reporting structural studies from this broad chemical spectrum, Section B continues to serve the needs of those working on charge-density studies, structural systematics from the inorganic and small-molecule databases, modelling and prediction of crystal structures, powder diffraction methodologies, studies of phase transitions *etc.* Impact statistics show that Section B remains fourth of 17 current crystallography journals, just behind three other IUCr publications. A citation half-life of more than 10 years reflects the lasting value of Section B papers.

During 1998, CIF requirements for Section B have become mandatory for structural papers, much typesetting has moved to the Chester office, and procedures have been tightened to reduce publication times. A major component of the longer publication times has been the time taken by authors to revise manuscripts in the light of referee comments. This time has now been reduced to a maximum of three months, with most authors revising in much shorter times than this. Now that the in-house typesetting is in place, we would expect to see shorter publication times from 1999 onwards.

4.1.3. *Acta Crystallographica* Section C (S. R. Hall, Editor). In 1998, Section C published 884 papers occupying 2026 printed pages, compared with 872 papers and 2004 pages in 1997. There were 76 CIF-access electronic publications compared with 32 in 1997. Section C published 1145 structure determinations in 1998 compared with 1061 in 1997. The combined rejection/withdrawal rate for Section C submissions in 1998 was 25% compared with 27% in 1997.

These statistics reflect publication objectives set at the 1996 Seattle Congress of applying acceptance criteria in the review process which are both consistent and in keeping with standards expected by the community for reliable structure determinations. The basic aim is both to raise the overall standard of studies submitted to the journal and to make the IUCr CIF archive a depository of reliable structural studies. The acceptance criteria currently used in the review process ensure that the number of papers published in Section C is maintained at a level that can be handled by the existing journal staff, and is economical at the current subscription rates.

Section C launched one major new initiative in 1998. This was the implementation of the complete data validation and checking suite of software into the CHECKCIF facility. As of July 1998, the use of CHECKCIF prior to submission has been mandatory for Section C authors. Although these checks are not exhaustive, they have been of real benefit to the authors, Co-editors and the journal in ensuring that problems in a submission are sorted out prior to the review process. The automatic validation facility will ultimately benefit the entire publication process by providing direct error reports to authors, simplifying submission requirements and reducing the overall editorial and publication times.

4.1.4. *Acta Crystallographica* Section D (J. P. Glusker, Editor). Section D, devoted to biological crystallography, published 6 Fast Communications, 1 Topical Review (protein crystallization methods), 91 Research Papers, 20 Short Communications, 105 Crystallization Papers and 3 Book Reviews in 1998. In addition, the Proceedings of the CCP4 Study Weekend, January 1998, entitled Databases for Macromolecular Crystallographers, was published as 17 articles in the first part of the November issue.

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	
A50	1994	798	4602	103	1189	91	306	8.1	7.7	12	36	1.4	2.1
B50		782		99		94		8.1		5		2.4	
C50		2102		852		847		2.5		5		0.6	
D50		920		135		121		7.2		14		3.0	
A51	1995	952	5888	125	1494	111	376	8.3	8.1	14	31	1.6	1.8
B51		1104		133		128		8.4		5		2.4	
C51		2726		1091		1087		2.5		4		0.5	
D51		1106		145		137		7.6		8		2.6	
A52¶	1996	1010	6596	96	1702	85	320	10.4	9.1	11	98	1.8	2.5
B52		1078		130		126		8.3		4		1.9	
C52		3262		1289		1284		2.5		5		0.5	
D52		1246		187		109		9.1		78		2.8	
A53	1997	863	4733	86	1201	76	273	10.7	9.1	10	59	1.8	2.7
B53		1045		113		111		9.0		2		4.5	
C53		2004		872		869		2.3		3		1.0	
D53		821		130		86		7.7		44		2.9	
A54	1998	1049	5518	113	1332	103	419	9.7	9.1	10	59	1.7	2.6
B54		943		106		103		8.8		3		2.3	
C54		2026		884		874		3.1		10		1.2	
D54		1500-		229		213		6.3		26		3.5	

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	Fast Communications Number	Fast Communications Average length	Computer Programs Number	Computer Programs Average length	Short items†† Number	Short items†† Average length
27	1994	1078	171	116	8.1	11	2.2	3	4.2	15	4.0	26	1.4
28	1995	860	144	95	7.2	10	2.8	5	3.9	16	4.7	18	1.8
29	1996	759	131	84	7.5	5	3.0	5	4.4	17	2.6	20	2.3
30	1997	1191	209	162	6.2	17	2.2	9	4.9	6	4.6	15	1.2
31	1998	988	162	104	7.7	27	3.4	4	3.5	86	4.6	19	1.7

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	Computer Programs Number	Computer Programs Average length	Short items†† Number	Short items†† Average length
1	1994	106	15	15	6.7	0	0	0	0	0	0
2	1995	319	50	47	5.9	3	1.7	0	0	0	0
3	1996	326	45	43	6.9	2	3.5	0	0	0	0
4	1997	405	50	49	7.6	2	2.5	0	0	0	0
5	1998	1431	371	86‡	6.0	285‡‡	3.0	0	0	0	0

§ Numbered pages excluding contents pages. Indexes are also excluded for Section C. † Including Lead Articles and Topical Reviews for Sections A, B and D, and Crystallization Papers for Section D. ‡ Including Fast Communications. ¶ Volume A52 includes, in addition, 688 pages of abstracts communicated to the Seattle Congress. †† Laboratory Notes, Letters to the Editor, Meeting Reports and Computer Program Abstracts. ‡‡ 34 Full Articles and 280 Short Communications were published in Part 3 of Volume 5 as the Proceedings of SRI '97.

The focus on crystallographic databases that was provided by the CCP4 Proceedings comes at a time when there is particular interest in this subject as a result of the general use of the web. The protein and nucleic acid databases currently in place were described together with other available databases, including those of structural motifs, intermolecular contacts and protein sequence alignment techniques ('validation, deposition, curation, exploration and exploitation of data'). The organizers, J. Murray-Rust, L. Potterton, B. Luisi, E. Dodson and S. Bailey, are to be thanked for a highly useful publication. Previous proceedings of CCP4 study weekends have been published as Daresbury Laboratory Technical Reports, but it was felt that *Acta Cryst*. Section D would reach a wider audience. We hope that the organizers will continue to publish with us in future years.

The subjects of research papers included structures of a wide variety of proteins and nucleic acids. Other articles considered techniques for cryogenic data collection, methods of analysis of diffraction patterns, synchrotron data collection and X-ray structure analyses combined with electron microscopy. Those involving crystallization research addressed heterogeneity effects, descriptions of

imperfections in protein crystals, crystal growth in magnetic fields and in space, and the use of isothermal microcalorimetry, dynamic light scattering, NMR and Raman spectroscopy to study nucleation, orientational disorder, and the mode of breakdown of protein crystals on melting. Articles on methods of phasing the diffraction data involved multiple-wavelength anomalous scattering with a variety of anomalous scatterers in the crystal, the various methods of density modification, phase improvement, molecular replacement and error estimates in macromolecular structure determinations. There were many interesting structures reported including those of a channel-forming integral membrane protein and an enzyme containing a transition-state structure. Hydrogen bonding between water and aromatic groups was also analysed.

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

4.1.5. *Journal of Applied Crystallography* (A. M. Glazer, Editor). During the past year, *Journal of Applied Crystallography* has published 988 pages, consisting of 102 Research Papers, 15 Short Communications, 12 Computer Abstracts, 8 Cryocrystallography Papers, 8 Computer Programs, 7 Laboratory Notes, 4 Fast Communications, 4 CIF Applications and 2 Teaching and Education Papers. It is particularly gratifying to see the Cryocrystallography section doing well and this is obviously becoming quite popular. The Teaching and Education section is new and looks as though it will become a valuable part of the journal in the future. Disappointingly, no Software Reviews were published in 1998.

As has always been the case with this journal, the spread of topics is vast covering everything from powder diffraction through small-angle scattering to certain aspects of biology. *J. Appl. Cryst.* continues to be the main repository of computer program information, especially with respect to abstracts.

4.1.6. *Journal of Synchrotron Radiation* (S. S. Hasnain, J. R. Helliwell, H. Kamitsubo, Editors). The main achievement of 1998 was the successful publication of the SRI '97 Proceedings, the largest ever undertaken by the IUCr journals team, comprising over 1050 pages. The papers for this issue were refereed to the usual standards, rather than at the meeting, and we believe that this effort is reflected in the improved quality of the Proceedings which formed the May 1998 issue. Many of the lessons learnt with SRI '97 were applied to the Proceedings of the XAFS X Meeting, held in Chicago, USA, in August 1998, which is to be published in May 1999. This was again fully refereed but was produced in camera-ready format, an innovation for IUCr journals springing from *Journal of Synchrotron Radiation* (*JSR*). *JSR*'s place in the citation ranking tables was sustained, being third out of 37 journals covering instruments and instrumentation, and with *Review of Scientific Instruments* placed fifth, *Nuclear Instruments and Methods B* placed sixth and *Nuclear Instruments and Methods A* placed eighth. The review and production times for the journal have continued to be rapid. Centralized submission, introduced in 1997, continued to allow fast review times and our current strategy is to cut production times by increasing electronification of the journal. We are currently compiling a Synchrotron Radiation and Structural Biology Special Issue (for the July 1999 issue of *JSR*) to celebrate J. Walker's (now Sir John Walker) share in the 1997 Nobel Prize in Chemistry, which is the first synchrotron-radiation-related Nobel prize. Finally, a five-year financial review of *JSR* is under way and steps have been taken to ensure that the journal is financially viable, provided that the advertising revenue is sustained at current levels. Overall, the high impact factor for the journal and its excellent review and publication turn-around times for authors are fine achievements, making it the best journal for the synchrotron-radiation community's papers in instrumentation, methods and applications. Whilst much energy and hard work are still necessary, the work targets are clear and within the grasp of a concerted marketing strategy, which has also been instigated in 1998.

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

4.2. Commission on *International Tables*

During 1998, extension and updating of the *International Tables* home page continued. It is accessible from the main IUCr home page (http://www.iucr.org/) and is maintained by U. Shmueli in Tel Aviv, Israel; its updated versions are retrieved by B. McMahon of the IUCr office in Chester. In the spring of 1998, a new volume of *International Tables* was proposed by U. Müller, Kassel, Germany; the volume is tentatively called A2 and has the title: *Relations of Wyckoff Positions between Space Groups and their Maximal Subgroups*. The proposal is presently being considered by the Executive Committee.

4.2.1. Volume A. *Space-Group Symmetry*; Editor Th. Hahn. Preparations for the Fifth, Revised Edition of Volume A continued throughout the year. The LaTeX files of the space-group tables (Sections 6 and 7), prepared by M. Aroyo and his colleagues in Sofia, Bulgaria, were completed by the end of 1998; checking of the data is in progress. The SGML conversion of the text sections will be carried out in Chester in the second half of 1999; the scheduled date for the publication of the Fifth Edition has now been set to the spring of 2000. The new edition will have a substantial number of corrections and small improvements. Two larger changes stand out: (i) the systematic introduction of the new symbol '*e*' for the 'double glide plane' throughout the volume; this symbol was first used in the Fourth Edition, but in a few places only; (ii) the addition of the new Section 9.4 entitled *Some Further Properties of Lattices* by B. Gruber, Prague, Czech Republic. The Fifth Edition of Volume A will also be the basis of the Fifth Edition of the *Brief Teaching Edition* of Volume A.

4.2.2. Volume B. *Reciprocal Space*; Editor U. Shmueli. There was practically no editorial activity during 1998, since (i) the final editorial work on all the revised and new contributions was completed during the early part of 1997 (see the report for 1997), and (ii) publication and, hence, proof-reading and indexes await the completion of the translation to SGML of the Second Edition of Volume B. The scheduled publication date of the Second Edition is now January 2000.

4.2.3. Volume C. *Mathematical, Physical and Chemical Tables*; Editor E. Prince. Typesetting and proof-reading of the Second Edition continued throughout 1998. Because some authors who had previously said that no revisions were necessary chose to make fairly extensive changes at the galley-proof stage, it was necessary to make further corrections to the page proofs of the Second Edition. Nevertheless, at the end of 1998, the entire volume was in page proof except for some front and back matter. Publication is therefore expected in the early summer of 1999, in time to have the finished product available for inspection at the Glasgow Congress.

4.2.4. Volume D. *Physical Properties of Crystals*; Editor A. Authier. The manuscripts which were already in the hands of the editor were updated by their authors in the course of 1998. The missing manuscripts are expected to be delivered during the first half

of 1999. It should, therefore, be possible to transmit the whole volume to the Technical Editor in July 1999. A meeting was held in Prague, Czech Republic, in January 1998, in order to evaluate the two accompanying software packages which will be included on a CD-ROM and form part of Volume D. A protocol was established for the preparation of α versions and a contract was prepared between the authors of the two software packages and the IUCr. The α versions were ready by mid-1998 and distributed to a restricted list of scientists. A β version of the CD-ROM including the two software packages and a presentation page prepared by the IUCr Research and Development Officer should be ready for distribution in the spring of 1999.

4.2.5. Volume E. *Subperiodic Groups*; Editors V. Kopsky and D. B. Litvin. All material for Volume E is with the Technical Editor in Chester. Because the SGML conversion of the material will begin only in January 1999, the tentative date of publication of Volume E is now April 2000.

4.2.6. Volume F. *Macromolecular Crystallography*; Editors M. G. Rossmann and E. A. Arnold. Preparation of articles for Volume F continued throughout 1998. As of January 1999, manuscripts have been received for approximately three quarters of the projected articles in the volume. The papers are reviewed for scientific content and overall consistency of style and expression; completed manuscripts following revisions are sent to the IUCr offices in Chester. The overall quality of the articles received is very high. We anticipate that most contributions will have been completed by the time of the Glasgow Congress and hope that Volume F will be completed and published in 2000.

4.2.7. Volume G. *Crystallographic Information*; Editors B. McMahon and S. R. Hall. The collection of manuscripts for the volume was delayed by the need to develop and implement procedures for the maintenance and usage of distributed dictionaries, and by the final stages of COMCIFS approval for the revised core, powder and macromolecular CIF dictionaries. Synopses for most chapters were requested in late 1998, and chapters are being collected to fulfil the original plan of the volume, which is divided into four parts: (1) Concepts and Specification; (2) CIF Data Definition and Classification; (3) Data Dictionaries; (4) Applications. Part (3) is essentially complete, inasmuch as it contains the CIF dictionaries accepted by COMCIFS (core version 3.1, powder version 1.0, macromolecular version 1.0.00). Chapters in Parts (1) and (4) will collate much information already documented on various aspects of the software development. It is hoped that the bulk of the material for the volume will be in hand during 1999, with publication in the later part of the year if possible. It is also intended that a CD-ROM will accompany the volume and include machine-readable versions of the dictionaries together with software utilities and libraries for using CIFs.

4.2.8. Volume A1. *Maximal Subgroups of Space and Plane Groups*; Editor H. Wondratschek. Volume A1 (renamed from Volume. H, to emphasize the strong relation to Volume A) provides complete tables and diagrams of the maximal subgroups of each space and plane group. For the Contents, see the report for 1995. The data of the subgroup tables are now complete and have been checked in several runs by hand, by the mathematical program system *GAP*, and by *ad hoc* programs. At a meeting in Karlsruhe, Germany, the homogenization of the data on isomorphic subgroups (derived by Y. Billiet in 1993/1994) and the data on non-isomorphous subgroups (derived in Karlsruhe before 1990) was carried out. Many transformations to standard settings have been changed in order to make the tables more user-friendly for the comparison of symmetry-related crystal structures. However, there are still problems to be settled, in particular for those space groups which are presented twice because of different settings (unique axis *b* or *c* for monoclinic space groups; two origin choices; hexagonal or rhombohedral coordinates for rhombohedral space groups). The user's guide and the theoretical part are in preparation. In addition to the tables, the subgroup relations will also be presented in the form of diagrams, separate for *translationengleiche* and *klassengleiche* subgoups. These diagrams have been completed.

Th. Hahn, Chair

4.3. Commission on Aperiodic Crystals

The Commission concentrated its efforts along two main directions. First, the establishment of rules and standards for the publication of crystal data for aperiodic structures and, second, the preparation and coordination of symposia and conferences on aperiodic crystals.

Following the establishment of a checklist for the publication of incommensurate crystals, the Commission pursued its work on the preparation of a CIF dictionary for modulated structures. The work is currently in progress and a proposition close to the final draft is already available on the web. This draft will be improved and completed from the feedback of the specialists working in the field of incommensurate crystals. A preliminary database containing more than 50 modulated structures has been prepared for test purposes. The checklist for the publication of incommensurate crystal structures is directly available from the IUCr web site.

The Proceedings of Aperiodic '97 have been edited by the organizers of the conference, M. de Boissieu, J.-L. Verger-Gaugry & R. Currat. They are currently available (World Scientific, Singapore, 1998). The book by C. Janot and J.-M Dubois entitled *Les Quasicristaux, Matière Paradoxe* has also been published (EDP Sciences, Les Ulis, 1998).

The Commission was actively involved in the preparation of ECM-18, Prague, Czech Republic, with a microsymposium dedicated to aperiodic crystals. Some members contributed actively to the creation of a special interest group (SIG) on aperiodic crystals within the European Crystallographic Association. The web site specially dedicated to this SIG (http://www-xray.fzu.cz/sgip/aphome.html) gives an exhaustive list of activities related to aperiodic crystals that occurred in 1998 in which members of this Commission were involved to various degrees. Let us mention in addition the organization of the Fall 1998 meeting of the Materials Research Society on Quasicrystals which took place in Boston, USA, and the French–German Colloquium on Quasicrystals which took place in Strasbourg, France, in April 1998.

The Commission contributed to the organization of two microsymposia dedicated to various aspects of aperiodic crystals, which will take place in 1999 during the Glasgow Congress. The Commission is presently working on the preparation of the next Aperiodic Conference which will be organized in Nijmegen, The Netherlands, in Summer 2000.

G. Chapuis, Chair

4.4. Commission on Biological Macromolecules

No report has been received from the Chair.

4.5. Commission on Charge, Spin and Momentum Densities

The Commission promotes the study of electron-density distributions in both real and momentum space by bringing together physi-

cists, chemists and crystallographers in conferences, workshops and schools, and by initiating and executing projects. The web page (http://www.tuwien.ac.at/theochem/iucr/csmd.html) contains updated information on the activities of the Commission.

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

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

Maximum Entropy Method (M. Sakata). Since 1991, the MEM has received the full attention of the community served by the Commission. Some highly controversial results have been reported at several conferences since. There was inconclusive and rather diffuse discussion about the MEM project mainly concerning the basis used in MEM. No subject led to more heated discussions than this.

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

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

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

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

4.5.3. Commission meetings. The Commission met in Oxford, UK, during the Gordon Research Conference. The location for the next Sagamore Conference was discussed and L. Dobrzynski was chosen as Chair for the Sagamore XIII Conference to be held in Poland. The projects were discussed and further activities were encouraged. The fields of multipole refinements and maximum entropy, magnetization densities and encounter of theory and experiment in charge-density studies were identified for microsymposia at the Glasgow Congress (all honoured). At the Gordon Research Conference, a proposal was made for new candidates and the next Chair. A special interest group on charge, spin and momentum densities of the European Crystallographic Association was approved at ECM-18, Prague, Czech Republic, thanks to D. Feil and other promoters. The Chair is P. Becker.

K. Schwarz, Chair

4.6. Commission on Crystal Growth and Characterization of Materials

In 1998, the Commission helped to organize the following two International Schools:

(1) The Tenth International Summer School on Crystal Growth (ISSCG-10), Rimini, Italy, 1–6 June 1998. This School was organized by Chairs R. Fornari (MASPEC, Parma, Italy) and C. Paorici (former Commission Chair, University of Parma) in connection with the Twelfth International Congress of Crystal Growth (ICCG-12), which was held 26–31 July 1998 in Jerusalem, Israel. The Commission was engaged in the lecturing programme with three former and two past Commission members as speakers. The school was sponsored and financially supported by the IUCr and other national and international institutions. It was attended by about 60 participants, mostly PhD students, from 19 different countries. The lectures are collected in the book *Theoretical and Technological Aspects of Crystal Growth* published by Trans Tech Publications Ltd, Zürich, Switzerland [*Materials Science Forum* (1998), Volumes 276–277].

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

Four Commission members attended the 12th International Congress of Crystal Growth (ICCG-12) in Jerusalem, Israel, 26–31 July 1998. They met during the Congress and discussed two main topics: (1) candidates for the Commission Chair and Commission members for the triennium 1999–2002; and (2) an International School on Crystal Growth (ISCG) in Brazil. The latter point was discussed with R. Caram, University of Campinas, Brazil. It was

decided to hold ISCG in Campinas, Brazil, 18–24 July 1999 with R. Caram as Chair and H. Klapper as Co-Chair.

During the 12th International Congress on Crystal Growth, 26–31 July 1998 in Jerusalem, the Commission Chair attended the business meetings of the International Organization of Crystal Growth (IOCG). It was again agreed to continue the cooperation of the IUCr and the IOCG in fields of common interest, in particular in the performance of International Schools for young scientists. The essential agenda of the IOCG business meetings and their results are presented in the report on the IOCG.

H. Klapper, Chair

4.7. Commission on Crystallographic Computing

The activities of the Commission in 1998 involved assisting in the preliminary planning for the Computing School to be held in Hinxton, Cambridge, UK, 14–20 August 1999. The School on Frontiers in Computational Crystallography is being organized by G. Bricogne and A. Bloomer with some input from Commission member D. Watkin. The web page for the School can be found at http://www.mrc-lmb.cam.ac.uk/IUCr99/School.html. Subsequent to the meeting, Proceedings will also be available through these web pages.

Preliminary plans are also underway for an Open Commission Meeting (on Improved Data Accuracy and Validation through Software) at the Glasgow Congress.

K. Bourne, Chair

4.8. Commission on Crystallographic Nomenclature

The Commission's primary activities in 1997 were related to the nomenclature of phases that form in phase-transition sequences, the nomenclature of crystallography in *n* dimensions, and cooperation with COMCIFS on matters of nomenclature. The first two culminated in 1998 in the final reports noted below, the third continued harmoniously. A new activity this year originated in a query regarding an earlier nomenclature report; that this issue was the only concern brought before the Commission in the course of the year is an indication of the current absence of nomenclature conflict in the crystallographic literature. All communications within the Commission and its committees during 1998 were electronic or by snail-mail.

The Working Group on Phase Transition Nomenclature, consisting of J.-C. Tolédano (Chair), A. M. Glazer, Th. Hahn, E. Parthé, R. S. Roth, R. S. Berry, R. Metselaar and S. C. Abrahams, completed its 1994 charge of studying the current multiple-choice nomenclature for naming the phases formed sequentially by a material as a function of temperature and/or pressure with a report entitled Structural Phase Transition Nomenclature published in *Acta Cryst.* (1998), A**54**, 1028–1033. The resulting notation uses six separate fields to specify the essential crystallographic and physical characteristics of each phase in the sequence the first time the phase is named in a paper. Following first use, it is recommended that, if the phase is commonly associated with a trivial label such as *a* or *I*, then the first two fields only be used subsequently in the paper to identify that phase; if not commonly associated with a label, then the second two fields should be used. Examples drawn from the sequence of phases formed by nine different materials are provided.

After the Report had been accepted, the Commission further charged the Working Group with extending its nomenclature to incommensurate, polytype, quasicrystal, magnetic and time-resolved phase transitions. Membership in the continued Working Group consists of J.-C. Tolédano (Chair), P. J. Brown, A. M. Glazer, R. S. Roth, R. S. Berry, R. Metselaar, D. Pandey, M. Perez-Mato and S. C. Abrahams.

The Sub-committee on the Nomenclature of *n*-Dimensional Crystallography, consisting of T. Janssen (Chair), J. L. Birman, V. A. Koptsik, M. Senechal, D. Weigel, A. Yamamoto, S. C. Abrahams and Th. Hahn, completed its 1990 charge of assessing the extent to which the representational symbolism then in use may have become so non-uniform as to be unacceptably ambiguous with a report entitled Symbols for Point Group Transformations, Families, Systems and Geometric Classes (in *n*-Dimensions). The Commission accepted the Report, with its unified nomenclature and symbolism for crystallography in arbitrary dimensions, on 16 November 1998; it appears in *Acta Cryst.* (1999), A**55**, 761–782.

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

The Commission Observer [see *Acta Cryst.* (1997), A**53**, 822] has noted that COMCIFS was very active in 1998, approving a new version of the core CIF dictionary and appointing a management group with responsibility for developing the powder dictionary. There were no nomenclature issues in contention.

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

S. C. Abrahams, Chair

4.9. Commission on Crystallographic Teaching

4.9.1. Visiting Professorships. D. Viterbo was Visiting Professor at the University of La Habana, Cuba, 1–14 July 1998, where he presented several lectures concerning X-ray diffraction and crystal structure determination as an introductory part to an International School on Materials which was taking place there. Professor Viterbo's lectures were attended by about 25 persons, and the participants came not only from Cuba but also from other Latin American countries, such as Mexico and Peru.

4.9.2. Contributions to Schools of Crystallography. Financial support from the IUCr was given to the International School in Crystallography on Implications of Molecular and Materials Structure for New Technologies, Erice, Italy, 28 May–7 June, 1998. C. P. Brock and C. M. Gramaccioli participated as teachers, and L. Riva di Sanseverino (a consultant to our Commission) was on the Organizing Committee.

An Open Session on Teaching Crystallography was organized by Å. Oskarsson and D. Puscharowsky at ECM-18 in Prague, Czech Republic. This session was attended by several persons, with considerable success.

The Commission is presently organizing an Open Commission Meeting at the Glasgow Congress.

C. M. Gramaccioli, Chair

4.10. Commission on Electron Diffraction

The Commission was involved with a School on Electron Crystallography in Stockholm, Sweden, with support from the IUCr. It

was organized by S. Hovmöller and X.-D. Zou with invited lecturers from overseas by G. L. Cascarano (Italy), Marks (USA), R. J. Cernik (UK) and J. W. Steeds (UK). It was a well attended school that stimulated a good deal of interest in the wide range of international participants.

Members of the Commission have been involved with the organization of several conference sessions related to electron diffraction. In particular, there were two relevant sessions at the 14th International Congress on Electron Microscopy in Cancun, Mexico, in August/September. One of these, on Electron Crystallography, was organized by S. Hovmöller, the other, on Convergent-Beam Electron Diffraction, had an invited talk by J. W. Steeds.

J. W. Steeds, Chair

4.11. Commission on High Pressure

In the final year of its first triennium, the Commission's principal activity has continued to be the organization of symposia and workshops. There is such rapid change and development in the field that regular meetings have proved essential to keep the community in touch with the latest science and techniques, and also to keep the Commission abreast of growth in the community and to draw in new people.

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

All members of the Commission met together during this workshop to agree the final Terms of Reference to recommend to the Executive Committee – which have since been approved. Amongst other things, the Commission has undertaken to work to strengthen the links between high-pressure crystallography and the wider field of high-pressure science; in so doing, to make the scope of 'high-pressure crystallography' as inclusive as possible without compromising its crystallographic identity; to make information about high-pressure methods and facilities widely available; and where possible to assist young scientists and others new to the field. The opportunity was also taken to discuss future membership of the Commission, the high-pressure sessions at the Glasgow Congress, and other future plans and activities.

Members of the Commission have been very actively engaged over much of the year in shaping the high-pressure sessions for the Glasgow Congress, particularly A. Katrusiak who is a member of the Programme Committee. All other members and consultants are acting as Chairs or Co-Chairs for the Commission's six microsymposia and one Open Commission Meeting (OCM). This OCM represents the Commission's first attempt to disseminate information about high-pressure techniques and best practice (in keeping with its Terms of Reference) – in this case for laboratory-based diffraction and spectroscopy. On a larger scale, plans are now under way to organize a School on High Pressure Crystallography at Erice, Italy, in May–June 2003. Commission member A. Katrusiak is to be the Director of the School. The Commission also intends to organize workshops in 2000 and 2001 at venues yet to be finally agreed.

R. J. Nelmes, Chair

4.12. Commission on Neutron Scattering

Neutron scattering conferences are now flourishing worldwide and subsequent to the International Conference on Neutron Scattering held in Toronto, Canada, 16–20 August 1997, there is the Second European Conference on Neutron Scattering, 1–4 September 1999, in Budapest, Hungary, organized by the European Neutron Scattering Association. A significant proportion of the Asian Crystallographic Association's meeting in Malaysia (October 1998) was devoted to a neutron scattering microsymposium organized by members of the Commission and in May and September 1999 there will be international meetings on small-angle neutron and X-ray scattering: SAS 99, Brookhaven National Laboratory, USA, 17–20 May 1999, and 6SXNS (surface X-ray and neutron scattering), The Netherlands, 12–17 September 1999. Despite this variety of international interests, the Commission has a full slate of microsymposia for the Glasgow Congress and a promising satellite meeting organized by C. Carlile set for Oxford, UK, just before the General Assembly and Congress.

Since 1992, the Neutron Scattering Association of Japan (NSAJ) has held its annual meeting every December; it is open to participants worldwide. Out of about 200 participants in 1998, about 10 came from outside Japan. It is hoped that such an activity may seed a regional meeting in Asia/Oceania in the near future. Commission member Y. Fujii has been President of NSAJ since 1997.

Two meetings devoted to neutron scattering were held in Russia: (1) Deuteration of Biological Molecules: Applications to Neutron Scattering and NMR, Dubna, 19–25 May 1998; and (2) Condensed Matter Physics with Neutrons at IBR-2, German–Russian User Meeting, Dubna, 2–4 April 1998.

An initial attempt to coordinate meeting dates for the long term was made at the Closed Commission Meeting in 1997 but matters were already too far advanced to have much effect. The Commission will continue to work for a proper intercalation of meetings through the participation of its members on the organizing committees of related activities but the news is not bad – neutron scattering seems to be of growing importance in the world and is likely to increase in its scope of applications as well as the number of adherents. The developments in the Asia/Australasia/Oceania region foreshadowed in the 1996/1997 report are continuing and it might well be that the next three-year period will begin to see more regular meetings of neutron scatterers in that region. At present, the numbers are not as large as those in Europe or even as those in North America. Recent decisions in Japan and Australia suggest a considerable investment in new instrumentation for neutron scattering in the region, which is sure to provide a scientific and technological stimulus to the communities.

In March 1998, Professor White attended, and was responsible for chairing, the exit session of the International Advisory Group for the

Japanese Atomic Energy Institute's spallation neutron source project as well as participating as a member of the advisory group for the KEK (Tskuba) Japanese Hadron Project at that Institute. In October 1998, a major decision by the Japanese government to bring the two projects together has led to the formation of the Japanese Atomic Energy Institute–KEK joint project which has three major goals, one of them being very important for the future development of neutron scattering.

In addition to providing a very powerful 50 GeV proton accelerator for fundamental particle physics and neutrino physics, the new joint project will provide accelerated protons at 3 GeV for a spallation neutron source capable of rivalling the new spallation neutron source (SNS) project under construction at the Oak Ridge National Laboratory, USA, and the foreseen SNS project for Europe. The spallation neutron source target will be of a power of at least 1 MeV and will have a mean neutron flux approaching that of the Institut Laue–Langevin (ILL), Grenoble, France, with a pulsed intensity about 100 times greater than that. This will be a major development in neutron scattering when built. A decision is expected on it during 1999. The third aspect of this project is to begin the research and development work for 'spallation neutron burning' – a possible future method for the destruction or great reduction in the activity of transuranic nuclear waste.

In addition to the major conferences mentioned above, members of the Commission have been involved in a number of workshops and major conference presentations. These include the Workshop on Powder Neutron Diffraction at ILL, Grenoble, France (March 1999) and the microsymposia celebrating the fiftieth anniversary of the IUCr in association with ECM-18, Prague, Czech Republic, August 1998, and AsCA '98, Selangor, Malaysia, October 1998.

Once again, it is a pleasure to thank members of the Commission for their independent action and effort in connection with the planning of the Glasgow Congress and their participation in also planning major neutron scattering events during 1998. The important contribution made to neutron scattering and the work of the Commission by *Neutron News* and by G. Lander through his editorship is again acknowledged with thanks.

J. S. White, Chair

4.13. Commission on Powder Diffraction

The Commission has expended a great deal of energy on the preparations for the Glasgow Congress. The Commission decided early in the triennium that it would not hold a separate satellite as it had in the past but would integrate the activities of the powder community with mainstream crystallographic activity. It was felt that this was more appropriate because of the advances made in the field since the Commission was founded 12 years ago. The Commission has also played an active role in promoting meetings and workshops. It has completed and nearly completed (respectively) its two major projects in publishing Rietveld refinement guidelines and establishing protocols for quantitative phase analysis. The results of the latter project will be presented at the Glasgow Congress. The mailing list for the *Newsletter* has now expanded to 1400. The establishment of the ECA and associated SIGs has raised interesting new ways of interacting with the European powder community that the Commission is investigating.

4.13.1. Meetings/workshops/schools. EPDIC 6 was held in Budapest with Commission-endorsed IUCr support. This was organized by T. Ungar with a focus on strains and stresses in materials. The meeting had a very broad range in addition to the major themes and covered structure solution to phase matching. The Commission held its business meeting in the old Department of Egyptology, now part of the science faculty. Commission consultant Shao Fan Lin produced a Chinese version of the *Newsletter*, and secured IUCr funding for visiting lecturers to a meeting on powder diffraction in Kunming, China, in 1999. Commission member S. P. Sen Gupta has edited the latest version of our *Newsletter* and organized a very successful workshop in Calcutta, India. A large local population in addition to visiting lecturers attended this meeting.

By far the most activity has been expended in assembling the suggestions for the Glasgow Programme Committee for the microsymposia, speakers, Chairs and Co-Chairs to present the very best scientific research using powder diffraction. We are especially grateful to Commission member L. B. McCusker who has been one of the coordinators on the Programme Committee. The other coordinator though not on the Commission was E. Antipov; we are grateful to him for his efforts in assembling these sessions. The whole Commission has actively participated in this activity and has with the Programme Committee produced the following programme. C. Giacovazzo and D. Cox are presenting keynote talks on structure solution and materials research, we have microsymposia on very applied themes such as thick coatings, on-line industrial processing, line broadening, nonstructural profile fitting and *in situ* experiments. The Commission also assembled the ideas for microsymposia on structure solution, difficult refinements, modelling and a session commemorating 30 years of Rietveld refinement. We have also been collaborating with other Commissions and have produced two combined sessions with electron diffraction and X-ray absorption spectroscopy.

4.13.2. Projects. *Quantitative phase analysis*. Four samples of carefully constituted multiple composition were distributed to those people who volunteered for the study. There was an excellent response to the original request for participants and 140 questionnaires were sent out. The original chemical specification has changed slightly and is now better defined. The samples are: (1) corundum + zincite + fluorite; (2) as (1), but with preferred orientation and brucite; (3) as (1), but with amorphous glass; and (4) corundum + magnetite + zircon. Thanks are due to I. C. Madsen particularly but also to Commission consultant R. J. Hill, member D. K. Smith and a large number of co-workers. I. C. Madsen will present the results of the study in full at the Glasgow Congress.

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

Newsletters. There have been two *Newsletters* produced in this period, one edited by L. M. D. Cranswick (guest editor), the other in production by Commission member S. P. Sen Gupta. Both editions are available on the World-Wide Web at http://www.iucr.org/iucr-top/comm/cpd/index.html. This web site has been considerably updated and is now fully operational containing useful links and information for the powder community. Mirror sites have been created in Australia and the USA.

R. J. Cernik, Chair

4.14. Commission on Small-Angle Scattering

During the past year, the Commission has continued in its tutorial and community building efforts with three workshops. An inter-

laboratory test programme to evaluate small-angle-scattering test methods is currently in its initial design stages. The Commission is providing considerable assistance to SAS 99, the XI Triennial World SAS Congress, taking place at Brookhaven National Laboratory, USA, 16–20 May 1999.

The first workshop, on Data Handling for Small-Angle Scattering, was held in conjunction with the 1998 American Crystallographic Association Annual Meeting in Arlington, VA, USA. Commission members J. D. Barnes and D. Svergun were aided by M. Capel and J. S. Pedersen as they explored issues ranging from proposed standard data formats to visualization tools for user facilities.

Another edition of this workshop will be conducted on 16 May 1999 in conjunction with SAS 99. The workshop title is canSAS II in recognition of the close relationship between the Commission and the canSAS (Collective Aid to Nomadic Small-Angle Scatterers) project (see http://www.ill.fr/lss/canSAS/welcome.html).

A second workshop, conducted as a tutorial for end users of SAS techniques in the polymer field, was held under the joint sponsorship of the Commission and the American Chemical Society Polymeric Materials Science and Engineering Division. The workshop was part of the ACS's August 1998 National Meeting in Boston, MA, USA. The workshop title was SAS in the Industrial Plastics Laboratory. Commission Chair J. D. Barnes was the instructor.

Technical activity in the standardization area is slowly ramping up. D. Svergun and M. Malfois of EMBL have circulated drafts of a sasCIF format and have worked with I. D. Brown and B. Toby of COMCIFS to bring sasCIF into conformance with the applicable standards. This work will be carried forward at canSAS II and it is expected that the sasCIF format will be used in the upcoming inter-laboratory test programmes.

At the time of writing, several compression-molded samples of various polyethylene resins are being evaluated as candidate samples for an interlaboratory test programme. The next stage of the project involves distributing these samples to a limited number of trusted laboratories. These laboratories will be asked to evaluate the samples using their standard procedures with the goal of providing the best possible description of the SAS properties of the samples. They will be asked to report the results using the sasCIF standard.

A task group will review the results from this preliminary study and then design a suitable protocol for a larger study involving any laboratories in the SAS community who wish to participate. Those members of the community who are aware of the project have been quite supportive. The intent and the approach are somewhat different from that of the 1978 effort [R. W. Hendricks *et al.* (1978). *J. Appl. Cryst.* **11**, 196–205], but we hope that it will prove to be equally useful.

J. D. Barnes, Chair

4.15. Commission on Structural Chemistry

1998 was a relatively quiet year for the Commission. Introducing a broad-based chemical audience to the benefits of X-ray crystallography by reaching out beyond the crystallographic meetings is a continuing goal of this Commission. A session on Advanced Methods of Structure Determination by Diffraction and Related Methods organized by A. Clearfield for the American Chemical Society meeting in Dallas, Texas, USA, in the spring of 1998 represented one way of accomplishing this goal. In 1998, the annual meetings of the regional crystallographic associations all included sessions and/or workshops on topics of interest to the community represented by the Commission. The Commission also gave its support to a workshop on Modern Techniques in Structural Chemistry of Microcrystalline and Amorphous Compounds, which was scheduled for October in Germany. Unfortunately, this workshop was cancelled for lack of participation. Commission member V. Belsky was involved in the organization of the first Russian National Conference on Crystal Chemistry. During 1998, the Commission also made further contributions to the organization of the programme for the Glasgow Congress.

The Commission continues to be concerned about the disappearance of crystallographic education from standard university course work, the tendency towards the use of 'black box' applications without any fundamental understanding of the science of crystallography, and the increasing number of errors appearing in the crystallographic literature. Therefore, in addition to sponsoring symposia and workshops, it must be one of the tasks of the Commission to develop recommendations for the appropriate approval of crystallographic research results in publications of related fields. The Commission also intends to work with the Commission on Biological Macromolecules and the Committee on Crystallographic Databases to develop guidelines for deposition of structure factors for all structures.

J. L. Flippen-Anderson, Chair

4.16. Commission on Synchrotron Radiation

It was decided that the venue for the Glasgow Congress Synchrotron Radiation Satellite Meeting would be Daresbury Laboratory, UK, 2–3 August 1999, prior to the main Glasgow Congress. R. J. Cernik agreed to chair the satellite meeting, entitled From Source to Science, covering topics such as coherence, polarization, high resolution, dynamic studies and anomalous scattering. The main aim is for a small well focused friendly meeting with a single set of sessions.

The Commission has also been heavily involved in the main Glasgow Congress. Three members (Y. Amemiya, R. Feidenhans'l and A. Yonath) served as members of the Programme Committee. Through the activities of the Commission, the interaction between users groups of synchrotron-radiation facilities all over the world has been enhanced.

Y. Amemiya, Chair

4.17. Commission on XAFS

The Commission, in coordination with the International XAFS Society, has continued to promote the development of XAFS through sponsorship of the International Conferences on XAFS, support of the IXS web page, development of standards and criteria for XAFS, creation and dissemination of educational materials regarding XAFS, and other activities.

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

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

The Standards and Criteria (S&C) Subcommittee has continued to be active. Prior to 1998, it consisted of three subgroups: experimental, analytical and error reporting. In 1998, a group of scientists in the area of X-ray magnetic circular dichroism (XMCD) asked to affiliate with the S&C committee. This idea was accepted and they are now actively working on a report dealing with standards for XMCD. Because their scope is a little broader than XAFS, they are working in a parallel and coordinated fashion with the main committee. It met in Seattle, USA, in July, 1997 and again in Chicago, USA, just prior to XAFS X. An oral report and summary of recommendations for error reporting which are under consideration by the S&C committee was made to the meeting. A draft report of the activities for the past two years is circulating in the committee. It is hoped that a final version will be ready soon. When it is, it will be posted on the IXS web page. There is also a set of recommendations for error reporting under final consideration by the S&C committee. If approved by them, these will be forwarded to the IXS Executive Committee for approval as official policy of the IXS. The mechanism for this is still being determined but will involve time for input and suggestions from the community. After adoption by the IXS, the recommendations will be posted on the IXS web page. In addition, it is hoped that wider dissemination will be possible through links to the IUCr web page and through publication in an IUCr journal (*e.g. Journal of Synchrotron Radiation*).

The web-page committee has recently been updating and expanding the web page. It now has on-line XAFS Society registration and a community listing as well as many links to other synchrotron and related sites. A listing of all committees is on the site and work is under way to add all committee reports to this site. The data listing provided by F. Lytle continues to receive attention from the community as well as a listing of analytical software and some preliminary descriptions of the features they contain. There are plans to expand other features of the site including a newsletter, and the abstracts from XAFS X and, hopefully, XAFS XI. An Education Committee is being formed under the leadership of G. Bunker. It hopes to coordinate with schools and courses that teach XAFS around the world regarding the content of their curricula, to develop standard educational materials and, possibly, to organize XAFS training courses at locations around the world that may not have the expertise or resources to run a course themselves.

Finally, as part of the effort to increase the coupling of the XAFS community with the IUCr, a session on XAFS was organized by the Commission at the ACA meeting in St Louis, USA, in 1997. It is planned to continue to sponsor related session such as this at other related meetings.

J. Penner-Hahn, Secretary

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 1998 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1998 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1999, but approved in 1998, are listed below:

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

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

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

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

The organizers of all IUCr-sponsored meetings are requested to recommend the journals of the IUCr as a suitable channel of publication for the original papers presented at the meeting. 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. Schenk. A new Chair will be appointed in Glasgow. 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.

H. Schenk, Chair

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

6.1. Information services

The Committee has continued its task as editorial body for the online web information services of the IUCr. A high priority is set on providing up-to-date information of use to the whole crystallographic community. The design of the pages has been restyled and a higher degree of uniformity of presentation has been achieved. The current design is judged by many to be rather austere but a considerable amount of work and design talent would be required to modify this. It is not evident that a much increased penetration of the community would result. The work of maintaining the content continues to be operated on a distributed basis with the major part of the input coming from Chester, Geneva and Paris. Further extension of the content requires the collaboration of the Commissions, Committees, Editors of the IUCr and individual crystallographers. The functioning

and software of the mirroring mechanism and its underlying file structure have been revamped. This has resulted in a greatly improved speed and efficiency in the file transfer and in the need for reduced storage space on the mirror servers. There is still a need for further mirrors to serve the needs of local communities whose access is limited by slow international transfer. National Committees and Regional Associates with a responsibility for areas that are currently poorly served are encouraged to make all possible effort to set up mirror servers.

6.2. List server

An IUCr e-mail-based discussion list server was put into operation in early 1998. For this purpose, the Committee drafted a *Policy Document on Creation and Management of Discussion Lists*, which received the approval of the IUCr Executive Committee. The IUCr list server provides facilities for e-mail-based discussion lists on topics relevant to the IUCr and the field of crystallography. It can greatly facilitate the work of IUCr Commissions, Committees *etc.* At present, the server is only lightly used.

6.3. *World Directory of Crystallographers*

A functional specification for a new implementation of the WDC as a relational database using technology parallel to, but not directly integrated into, the IUCr editorial office production database is currently at the discussion stage. The design of this database is centred around the need to allow rapid, but supervised, updating of records in a secure manner. It is intended that it should be possible to consult the database online by a variety of the most popular industry-standard protocols.

6.4. Glasgow CD-ROM

The Committee is collaborating in the project to produce the CD-ROM for the Glasgow Congress. This is the first time that the IUCr has ventured into the realm of publication on CD-ROM. On arrival, Congress participants and, in September 1999, subscribers to *Acta Crystallographica* Section A will receive a copy of the CD-ROM. Printed copies of the Congress Abstract Book will be distributed to Congress participants but not to subscribers to *Acta*. The CD-ROM is sponsored by a commercial organization. The CD-ROM will contain the Congress Abstracts, the sponsoring organization's web site, a selection from the IUCr's web information service, including the General Assembly papers, and the contents of a book, now out of print, for which the IUCr holds the copyright. Many aspects concerning the design and technical aspects of this production were discussed at a meeting in Chester in November 1998 between the Congress organizers, the sponsoring organization, the Committee, the Promotions Officer and the Executive Secretary. The scanning and digitization of the book by a commercial service will also provide excellent experience for the electronification of all back numbers of the IUCr journals.

6.5. Online access for journal content in *Acta Crystallographica* Section D

Negotiations were carried out with Munksgaard to provide an online version of *Acta Crystallographica* Section D on their Synergy server, which is operated by Healthgate. Healthgate were supplied SGML, PDF and image files of the journal, and the Managing Editor visited their offices in Boston at the time of the ACA Meeting. Development has been slower than expected, but the journal should become available online during 1999.

6.6. Checking

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

The Committee was pleased to welcome L. M. D. Cranswick as a new member in 1998. The Chair of the Committee visited the IUCr editorial office in Chester, UK, in November 1998.

H. D. Flack, Chair

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

7.1. Report on the future structure of COMCIFS

In May 1998, COMCIFS presented the Executive Committee with a report on its work up to that date and proposals for the future structure of COMCIFS. Among the recommendations accepted by the Executive Committee was one that required COMCIFS to recommend to the Executive Committee, after each General Assembly, a slate of about six names of people willing to serve as full (voting) members of COMCIFS for the following triennium. This procedure will be followed starting with the Glasgow Congress.

7.2. Established Dictionaries

Following the recommendations in the report mentioned above, Dictionary Maintenance Groups (DMG) have been established for each of the approved dictionaries. The first DMG to be established was that for the mmCIF dictionary. It is headed by P. M. D. Fitzgerald. This was followed by a DMG for the coreCIF dictionary headed by I. D. Brown and one for the pdCIF dictionary headed by B. Toby. The first two DMGs have been active in preparing new versions of their respective dictionaries, both of which are expected to come to COMCIFS for approval before the Glasgow Congress.

7.3. Dictionaries in progress

Now that the three principal dictionaries are approved, attention is being given to those under preparation.

1. The Modulated Structures (msCIF) Dictionary is being prepared by a group headed by G. Madariaga. This dictionary is in an advanced stage and should receive preliminary approval before the Glasgow Congress.

2. The Images and Higher Dimensional Data (imgCIF/CBF) Dictionary is in an advanced state of preparation by a group headed by A. Hammersley. It, too, is expected to receive preliminary approval before the Glasgow Congress. The purpose of this dictionary is to provide a file structure for recording images, initially diffraction patterns recorded by two-dimensional detectors, but ultimately any image, with extensions to higher dimensions possible. Because image files can be large, it will also be possible to store imgCIFs as binary imgCBFs (Crystallographic Binary Files). The two files have the same structure, the differences lying only in the different requirements of ASCII and binary representations.

3. The Small-Angle Scattering (sasCIF) Dictionary is being prepared by a group under the leadership of M. Malfois. A draft of this Dictionary is being refined.

4. The Magnetic Structures (magCIF) Dictionary is being prepared in conjunction with the magnetic structure database constructed by W. Sikora and her colleagues.

5. The Symmetry (symCIF) Dictionary is at the stage of an early draft prepared by a group headed by I. D. Brown. Its purpose is to cover all the concepts used in describing symmetry, initially focusing on those in Volume A of *International Tables for Crystallography* but with extension to other symmetry concepts and not restricted to three dimensions.

6. After a slow start, preparation of the Electron Density (rhoCIF) Dictionary will soon be undertaken by a group being assembled by P. Mallinson.

7.4. Other matters

B. McMahon and H. Bernstein are working on a scheme to allow dictionaries to be concatenated. This means that when a specialized dictionary such as the mmCIF dictionary is called, it would automatically merge with any other dictionaries, such as coreCIF, needed to read or write a complete CIF. In this way, it would not be necessary to include the core data items (such as space group and unit cell) in every dictionary. The intent is that all dictionaries would be loaded from the web as needed, so the process of concatenation would be transparent to the user. The problem of merging dictionaries is complicated by the use of two different and incompatible Dictionary Definition Languages (DDL). The coreCIF and pdCIF dictionaries use DDL1 while the mmCIF dictionary uses the much more structured (but more cumbersome) DDL2. At present, COMCIFS does not have a policy on whether to maintain two different sets of dictionaries indefinitely or whether to move all dictionaries to DDL2. Many of the new dictionaries are being written using DDL2, partly because it forces a more rigorous structure on the dictionary and partly because converting DDL2 to DDL1 is much easier than converting DDL1 to DDL2. COMCIFS will be looking at a number of other items relating to the future of data representations such as the relation between XML (or SGML) and CIF and ways in which functional relationships between different data items in a CIF can be encoded within the dictionary.

7.5. Thanks

It gives me great pleasure to acknowledge the hard work that many of my colleagues have contributed to this project. I would particularly like to thank COMCIFS' Secretary, B. McMahon, whose patient manner and wise judgement has guided us safely through uncharted waters.

I. D. Brown, Chair

8. Committee on Crystallographic Databases

The present membership is H. M. Berman (USA; Chair), F. H. Allen (UK), H. Behrens (Germany), P. M. D. Fitzgerald (USA), G. L. Gilliland (USA), S. R. Hall (Australia), J. R. Helliwell (UK), J. Faber (USA), J. R. Rodgers (Canada), J. L. Sussman (Israel) and the IUCr President.

9. Promotion Committee

A Promotions Officer, Miss A. J. Sharpe, was appointed in February 1998 and this was accompanied by the start of a more aggressive campaign to market the IUCr publications and services to the crystallographic community as well as to other structural science communities. Particular attention was given to the relatively new *Journal of Synchrotron Radiation*, and early results show that the number of personal subscriptions has risen owing to increased exposure at relevant conferences and users' meetings. 1999 will see the results of an initiative to promote all journals by highlighting articles within the *IUCr Newsletter*.

Advertisers were solicited to the three Special Issues published in 1998, generating a revenue of nearly USD 40 000. The provision of the *World Directory of Crystallographers* (*WDC*) database was recognized as a potential source of revenue, and a charging policy was introduced. The scale of charges used for providing specific mailing lists from the *WDC* was reviewed.

A. M. Glazer, Chair

10. *IUCr Newsletter*

The *IUCr Newsletter* is a vehicle to broadcast and promote the interests and activities of the IUCr and its Commissions and Committees and to strengthen communication in the world community of crystallographers. Four issues of the *Newsletter* were published in 1998. Each 24 page issue contained a letter from the President, news of IUCr Commission activities, crystallographic meeting announcements and reports, obituaries of prominent crystallographers, notices of elections, awards to crystallographers, and information on books, web sites, resources, and activities of interest to crystallographers. Contributions from crystallographers everywhere are sought, material is gathered from newsletters of crystallographic associations and societies and from leading science news magazines. Photographs are provided by contributors or drawn from the personal collection of the editor. Almost all contributions are published and all material is edited to varying degrees. In 1998, special articles on advances in synchrotron research and protein crystal growth were solicited and generously contributed by J. R. Helliwell and A. McPherson, extensive coverage of ECM-17, ECM-18 and the BCA 1998 Spring meeting were published, and five pages were devoted to information concerning the Glasgow Congress. The Second Circular for the Glasgow meeting was distributed with Volume 6, No. 4.

The *Newsletter* is distributed to 587 libraries and 15 000 crystallographers and other interested individuals in 39 countries. Cost of distribution in Australia, Colombia, Croatia, Cuba, Czech Republic, France, India, Italy, Japan, New Zealand, Poland, South Africa, Switzerland, Taiwan, The Netherlands and Venezuela is borne by crystallographic associations or institutions or by individual crystallographers in these countries. Copies of the *Newsletter* are sent upon request to organizers of meetings sponsored by the IUCr.

A *Newsletter* exhibit was set up at the 1998 European Crystallographic Meeting and the 1998 meeting of the Asian Crystallographic Association where copies of the *Newsletter* were distributed and material for reports on the meetings was gathered.

W. L. Duax, Editor

11. Regional Associates and Scientific Associates

11.1. American Crystallographic Association (ACA)

During the reporting period, there was no official contact between the ACA and the IUCr Representative to the ACA.

P. Coppens, IUCr Representative

11.2. Asian Crystallographic Association (AsCA)

The third Asian Crystallographic Association Conference (AsCA '98) was held in Hotel Equatorial, Bangi, Malaysia, 13–15

October 1998. More than 300 scientists and students from 14 countries and/or regions participated in this conference. During the three-day programme, all the participants had successful academic exchanges and helpful discussions. There were four plenary lectures and 14 microsymposia. The topics ranged from Diffraction theory, Structure refinement, Aperiodic structures, Biocrystallography and Proteins *etc.* to Instrumentation and other categories.

To celebrate the 50th anniversary of *Acta Crystallographica* and the IUCr, a symposium was also held during AsCA '98. This symposium was sponsored by the IUCr and consisted of four lectures. E. N. Baker, the President of IUCr, gave a lecture on the history of IUCr, and his talk received a warm welcome.

A small instrumentation exhibition was also held at AsCA '98. Contributions were received from seven professional bodies and institutions, such as the IUCr, the Crystallography Society of Japan, the University of Kebangsaan Malaysia *etc.* Financial support from Rigaku International Japan, MAC Science, the International Centre for Diffraction Data, Bruker AXS and Marresearch are gratefully acknowledged. At the opening ceremony, Z. Zhang, the President of AsCA, welcomed all the participants and at the closing ceremony thanked those who made the conference possible.

M. Tanaka, IUCr Representative

11.3. European Crystallographic Association (ECA)

The Eighteenth European Crystallographic Meeting (ECM-18) was held in Prague, Czech Republic, 15–20 August 1998, and gathered about 1000 participants. The conference was organized in the Technical University of Prague and followed the usual scheme of plenary lectures, microsymposia and poster sessions. All areas of crystallography were well represented with a special emphasis on materials sciences.

The ECA is now officially registered in Nijmegen, The Netherlands, and thus established as a legal organization. The Council met together with the Executive Committee on 17 August 1998. As a consequence of the legislation of The Netherlands, modifications to the Statutes and By-Laws were proposed by the Secretary P. Beurskens and accepted by those present. As stated by the President C. Giacovazzo, members in all three categories (national, affiliate and individual) were admitted to ECA. It was noted that South Africa was accepted as a National Member of the association. The Council approved with pleasure several Special Interest Groups (SIGs), which asked for admission according to the By-Laws. ECM-19 will be held in Nancy, France, 25–31 August 2000. The site for ECM-20 will be Cracow, Poland.

H. Fuess, IUCr Representative

11.4. International Organization of Crystal Growth (IOCG)

During 1998, the activities of the IOCG were mainly governed by the preparation and performance of the following scientific meetings.

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

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

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

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

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

The following Officers and Executive Committee members are elected for the period 1998–2001: President: T. Nishinaga (Japan); Vice-Presidents: K. W. Benz (Germany), R. F. Sekerka (USA); Secretary: T. E. Kuech (USA); Treasurer: C. F. Woensdregt (The Netherlands); Past President: B. Cockayne (UK); Honorary Principal Founder IOCG: M. Schieber (Israel); Executive Committee members: J. J. Favier (France), A. Horowitz (Israel), Jiang Min-Hua (People's Republic of China), T. Ohachi (Japan), V. V. Osiko (Russia), C. Paorici (Italy), H. J. Scheel (Switzerland), J. N. Sherwood (UK). *Ex officio* members of the Executive Committee: J. Buttrey (USA), P. M. Dryburgh (UK) (IOCG Representative to the IUCr), H. Klapper (Germany) (IUCr Representative to the IOCG), J. P. van der Eerden (The Netherlands) (IOCG Representative to IUPAP), J. N. Sherwood (UK) (IOCG Representative to IUPAC), and others.

In addition, 35 Councillors representing 18 national associations, five Councillors representing nations who do not have a national association, and four *ex officio* Councillors representing International Unions were approved. The *ex officio* Councillor representing the IUCr is M. H. Dacombe, the Executive Secretary of the IUCr. The following IOCG prizes, sponsored by the ICCG-12/ICVGE-12 Organizing Committee, were awarded: The Frank Prize to K. A. Jackson (USA) and the Laudise Prize to I. Akasaki (Japan). The Thirteenth International Congress on Crystal Growth (ICCG-13) and the Eleventh International School on Crystal Growth (ISSCG-11) will be held in Kyotanabe, Japan, 29 July–3 August 2001.

H. Klapper, IUCr Representative

11.5. International Centre for Diffraction Data

The ICDD membership has grown to 266 with the infusion of many new overseas members. At present, it has 133 members in the USA and exactly the same number from outside the USA. The second major change is that it has pursued joint activities with other database organizations, notably Fachinformationszentrum (Inorganic Crystal Structure Database) and the Cambridge Crystallographic

Data Centre (Cambridge Structural Database). It has drawn up contracts with both of these organizations that allow the ICDD to calculate powder patterns from the crystallographic data. In addition, each of the three organizations has pledged to add cross references in their databases, thus allowing user interaction between several databases – permitting new extensions of Computational Materials Design. The sub-committees and task groups are actively engaged in screening and reviewing all new and historical data. The Technical Committee has established Co-Chairs on each of the world's continents and is looking forward to the ICDD operating as a truly international organization. Associated with this internationalization of the ICDD has been its support of the Denver X-ray Conference's organizing committee in establishing an International X-ray Analysis Society. ICDD is sponsoring various international institutions to produce experimental powder data, it sponsors scholarship programmes, and gives financial support to selected national and international meetings. Last year, the ICDD took over the administration of the Denver X-ray Conference, and it continues to support domestic and overseas clinics and training courses.

R. J. Cernik, IUCr Representative

12. Representatives on Other Bodies

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

The International Union of Pure & Applied Chemistry (IUPAC) closed its offices in Oxford, UK, in October 1997, re-establishing its Secretariat in Triangle Research Park, North Carolina, USA. The annual meeting of IDCNS in 1998 was held 14–15 August in nearby Durham, NC. A major responsibility of IDCNS is the review of nomenclature reports that originate in one or more IUPAC Commissions, primarily for the resolution of potential interdivisional nomenclature conflicts, before the report is published in *Pure & Applied Chemistry*. 21 such reports were reviewed since the last meeting. All provisional and all final IUPAC nomenclature recommendations, also all IUPAC books, are in the process of becoming accessible at http://www.iupac.org as IUPAC moves toward full electronic publishing. Among recent IUPAC publications of possible interest to crystallographers are *Principles of Chemical Nomenclature, a Guide to IUPAC Recommendations* by G. J. Leigh, H. A. Favre & W. V. Metanomski (1998, Oxford: Blackwell), and *Compendium of Chemical Terminology, IUPAC Recommendations*, Second Edition, by A. D. McNaught & A. Wilkinson (1997, Oxford: Blackwell). A related publication of interest is the 7th Edition of *Le Système International d'Unités* (the SI Brochure) published in 1998 by the Bureau International des Poids et Mesures (BIPM).

The International Standardization Organization (ISO) and IUPAC recommend that numerical values of physical quantities in tables and figures be labelled by their international symbol divided by the SI unit, for example lambda/nm, not lambda (nm) [the IUCr would use lambda/Å [not lambda (Å)]. The reason is to allow manipulation of physical quantities, numerical values and units by the ordinary rules of algebra and to eliminate possible ambiguity by representing numerical quantities with an unambiguous dimension of unity. ISO practice for displaying dates uses the order year/month/day, thereby eliminating the present ambiguity between the European order day/month/year and the US order month/day/year. The correct international use of italic and roman fonts for symbols in scientific text was reiterated, in view of the common failure of many manuscripts to follow them. The usage is given in detail in the IUPAC Green Book *Quantities, Units and Symbols in Physical Chemistry*, in ISO 31 and in the SI Brochure. The overall rule is that symbols, including single letters of the Greek alphabet, representing physical quantities (or variables) should be italic, but symbols representing units, or labels, should be roman. The recommendation that unusual abbreviations always be defined in a paper at its first use was also emphasized.

A new list of fundamental constant values will appear in the next edition of the IUPAC Green Book, currently in preparation. A strong need exists for an internationally agreed set of 'preferred' names of organic compounds for use in legal, medical and related fields.

The Comité International des Poids et Mesures supervises the work of the BIPM in Sèvres, France; it generally accepts the advice of its Comité Consultatif des Unités (CCU) on all matters referred to them. The Chair of IDCNS, currently serving also as President of CCU, reported on CCU activities. Among these is the agreement to delete the class of supplementary SI units so there are now only base and derived units; the proposal to extend the range of SI prefixes from the present $10^{\pm 24}$ to $10^{\pm 48}$; and important progress made toward a new and fundamental definition of the kilogram.

A major concern of IDCNS was the recent Report of the IUPAC Strategy Development and Implementation Committee (SDIC), which proposes to terminate most of the long-term Commissions of IUPAC and replace them by short-term Task Groups to carry out scientific projects. IDCNS proposed more evolutionary means for improving the less-effective Commissions rather than SDIC's revolutionary proposals.

The next meeting of IDCNS will be in Berlin, Germany, 11–12 August 1999, dates that completely overlap the Glasgow Congress.

S. C. Abrahams, IUCr Representative

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

ICSTI has reoriented its mission away from the consideration of purely technical issues so prevalent with the onset of the era of electronic publishing into that of the strategy of the scientific and technical information industry in all its forms. This action is coordinated through its Information Policy Committee. ICSTI's membership is drawn from diverse sectors of learned societies, the commercial publishing industry, national and academic libraries, patent offices, intellectual property consultants, secondary services *etc*. Over the years, ICSTI's links with ICSU have weakened and within its membership the user community is now poorly represented. Only those scientific unions directly involved in the publishing field are members. ICSTI is a most useful source of information and contacts for the IUCr with regard to its considerable involvement in publication for the crystallographic community.

ICSTI has undertaken a drive to improve its finances by reducing staff at the secretariat, by switching from print to electronic distribution for its quarterly newsletter and by charging a registration fee for its Annual General Meeting and opening the discussion sessions to non-members. A considerable effort has also been undertaken to increase the membership. It is intended that some future AGMs will be joint efforts with associated organizations.

The current technical activities, especially those relevant to the interests of the IUCr, include: (i) a networking survey of user needs; (ii) access to telematics facilities in the Eastern Caribbean; (iii) an international classification scheme for physics; (iv) the addition of information on A&I services to the ISSN register; and (v) a multilingual thesaurus of geosciences. Moreover, ICSTI has a group active in the area of legal issues that surveys developments in copyright, database and patent law throughout the world. The Information Policy Committee has given considerable attention to the problem of

the electronic archive and this subject will form the theme of ICSTI's contribution Sharing Scientific Knowledge to the World Science Conference in collaboration with ICSU Press and CODATA. It has also been mooted that the implementation of a registry defining the location of each current master archive could be created.

New proposals include collaboration in an IUPAC/CODATA project on standardization of physicochemical property electronic data files (IUCOSPED). The goal of this project is to develop standards for the publication, dissemination and storage of numerical data files in electronic form and thereby avoid the proliferation of incompatible formats as journals move to dissemination on the Internet. One aspect of the project is to link the standard numerical data formats to literature sources for which ICSTI could provide the contact with publishers and with the organizations responsible for identification codes: ISSN, CAS Registry Number, DOI *etc.*

In order to cut costs, ICSTI now undertakes its publication programme entirely by way of the Internet. The quarterly newsletter *ICSTI Forum* and other general information are made available on the public web site at http://www.icsti.org/. 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.

12.2.1. Winter Committee and Discussion Meetings. One was held 10–11 January 1998 in Paris, France. The presentation and discussion sessions concerned recent developments in copyright law in the European Union and in the USA, and a presentation of the activity or initiatives of IFLA. A second was held 12–13 December 1999 in London, UK. The presentation and discussion sessions focused on the electronic publications archive, ICSTI participation in the ICSU World Science Conference, and the European Union proposed directive on copyright. The recent EBLIDA/ECUP/STM (European Bureau of Library, Information and Documentation Associations/European Copyright User Platform/International Association of Scientific, Technical, and Medical Publishers) interim joint statement on guidelines for incidental digitization and permanent storage of scientific, technical and medical journal articles was also noted.

12.2.2. AGM 1998. The IUCr Representative attended the annual general meeting in Loch Lomond, UK, 20–24 May 1998. Over 50 people attended from all walks of scientific, technical and medical publishing. In the session on *Electronic libraries – relationship between suppliers and customers*, the points of view of a large (Blackwell Science) and a small (ASLIB) publisher, secondary publishers (Chemical Abstracts, NFAIS), intermediaries (Blackwell, Dawson) and purchasers (University librarians from Heriot-Watt and Newcastle) were presented. Users were talked about but were not represented. The use of electronic services gives rise to an enigma in that the providers are now in much closer contact with the user whereas it is really the editor that needs to be in contact with the user, and for preference the provider would like to be in contact with the purchaser. *Restructuring/rationalization in the information industry* presented the situation of JST (Japan Science and Technology Corporation), VINITI – the Russian information industry, EPO (European Patent Office), DTIC (US federal science and technical information organizations) and the newly formed DOI foundation (Digital Object Identifier).

H. D. Flack, IUCr Representative

12.3. International Council for Science (ICSU)

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

P. Coppens, IUCr Representative

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

No significant meetings occurred in 1998 but the IUCr's Visiting Professorship Programme, which receives support from the ICSU/UNESCO subvention, continues.

C. Gramaccioli, IUCr Representative

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

No report has been received from the IUCr Representative.

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

COSTED is continuing its discussions on technology management, coping with hazardous wastes, facilitating technology transfer, leadership development for science and technology in developing countries, and undertaking natural resource surveys for economic development.

P. Coppens, IUCr Representative

12.7. ICSU Committee on Space Research (COSPAR)

The main COSPAR activities in 1998 were the preparation and performance of the 32nd COSPAR Scientific Assembly and Related Events, which was held 12–19 July 1998 in Nagoya, Japan, under the Chair of Y. Kamide, Solar–Terrestrial Environment Laboratory, Nagoya University. It was connected with the 40th Anniversary of COSPAR, commemorating its founding by ICSU in October 1958. During the opening ceremony, M. Oda gave a retrospective survey on the rapid development, during the past 40 years, of space observatories and space missions, and of the many exciting results that they yielded in the fields of X-ray astronomy, radio astronomy and radio interferometry, and in the study of the solar corona and solar flares.

The COSPAR meeting was attended by about 1 700 registered participants, among them 279 students. The papers accepted for oral or poster presentation numbered about 2 500 and were presented in 20 parallel sessions. About 1 200 papers were submitted for publication in *Advances in Space Research* and will appear in volumes 23 to 26. The evening lecture was entitled 'Recent Discoveries about Life in the Universe: Earth, Mars and Beyond' and consisted of the three chapters 'Earth's Earliest Biosphere', 'The Possible Origin of Life on Mars' and 'The Biopotential of Extrasolar Planets'.

During the Congress, the 58th COSPAR Bureau Meeting and the 32nd COSPAR Council Meeting were held. The most important item on the agenda was the election of the President, the Vice-Presidents, the remaining Bureau members and the Finance Committee members for the period 1998–2002. The presiding President G. Haerendel (Germany) as well as the Vice-Presidents L. J. Lanzerotti (USA) and A. Nishida (Japan) were re-elected.

Another item on the agenda concerned the election of the Nomination Committee, which has the important task of preparing the slates for the next COSPAR Council elections. Under current COSPAR By-laws, a new Nomination Committee must be elected every two years, whereas the COSPAR Council Officers are elected

for a period of four years. In order to homogenize the rules, a modification of the By-laws allowing an extension of the term of Nomination Committee members from two to four years was discussed and subjected to voting by correspondence.

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

H. Klapper, IUCr Representative

13. Finances

The audited accounts of the year 1998 are given at the end of this Report. For comparison, the figures for 1997 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 1998 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 318 743. 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 1998. It should be noted that this loss of CHF 318 743 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 1998. The total of CHF 441 264 with the banks at the end of the year was represented by USD 232 424 with Merrill Lynch, GBP 49 461 with National Westminster Bank and CHF 9 052 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, including the loss of CHF 318 743 resulting from fluctuations in rates of exchange, have reduced during the year, from CHF 7 151 105 to CHF 6 916 067.

A transfer of CHF 150 000 was made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund. A transfer of CHF 50 000 was made to the Research and Education Fund from the General Fund. A transfer of CHF 20 000 was made to the President's Fund from the General Fund. Transfers of CHF 30 000 and CHF 50 000 were made to the *Newsletter* Fund from the General Fund and the *Acta Crystallographica* Fund. A transfer of CHF 100 000 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 25 130 before the transfers totalling CHF 100 000, as compared with a surplus in 1997 of CHF 39 834 before transfers totalling CHF 50 000. The administrative expenses were CHF 348 751 in 1998 as compared with CHF 313 338 in 1997. Of this amount, CHF 109 476 was charged to the publications of the Union.

CHF 72 990 was spent on the Eighteenth General Assembly and Congress and CHF 5 495 in assisting the work of the non-publishing Commissions. The expenses of the Union Representatives on other bodies were CHF 3 377. The cost of the Finance Committee meetings held in 1998 was CHF 21 223, while the Executive Committee meeting cost CHF 33 201. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 7 320. The Union received CHF 16 072 from the UNESCO subvention to ICSU. The subscriptions from Adhering Bodies were CHF 159 692. Interest on bank accounts and investments credited to the General Fund was CHF 285 144.

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

The President's Fund therefore received interest of CHF 2 216. Grants totalling CHF 2 403 were paid from the fund.

The *Acta Crystallographica* account for 1998 shows a surplus of CHF 340 167 before the transfer of CHF 300 000 to other fund accounts, as compared with a surplus of CHF 269 302 in 1997 before transfers of CHF 125 000.

The subscription rates were increased for 1998. In 1998, the number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 52 (54) personal subscriptions, was 612 (638) (values for 1997 are given in parentheses). The number of paid subscriptions to *Sections A+B+C*, including 16 (15) personal subscriptions, was 135 (137). The number of paid subscriptions to the separate sections of the journal were: *Section A* 270 (258 for 1997), *Section B* 213 (204), *Section C* 163 (151) and *Section D* 195 (186). The cost of the technical editing office has been divided between the *Acta Crystallographica*, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation* accounts in percentages based on the number of text pages published during the year. The technical editing costs for *Acta Crystallographica* were CHF 951 380 (for 5 518 published pages) as compared with CHF 878 571 in 1997 (4 733 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 deficit of CHF 61 263, as compared with a deficit of CHF 15 583 in 1997 before transfers of CHF 150 000. In 1998, the number of paid subscriptions, including 106 (102 in 1997) personal subscriptions, was 780 (820 in 1997).

The *Journal of Synchrotron Radiation* account shows a deficit of CHF 118 134 before receiving a transfer of CHF 100 000 from the *Acta Crystallographica* Fund, as compared with a deficit of CHF 142 541 in 1997 before receiving a transfer of CHF 50 000. In 1998, the number of paid subscriptions, including 137 (120 in 1997) personal subscriptions, was 288 (269 in 1997).

The *International Tables* account shows a deficit of CHF 8 788, as compared with a surplus of CHF 8 095 in 1997. The net sales income was CHF 94 193 in 1998 as compared with CHF 146 020 in 1997.

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

The *Newsletter* Fund Account received transfers of CHF 30 000 from the General Fund and CHF 50 000 from the *Acta Crystallographica* Fund in 1998. The cost to the Union of producing the *Newsletter* in 1998 was CHF 74 059 (CHF 84 574 in 1997).

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 expenses of CHF 292 288 for computer expenses, including the purchase of computing equipment for the Chester office, relate to the technical editing of the journals and software. The programming and development costs are now divided between the General Fund, the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Journal of Synchrotron Radiation* Fund and the *International Tables* Fund in percentages based on the total expenditure in those Funds. Expenses of a project to develop an SGML implementation for the Union's journals, promotional costs and web input costs are also charged to the Publication and Journals Development account. CHF 76 399 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union, and CHF 8 837 for the Visiting Professorship Programme were charged to the Research and Education Fund. Part of the costs of these activities is met by funds received under the ICSU/UNESCO grants programme.

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

We have audited the financial statements on pages 212 to 225 which have been prepared under the accounting policies set out on page 213.

Respective responsibilities of Executive Committee and Auditors

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

Basis of opinion

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

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

Opinion

In our opinion, the financial statements give a true and fair view of the state of the Union's affairs as at 31 December 1998 and of the result for the year then ended.

Deloitte & Touche
Chartered Accountants and Registered Auditors
24 June 1999

Table 2
Income and Expenditure Account for the year ended 31 December 1998.

	Note	1998		*1997*	
		Swiss Francs			
Income					
Membership subscriptions			159,692		*151,562*
Sales					
Journals		3,069,887		*2,740,553*	
Books		269,298		*196,741*	
Back numbers and single issues		22,309	3,361,494	*36,798*	*2,974,092*
Investment income					
Income from investments	15.7	334,837		*280,164*	
Bank interest	15.8	41,440		*32,148*	
(Loss)/Profit on sale of investments	15.9	(45,592)	330,685	*15,566*	*327,878*
Other income					
Grants		16,145		*23,200*	
Royalties and copyright fees		3,327		*12,136*	
Advertising income		188,852		*87,957*	
General Assembly refund		–	208,324	*7,150*	*130,443*
Total Income			4,060,195		*3,583,975*
Expenditure					
Journals					
Publication costs		1,656,050		*1,297,065*	
Editorial expenses		156,779		*143,523*	
Technical editing		1,315,530	3,128,359	*1,052,692*	*2,493,280*
Books					
Publication costs		60,093		*105,969*	
Editorial expenses		45,263	105,356	*46,198*	*152,167*
Newsletter					
Publication costs		120,687		*118,790*	
Editorial expenses		81,215	201,902	*48,032*	*166,822*
President's Fund					
Grants and Young Scientists' support			78,802		*99,374*
General Assembly costs			72,990		*27,705*
Ewald Prize			1,537		–
Committee meetings and expenses			54,424		*60,982*
Publications and journals development					
General		266,686		*231,464*	
Electronic Publishing Committee/Section Editors meeting expenses		986		*1,343*	
Electronic publishing project		5,333	273,005	*27,545*	*260,352*
Subscriptions paid			10,598		*8,661*
Visiting Professorship programme			8,837		*16,661*
Administration expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		9,345		*9,365*	
Secretarial assistance		274		*346*	
Audit and accountancy charges		34,822		*39,721*	
Legal and professional fees		7,570		*2,293*	
Postage and sundries		–		*206*	
Travelling expenses		7,733		*2,940*	
Bank charges		2,050	61,794	*3,156*	*58,027*
Executive Secretary's office:					
Salaries and expenses		267,625		*242,130*	
Travel expenses of IUCr representatives on other bodies		3,377		*1,958*	
STAR/CIF		1,943		*22,656*	
Commission expenses		5,495		*2,945*	
Sponsorship of meetings		5,475		*10,525*	
President's secretary		4,486		*1,206*	
IUCr/FIZ agreement		(7,320)		*(4,569)*	
IUCr50 symposia		22,103		–	
Bad debts – subscriptions		2,000	305,184	*(6,000)*	*270,851*
Depreciation			61,615		*57,719*

Table 2 (continued)

	Note	1998		*1997*	
			Swiss Francs		
TOTAL EXPENDITURE			4,364,403		*3,672,601*
Deficit of income over expenditure (carried forward)			(304,208)		(*88,626*)
Movement in market value of investments in year	15.5		387,913		*412,142*
			83,705		*323,516*
Fluctuation in rates of exchange					
Trading activities	15.2	(25,684)		*49,454*	
Investment activities	15.2	(293,059)	(318,743)	*688,535*	*737,989*
Total recognized gains and losses relating to the year			(235,038)		*1,061,505*
Opening fund accounts at 1 January			7,151,105		*6,089,600*
Closing fund accounts at 31 December			6,916,067		*7,151,105*

All the income and expenditure related to continuing activities. Historic cost results would only differ from above by the profit on sale of investments – see Note 15.9. 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.

15. Notes to the Accounts

The Income and Expenditure Account, the Balance sheet and the Cash Flow statement for the year ended 31 December 1998 are given in Tables 2, 3 and 4.

15.1. Accounting policies

(*a*) *Accounting convention*

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

(*b*) *Rates of exchange*

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

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

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

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

(*c*) *Publication costs*

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

(*d*) *Stocks*

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

(*e*) *Expenditure on premises*

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

(*f*) *Depreciation*

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

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

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

(*g*) *Investment income*

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

(*h*) *Investments*

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

(*i*) *Lease costs*

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

15.2. 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

Table 3
Balance sheet as at 31 December 1998.

	Note	1998		*1997*	
		Swiss Francs			
FIXED ASSETS					
Tangible fixed assets	15.4		130,413		*167,852*
CURRENT ASSETS					
Stock			26,061		*38,180*
Cash at bank					
Current accounts		19,765		*55,310*	
Deposit and savings accounts		421,499		*241,592*	
Cash with Union officials		30,763	472,027	*26,243*	*323,145*
Investments at market value	15.5		6,163,824		*6,627,615*
Debtors, accrued income and payments in advance			293,490		*262,437*
Subscriptions from Adhering Bodies			60,000		*29,192*
TOTAL CURRENT ASSETS			7,015,402		*7,280,569*
Creditors: amounts falling due within one year	15.6		(229,748)		(*297,316*)
NET CURRENT ASSETS			6,785,654		*6,983,253*
TOTAL FUNDS			6,916,067		*7,151,105*

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

	1998	*1997*
Netherland Guilders (NLG)	1.3664	*1.3908*
Danish Crowns (DKK)	4.6337	*4.5501*
Pounds Sterling (GBP)	0.4376	*0.4219*
US Dollars (USD)	0.7280	*0.7042*

compared with the Swiss Franc were as follows:

The net assets of the Union at 1 January 1998 (CHF 7,151,105) would have had the value of USD 5,206,000 or GBP 3,129,324 if expressed in those currencies.

At 31 December 1998, the net assets (CHF 6,916,067) would have had the value of USD 5,048,224 or GBP 3,026,725, respectively, being a decrease of USD 157,776 or a decrease of GBP 102,599 from the previous year.

15.3. 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.

15.4. Tangible fixed assets

Table 5 lists the tangible fixed assets.

15.5. Investments

Table 6 lists the investments of the IUCr, their disposals and additions and the holding at 31 December 1998.

15.6. Creditors

Table 7 lists the creditors, with the amounts falling due within one year for 1997 and 1998.

15.7. Investment income

Table 8 lists the income from investments for 1997 and 1998.

15.8. Bank interest

Table 9 lists the bank interest for 1997 and 1998.

15.9. Loss/profit on disposal/redemption of investments

Table 10 lists the loss or profit on disposal/redemption of investments for 1997 and 1998.

15.10. Exchange rate fluctuations

Table 11 lists exchange rate fluctuations attributable to operating activities for 1997 and 1998.

15.11. Changes in cash during the year

Table 12 is an analysis of cash changes during 1997 and 1998.

15.12. Balances of cash as shown in the balance sheet

Table 13 is an analysis of cash balances as shown in the balance sheet.

15.13. Operating lease commitments

At 31 December 1998, the Union was committed to making the payments listed in Table 14 during the next year in respect of operating leases.

Table 4
Cash Flow statement for the year ended 31 December 1998.

	Note	1998	Swiss Francs *1997*
Net cash outflow from operating activities (see below)		(671,499)	(*374,526*)
Returns on investments			
Interest received		41,440	*32,148*
Investment income (net of notional dividends)		92,909	*116,598*
Net cash inflow from returns on investments		134,349	*148,746*
Investing activities			
Purchase of fixed assets		(28,931)	(*52,569*)
Purchase of investments	15.5	(969,649)	(*1,389,353*)
Disposal of investments	15.9	1,725,028	*1,554,768*
Net cash inflow from investing activities		726,049	*112,846*
Increase/(decrease) in cash	15.11	188,899	(*112,934*)
Reconciliation of Deficit of Income over Expenditure to Net Cash Outflow from Operating Activities			
Deficit of income over expenditure		(304,208)	(*88,626*)
Exchange rate fluctuations attributable to operating activities	15.10	14,333	(*17,767*)
Interest received	15.8	(41,440)	(*32,418*)
Investment income	15.7	(334,837)	(*280,164*)
Loss/(profit) on disposal of investments	15.9	45,592	(*15,566*)
Depreciation charges		66,370	*57,719*
Decrease in stock		12,120	*21,094*
(Increase) in debtors		(61,861)	(*27,720*)
(Decrease)/increase in creditors		(67,568)	*8,652*
Net cash outflow from operating activities (see above)		(671,499)	(*374,526*)

Table 5
Tangible fixed assets.

	Leasehold property improvements CHF	Office equipment CHF	Computer equipment CHF	Total CHF
Cost				
As at				
1 January 1998	102,987	62,695	107,419	273,101
Additions	–	3,564	25,367	28,931
As at				
31 December 1998	102,987	66,259	132,786	302,032
Accumulated depreciation				
As at				
1 January 1998	22,936	31,024	51,289	105,249
Charge for the year	10,299	12,252	43,819	66,370
As at				
31 December 1998	33,235	43,276	95,108	171,619
Net book value				
31 December 1998	69,752	22,983	37,678	130,413
31 December 1997	80,051	31,671	56,130	167,852

15.14. Sponsorship commitments

At 31 December 1998, the Union had authorized, but not contracted for, sponsorship grants of CHF 24,036 (1997: CHF 57,631).

15.15. Contingencies

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

Tables 15–26 give the accounts for the year ended 31 December 1998 for the various Fund Accounts.

Table 6
Investments.

	Swiss Francs								
	Holding at market value 1 January 1998	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 1998	Holding at revalued cost 31 December 1998	Holding at revalued cost 31 December 1997
Held by Merrill Lynch									
GNM P146535-2016 (USD)	3,884	–	–	(3,636)	(248)	–	–	–	3,444
GNM P169332-2016 (USD) 11,040 Units	27,419	–	–	(9,110)	(1,796)	(227)	16,286	14,639	28,694
Haussmann Holdings (USD) 122 Units	199,213	–	–	–	(11,674)	4,623	192,162	79,214	84,176
British Gas Finance (USD)	110,043	–	–	(114,945)	4,902	–	–	–	112,511
Global Allocation Portfolio Class A (USD) 5,700 Units	125,660	–	–	–	(7,365)	4,541	122,836	82,565	87,737
Meridian Funds Global	170,187	–	–	(177,769)	7,582	–	–	–	193,357
Meridian Charter Income Fund (USD) 14,661 Units	210,347	–	12,339	–	(12,697)	(7,009)	202,980	210,676	211,158
Lehman Brothers Holdings (USD)	116,952	–	–	(121,601)	4,649	–	–	–	115,399
Permal Investment Holdings NV (USD) 53 Units	166,902	–	–	–	(9,780)	(2,290)	154,832	96,088	102,106
Repsol International Capital Limited 2000 Units	73,495	–	–	–	(4,306)	1,203	70,392	70,050	74,438
Santander Finance Limited 2,700 Units	71,552	31,013	–	–	(6,030)	1,739	98,274	99,410	74,644
Aetna Emerging Europe FD	52,608	–	–	(52,146)	(462)	–	–	–	59,301
Lord Abbett Developing	54,936	–	–	(54,446)	(490)	–	–	–	63,125
ML ECS Capital Portfolio CLB	418,369	–	–	(414,640)	(3,729)	–	–	–	302,946
ML Global Alloc A (Offshore) 3,286 Units	71,962	–	–	–	(4,218)	2,518	70,262	73,222	77,808
MLBS SP PF EU EQ (US) B 5,825 Units	–	146,817	–	–	(8,699)	19,735	157,853	138,068	–
ML Debt Strategy PF CL B 5,118 Units	–	72,702	4,451	–	(4,482)	(6,944)	65,727	72,644	–
Sector SPDR Energy 2075 Units	–	68,170	–	–	(1,766)	115	66,519	66,380	–
Seligman US Large Cap 7,500 Units	–	112,827	–	–	(10,199)	(3,118)	99,510	102,591	–
Banco Bilbao 1,500 Units	–	61,010	–	–	(3,616)	(416)	56,978	41,787	–
Held by Foreign & Colonial									
Reserve Asset Fund Class D (USD) 11,520 Units	675,687	–	22,093	(228,016)	(28,805)	38,830	479,789	429,316	663,483
Reserve Asset Fund Class L (GBP) 23,826 Units	1,359,132	–	97,611	–	(67,403)	80,103	1,469,443	784,070	876,835
Reserve Asset Fund Class X (GBP) 10,657 Units	1,012,295	–	28,446	(594,311)	(15,573)	(1,960)	428,897	452,131	1,034,637
Reserve Asset Fund Class M (USD) 5,144 Units	293,285	–	17,739	–	(17,702)	56,127	349,449	81,342	68,140
Reserve Asset Fund Class E (GBP) 16,425 Units	428,749	477,110	59,647	–	(42,039)	74,591	998,058	910,504	415,135
Treasury Stock									
Treasury stock UK Treasury 2006	984,938	–	–	–	(47,113)	125,752	1,063,577	907,766	953,369
	6,627,615	969,649	242,326	(1,770,620)	(293,059)	387,913	6,163,824	4,712,462	5,602,443

Table 7
Creditors: amounts falling due within one year.

	Swiss Francs	
	1998	*1997*
Trade creditors	25,356	*53,859*
Accruals	142,384	*174,731*
Other creditors	–	*4,067*
Payroll creditor including tax and social security	46,469	*52,179*
Lease creditor relating to property	15,539	*12,480*
	229,748	*297,316*

Table 8
Investment income.

	Swiss Francs 1998	*1997*
ML Global Allocation A (offshore)	–	*446*
GNM P146535 - 2016	1,240	*404*
GNM P169332 - 2016	1,694	*2,417*
ML Capital Fund/CLB	–	*3,450*
Haussmann Holdings	327	*342*
Meridian Funds Global – Government Fund	–	*7,927*
Meridian Charter – Income Fund	12,339	*11,395*
British Gas Finance	4,791	*9,745*
Global Allocation	–	*1,295*
Foreign and Colonial – Reserve Asset Fund Class D	22,093	*27,614*
Foreign and Colonial – Reserve Asset Fund Class L	97,611	*25,880*
Foreign and Colonial – Reserve Asset Fund Class X	28,446	*57,826*
Foreign and Colonial – Reserve Asset Fund Class M	17,739	*3,525*
Foreign and Colonial – Reserve Asset Fund Class E	59,647	*24,493*
Lehman Brothers	3,774	*7,217*
UK Treasury 7.75% 22.9.2006	63,862	*73,371*
Lord Abbett Developing	–	*4,460*
Altos Hornos Demex	–	*15,944*
Repsol International Capital Ltd	5,429	*1,043*
Santander Finance Ltd	7,400	*1,370*
Banco Bilbao	3994	–
ML Debt Strategy	4,451	–
	334,837	*280,164*
Allocated to:		
President's Fund	2,216	*2,210*
Ewald Fund	23,850	*19,580*
Publication and Journals Development Fund	17,518	*33,986*
Research and Education Fund	47,549	*43,671*
Balance left in General Fund	243,704	*180,717*
	334,837	*280,164*

Table 9
Bank interest.

	Swiss Francs 1998		*1997*	
National Westminster Bank Plc				
Manchester Business Reserve Account	8,732		*7,480*	
Manchester Capital Reserve Account	2,569		*2,747*	
		11,301		*10,227*
Merrill Lynch				
CMA Account		11,787		*6,033*
Foreign & Colonial				
Cash balance	755		*580*	
Interest from Munksgaard	17,597		*15,308*	
		18,352		*15,888*
Allocated to General Fund		41,440		*32,148*

Table 10
Loss/(profit) on disposal/redemption of investments.

	Swiss Francs 1998	*1997*
Proceeds	1,725,028	*1,554,768*
Book value	1,770,620	*1,539,202*
(Loss)/Profit allocated to General Fund	(45,592)	*15,566*

Book value represents market value at 1 January 1998. The profit on disposal based on historic cost was CHF 30,502 (1997: CHF 378,338). Therefore historic cost results would be as follows:

	Swiss Francs 1998	*1997*
(Deficit)/excess of income over expenditure	(195,806)	*274,146*

Table 11
Exchange rate fluctuations attributable to operating activities.

	Swiss Francs 1998	*1997*
Total fluctuations in exchange rates dealt with in Fund accounts	(318,743)	*737,989*
Adjustments for exchange differences attributable to:		
Investments (Note 15.5)	293,059	(*688,535*)
Cash and bank balances	40,017	(*67,221*)
	14,333	(*17,767*)

Table 12
Analysis of cash changes during the year.

	Swiss Francs 1998		*1997*	
Balance at 1 January 1998		323,145		*368,858*
Net cash inflow/(outflow)	188,899		(*112,934*)	
Fluctuations in rates of exchange on cash and bank balances	(40,017)		*67,221*	
		148,882		(*45,713*)
Balance at 31 December 1998		472,027		*323,145*

Table 13
Analysis of cash balances as shown in the Balance sheet.

	Swiss Francs 1998	*1997*	Change 1998	*Change 1997*
Cash at bank and in hand	472,027	*323,145*	148,882	(*45,713*)

Table 14
Operating lease commitments.

	Swiss Francs 1998	1997
Leases which expire:		
within one year	22,852	–
within two to five years	41,912	*28,739*
after five years	59,415	*62,400*
	124,179	*91,139*

Table 15
Fund Accounts as at 31 December 1998.

	Swiss Francs						
	As at 1 January 1998	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Gain on market value of investments	Fluctuations in exchange rates (Note 15.2)		Balance at 31 December 1998
					Trading	Investments	
FUND ACCOUNTS							
General Fund	3,101,978	(100,000)	(25,130)	387,913	(11,945)	(293,059)	3,059,757
President's Fund	39,344	20,000	(187)	–	(210)	–	58,947
Acta Crystallographica	1,548,726	(300,000)	340,167	–	(5,641)	–	1,583,252
Journal of Applied Crystallography	213,838	–	(61,263)	–	(542)	–	152,033
International Tables	204,753	–	(8,788)	–	(695)	–	195,270
Book Fund	20,719	–	4,972	–	(91)	–	25,600
Publications and Journals Development Fund	655,433	150,000	(345,955)	–	(1,631)	–	457,847
Research and Education Fund	878,247	50,000	(38,217)	–	(3,160)	–	886,870
Ewald Fund	398,968	–	22,386	–	(1,496)	–	419,858
Newsletter Fund	51,505	80,000	(74,059)	–	(204)	–	57,242
Journal of Synchrotron Radiation	37,594	100,000	(118,134)	–	(69)	–	19,391
	7,151,105	–	(304,208)	387,913	(25,684)	(293,059)	6,916,067

Table 16
General Fund Account for the year ended 31 December 1998.

	Note	1998		*1997*	
		Swiss Francs			
Income					
Grant received from UNESCO subvention to ICSU			16,072		*23,200*
Subscriptions from Adhering Bodies			159,692		*151,562*
Income from investments	15.7		243,704		*180,717*
Interest on bank accounts	15.8		41,440		*32,148*
Profit on disposal/redemption of investments	15.9		(45,592)		*15,566*
General Assembly refund			–		*7,150*
Amounts charged to the following journals and publications:					
Acta Crystallographica		76,634		*60,398*	
Journal of Applied Crystallography		13,136		*15,508*	
Journal of Synchrotron Radiation		19,706	109,476	*5,713*	*81,619*
Total Income			524,792		*491,962*
Expenditure					
Subscriptions to ICSU and ICSU bodies			10,598		*8,661*
Administrative expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		9,345		*9,365*	
Secretarial assistance		274		*346*	
Audit and accountancy charges		34,822		*39,721*	
Legal and professional fees		7,570		*2,293*	
Postage and sundries		–		*206*	
Travelling expenses		7,734		*2,940*	
Bank charges		2,050		*3,156*	
Executive Secretary's office:					
Salaries and expenses		267,625		*242,130*	
Depreciation of office equipment		9,032		*2,882*	
Depreciation of freehold property		10,299	348,751	*10,299*	*313,338*
Eighteenth General Assembly and Congress expenses		72,990		*27,705*	
Meeting of the Executive Committee		33,201		*38,219*	
Finance Committee expenses		21,223		*22,763*	
Travel expenses of IUCr Representatives on other bodies		3,377		*1,958*	
STAR/CIF		1,943		*22,656*	
Commission expenses		5,495		*2,945*	
Sponsorship of meetings		5,475		*10,525*	
President's secretary		4,486		*1,206*	
IUCr/FIZ agreement		(7,320)		*(4,569)*	
IUCr 50 Symposia		22,103		–	
Bad debts – subscriptions		2,000		*(6,000)*	
Programming and development costs		25,600	190,573	*12,721*	*130,129*
Total Expenditure			549,922		*452,128*
(Deficit)/excess of income over expenditure			(25,130)		*39,834*
Reconciliation of movements					
Balance at 1 January			3,101,978		*1,992,999*
Transfers to other funds:					
Research and Education Fund		50,000		*50,000*	
President's Fund		20,000		–	
Newsletter Fund		30,000	(100,000)	–	(*50,000*)
(Deficit)/excess of income over expenditure		(25,130)		*39,834*	
Movement in market value of investments in the year	15.5	387,913	362,783	*412,142*	*451,976*
Fluctuations in rates of exchange			(305,004)		*707,003*
Balance at 31 December			3,059,757		*3,101,978*

Table 17
President's Fund Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998	*1997*
Income			
Investment income	15.7	2,216	*2,210*
TOTAL INCOME		2,216	*2,210*
Expenditure			
Grants		2,403	*7,558*
Deficit of income over expenditure		(187)	(*5,348*)
Reconciliation of movements			
Balance at 1 January		39,344	*44,391*
Transfers from other Funds			
General Fund		20,000	–
Deficit of income over expenditure		(187)	(*5,348*)
Fluctuations in rates of exchange		(210)	*301*
Balance at 31 December		58,947	*39,344*

Table 18
Acta Crystallographica Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998		*1997*	
Income					
Subscriptions to Volume 54 (*1997 Volume 53*)		2,535,290		*2,229,054*	
Sale of back numbers and single copies		13,503		*29,327*	
Airfreight charged to subscribers		51,687		*52,914*	
Royalties and copyright fees		10,441		*8,531*	
Special Issue income		20,852		–	
		2,631,773		*2,319,826*	
Less Publisher's commission on sales		178,416	2,453,357	*158,087*	*2,161,739*
Income from advertisements (net)			37,946		*1,459*
Recharge for Special Issue			36,428		–
TOTAL INCOME			2,527,731		*2,163,198*
Expenditure					
Publication expenses:					
Printing and binding Volume 54 (*1997 Volume 53*)		651,293		*559,821*	
Distribution and postage		121,594		*90,611*	
Airfreight costs		5,984		*18,531*	
		778,871		*668,963*	
Net loss on reprints		27,515		*1,313*	
Index/other incidental costs		36,043		*2,046*	
Special Issue costs		59,019	901,448	–	*672,322*
Editorial expenses:					
Editorial honoraria		76,915		*75,110*	
Secretarial assistance		10,061		*11,145*	
Postage, travel and sundries		17,517		*27,603*	
Technical editing:					
Salaries and expenses		880,699		*809,494*	
Computer expenses		38,634		*36,119*	
Depreciation of office equipment		32,047	1,055,873	*32,958*	*992,429*
Programming and development costs			153,609		*168,747*
Administration expenses recharged from General Fund			76,634		*60,398*
TOTAL EXPENDITURE			2,187,564		*1,893,896*
Excess of income over expenditure			340,167		*269,302*
Reconciliation of movements					
Balance at 1 January			1,548,726		*1,392,573*
Transfers to other funds					
Publications and Journals Development Fund		150,000		*50,000*	
Journal of Synchrotron Radiation		100,000		–	
Newsletter Fund		50,000	(300,000)	*75,000*	(*125,000*)
Excess of income over expenditure			340,167		*269,302*
Fluctuations in rates of exchange			(5,641)		*11,851*
Balance at 31 December			1,583,252		*1,548,726*

Table 19
Journal of Applied Crystallography Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998		*1997*	
Income					
Subscriptions to Volume 31 (*1997 Volume 30*)		344,372		*333,119*	
Sale of back numbers and single copies		3,366		*3,589*	
Airfreight charged to subscribers		7,541		*7,604*	
Royalties and copyright fees		1,240		*2,328*	
Special Issue income		–		*21,885*	
Advertising income		3,207		–	
		359,726		*368,525*	
Less Publisher's commission on sales		24,342	335,384	*23,570*	*344,955*
Recharge for Special Issue			–		*96,488*
Total Income			335,384		*441,443*
Expenditure					
Publication expenses:					
Printing and binding Volume 31 (*1997 Volume 30*)		116,019		*82,601*	
Distribution and postage		31,133		*15,181*	
Airfreight costs		1,050		*2,913*	
		148,202		*99,975*	
Net loss/(profit) on reprints		22,542	170,744	*(1,894)*	*98,081*
Editorial expenses:					
Special Issue costs		–		*118,373*	
Editorial honoraria		2,257		*12,224*	
Secretarial assistance		1,963		*6,029*	
Postage, travel and sundries		2,151		*3,727*	
Technical editing:					
Salaries and expenses		165,636		*164,660*	
Computer expenses		6,786		*6,788*	
Depreciation of office equipment		8,372	187,165	*6,194*	*317,995*
Programming and development costs			25,602		*25,442*
Administration expenses recharged from General Fund			13,136		*15,508*
Total Expenditure			396,647		*457,026*
Deficit of income over expenditure			(61,263)		(*15,583*)
Reconciliation of movements					
Balance at 1 January			213,838		*377,785*
Transfers to other funds					
Ewald Fund		–		*50,000*	
Research and Education Fund		–		*50,000*	
Journal of Synchrotron Radiation		–	–	*50,000*	(*150,000*)
Excess of income over expenditure			(61,263)		(*15,583*)
Fluctuations in rates of exchange			(542)		*1,636*
Balance at 31 December			152,033		*213,838*

Table 20
Journal of Synchrotron Radiation Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998		*1997*	
Income					
Subscriptions to Volume 5 (*1997 Volume 4*)		115,323		*93,282*	
Sales of back numbers and single issues		5,038		*3,408*	
Airfreight charged to subscribers		5,233		*2,695*	
Special Issue income		108,040		–	
		233,634		*99,475*	
Less Publisher's commission on sales		8,482	225,152	*6,775*	*92,700*
Income from advertisements			19,667		*2,356*
Income from copyright fees			273		*187*
Recharge for Special Issue			194,704		–
Total Income			439,796		*95,243*
Expenditure					
Publication expenses:					
Special Issue costs		302,744		–	
Printing and binding Volume 5 (*1997 Volume 4*)		62,348		*70,300*	
Distribution and postage		19,957		*8,213*	
Airfreight costs		1,729		*437*	
		386,778		*78,950*	
Net loss on reprints		25,730	412,508	*10,655*	*89,605*
Editorial expenses:					
Editorial honoraria		12,340		*16,181*	
Secretarial assistance		3,066		*5,929*	
Postage, travel and sundries		79		*5,504*	
Technical editing:					
Salaries and expenses		79,506		*82,875*	
Computer expenses		3,257		*3,417*	
Depreciation of office equipment		1,866	100,114	*3,118*	*117,024*
Programming and development costs			25,602		*25,442*
Administration expenses recharged from General Fund			19,706		*5,713*
Total Expenditure			557,930		*237,784*
Deficit of income over expenditure			(118,134)		(*142,541*)
Reconciliation of movements					
Balance at 1 January			37,594		*129,847*
Transfers from other funds					
Acta Crystallographica		100,000		–	
Journal of Applied Crystallography		–	100,000	*50,000*	*50,000*
Deficit of income over expenditure			(118,134)		(*142,541*)
Fluctuations in rates of exchange			(69)		*288*
Balance at 31 December			19,391		*37,594*

Table 21
International Tables Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998		*1997*	
Income					
Sales of copies					
Volume A		74,067		*69,461*	
Volume B		32,791		*33,918*	
Volume C		16,562		*77,726*	
Teaching Edition of Volume A		3,899		*5,556*	
Volumes II, III and IV		59		–	
		127,378		*186,661*	
Less Publisher's commission on sales		33,185		*40,641*	
Total Income			94,193		*146,020*
Expenditure					
Publication expenses:					
Printing and typesetting Volume A		26,318		*16,426*	
Printing and typesetting Volume B		3,508		*47,209*	
Printing and typesetting Volume C		18,693		*32,288*	
Printing and typesetting Teaching Edition of Volume A		2,194	50,713	*1,987*	*97,910*
Editorial expenses:					
Editorial honoraria		13,834		*11,345*	
Secretarial assistance, postage and office equipment		11,437		*5,557*	
Technical editing		1,392	26,665	*214*	*17,117*
Programming and development			25,603		*22,898*
Total Expenditure			102,981		*137,925*
Excess of income over expenditure			(8,788)		*8,095*
Reconciliation of movements					
Balance at 1 January			204,753		*195,091*
Excess of income over expenditure			(8,788)		*8,095*
Fluctuations in rates of exchange			(695)		*1,567*
Balance at 31 December			195,270		*204,753*

Table 22
Book Fund Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998	*1997*
Income			
Sales of copies, net of Publisher's commission on sales			
Historical Atlas of Crystallography		–	*436*
World Directory of Crystallographers 10th edition		12,108	*8,468*
Escher *Kaleidozyklen*		27	*83*
Sundry publications		–	*1,093*
Structure Reports		402	*384*
Royalties			
IUCr/OUP Book series		1,814	*1,090*
Total Income		14,351	*11,554*
Expenditure			
Publication expenses:			
Book series		105	–
World Directory of Crystallographers 10th edition		9,274	*8059*
Total Expenditure		9,379	*8,059*
Excess of income over expenditure		4,972	*3,495*
Reconciliation of movements			
Balance at 1 January		20,719	*17,065*
Excess of income over expenditure		4,972	*3,495*
Fluctuations in rates of exchange		(91)	*159*
Balance at 31 December		25,600	*20,719*

Table 23
Publications and Journals Development Fund Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998		*1997*	
Income					
Investment income	15.7		17,518		*33,986*
Expenses					
Computer expenses:					
Purchase of computer equipment and software		36,272		*2,485*	
Programming and development		256,016		*254,423*	
Recharged to other funds		(256,016)	36,272	(*254,423*)	*2,485*
Electronic Publishing Committee/ Section Editors' Meeting			985		*1,344*
Special Issue costs			231,132		*96,488*
Electronic Publishing Project			5,333		*27,545*
Promotions Representative			87,888		*17,334*
No. 6 Abbey Square			–		*1,194*
Web input			1,863		*3,676*
Total Expenditure			363,473		*150,066*
Deficit of income over expenditure			(345,955)		*(116,080)*
Reconciliation of movements					
Balance at 1 January			655,433		*716,497*
Transfers from other funds					
Acta Crystallographica		150,000	150,000	*50,000*	*50,000*
Deficit of income over expenditure			(345,955)		*(116,080)*
Fluctuations in rates of exchange			(1,631)		*5,016*
Balance at 31 December			457,847		*655,433*

Table 24
Research and Education Fund Account for the year ended 1998.

	Note	Swiss Francs 1998		*1997*
Income				
Investment income	14.7	47,549		*43,671*
Expenditure				
Young Scientists' Support		76,399	*91,816*	
Moscow ECM Funds		530	–	
Visiting Professorship Programme		8,837	*16,661*	
Total Expenditure		85,766		*108,477*
Deficit of income over expenditure		(38,217)		(*64,806*)
Reconciliation of movements				
Balance at 1 January		878,247		*836,332*
Transfers from other funds				
General Fund		50,000	*50,000*	
Journal of Applied Crystallography		– 50,000	*50,000*	*100,000*
Deficit of income over expenditure		(38,217)		(*64,806*)
Fluctuations in rates of exchange		(3,160)		*6,721*
Balance at 31 December		886,870		*878,247*

Table 25
Ewald Fund Account for the year ended 31 December 1998.

	Note	Swiss Francs 1998		*1997*
Income				
Investment income	15.7	23,850		*19,580*
Income bequest		73		–
		23,923		*19,580*
Expenditure				
Selection Committee and expenses		1,537		–
Excess of income over expenditure		22,386		*19,580*
Reconciliation of movements				
Balance at 1 January		398,968		*326,335*
Transfers from other funds		–		
Journal of Applied Crystallography		– –	*50,000*	*50,000*
Excess of income over expenditure		22,386		*19,580*
Fluctuations in rates of exchange		(1,496)		*3,053*
Balance at 31 December		419,858		*398,968*

Table 26
Newsletter Fund Account for the year ended 1998.

	Note	Swiss Francs 1998		*1997*
Income				
Income from advertisements		121,456		*82,248*
Re-imbursement of 18GAC circular		6,387		–
Total Income		127,843		*82,248*
Expenditure				
Editorial honoraria		5,360		*5,600*
Editorial expenses		75,855		*42,432*
Newsletter printing and distribution		90,323		*98,228*
Advertising costs		30,364		*20,562*
Total Expenditure		201,902		*166,822*
Deficit of income over expenditure		(74,059)		(*84,574*)
Reconciliation of movements				
Balance at 1 January		51,505		*60,685*
Transfers from other funds				
Acta Crystallographica		50,000	*75,000*	
General Fund		30,000 80,000	–	*75,000*
Deficit of income over expenditure		(74,059)		(*84,574*)
Fluctuation in rates of exchange		(204)		*394*
Balance at 31 December		57,242		*51,505*