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International Union of Crystallography
Report of the Executive Committee for 1997

1. Meetings

The IUCr sponsored the following meetings held during 1997:

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

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

3. 26th International School of Crystallography: Electron Crystallography, Erice, Italy, 22 May–2 June.

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

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

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

7. Sagamore XII Conference, Waskesiu, Saskatchewan, Canada, 27 July–1 August.

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

9. Symposium on Organic Crystal Chemistry, Rydzyna, Poland, 17–21 August.

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

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

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

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

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

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

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

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

The Executive Committee met in Lisbon, Portugal, in August. The Finance Committee met twice, in Copenhagen, Denmark, in March, and then in August in Lisbon 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 Co-editors, electronic publishing, Special Issues, format of offprints, and other matters concerning the IUCr journals;

(2) appointment of a Promotions Representative;

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

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

(5) the IUCr *Newsletter*; the Tenth Edition of the *World Directory of Crystallographers*;

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

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

(8) investment policy;

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

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

(11) fiftieth anniversary of the IUCr;

(12) appointment of the Selection Committee for the fifth Ewald Prize;

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

(14) importance of crystallography.

Other items dealt with in this way were:

(15) consideration of a proposal to establish an Inter-Union Bioinformatics Group;

(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;

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

(18) charges for visas;

(19) crystallography in Africa;

(20) use of financial support through ICSU;

(21) access to large-scale research facilities;

(22) review of the activities of the Commissions;

(23) review of the activities of Regional Associates.

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 53 of *Acta Crystallographica*, Volume 30 of *Journal of Applied Crystallography*, Volume 4 of *Journal of Synchrotron Radiation* and the Tenth Edition of the *World Directory of Crystallographers* were published.

3. Adhering Bodies

A list of Adhering Bodies of the IUCr, 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

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	
A49¶	1993	901	4766	121	1228	108	319	7.9	7.7	13	40	2.1	2.0
B49		1075		155		149		7.1		6		2.0	
C49		2186		880		869		2.5		11		0.9	
D49		604		72		62		9.0		10		3.0	
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	

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
26	1993	848	144	99	7.2	18	2.6	0	0	14	4.2	13	1.0
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

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

§ 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 A49, includes, in addition, 515 pages of abstracts communicated to the Beijing Congress, and 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.

Congress of Crystallography [*Acta Cryst.* (1997), A**53**, 692–748].

4. Work of the Commissions

4.1. *Commission on Journals*

This Commission, representing the three individual Editorial Boards of *Acta Crystallographica* (*Acta*), *Journal of Applied Crystallography* (*JAC*) and *Journal of Synchrotron Radiation* (*JSR*), had a very active year especially in terms of its broad remit (including nearly 100 editorial members), the number of journal pages published and work on two major Special Issues. 1997 has also seen extensive work towards electronic publishing and preparations for *Acta*'s 50th anniversary and *JAC*'s 30th anniversary which will both occur in 1998. Moreover, centralized submission to *JSR* has shown the way for organizational streamlining for the other journals,

especially the setting of improved targets for the reduction of review and publication times to benefit authors, the reduction of administrative burdens on Co-editors and more systematized control of all stages of the submission and publication process by the Chester office. The work of the Chester staff in sustaining the regular work of the journals' production, the heavy workload involved with the Special Issues and the R&D associated with the technical innovations involved in all stages of the publication process have been outstanding. I would especially like to thank them for their hard work in exploring new procedures and willingly taking on board major items such as the two Conference Proceedings Special Issues. In particular, the Synchrotron Radiation Instrumentation (SRI'97) Conference took place in Japan (at SPring-8) in August 1997. The publication of the Proceedings in 1998 in *JSR* comprising approximately 1100 pages, all fully refereed, has involved a great deal of work for *JSR* Co-editors and for Chester. Also, the Proceedings of the Small-Angle Scattering Conference from the International Conference on Small Angle Scattering held in Brazil in 1996 were published in *JAC* and comprised 62 papers. Thus some 20% of the journal pages published have come from these two Special Issues alone. Special Issues have become a substantial part of the Commission's activities. The number of proposals for these is growing, representing as they do the activities of particular communities within the IUCr. These are important and ways have to be explored for streamlining production methods.

The summary over *Acta*, *JAC* and *JSR* is as follows (see Table 1 for full details). The total number of pages published in 1997 was 6329, which compares with 7681 in 1996, 7067 in 1995 and 5786 in 1994. The decrease over 1996 and 1995 can be attributed to a shorter publication format and higher rejection and withdrawal rates in *Acta Section C*, for which it was agreed at the Seattle Congress that the growing number of pages in *Section C* (due to the greatly increasing numbers of chemical structures) should be capped and indeed reduced. The median publication times were *Section A* (4.4 months), *Section B* (5.7 months), *Section C* (4.6 months), *Section D* (5.4 months), *JAC* (7.0 months) and *JSR* (2.9 months). Citation statistics showed that the top four rankings amongst crystallographic journals were, in order of ranking, *Section D*, *JAC*, *Section A* and *Section B*. Moreover, *Section D* was ranked first out of 21 journals reporting Biochemical Research Methods. *JSR*, entering the citation rankings for the first time, having now been in existence for four years, was ranked third out of 37 instrumentation journals. Initiatives are in hand to promote the journals much more actively with a view to increasing subscriptions and to moving up the citation rankings, especially in those lists covering biological and chemical results. The individual Editors' comments are summarized below.

4.1.1. *Acta Crystallographica Section A (A. Authier, Editor)*. *Section A* contained 863 pages in 1997, comprising 1 Lead Article, 75 Research Papers and 10 Short Communications. This represents a decrease with respect to preceding years and it is hoped that this tendency will not continue. As usual the major concerns are on the one hand the need to decrease publication times for which every effort is made and on the other hand the lack of suggestions by readers and Co-editors of good suggestions for Lead Articles and Topical Reviews.

One important feature of 1998 will be the Special Issue to celebrate the fiftieth anniversary of *Acta*. The Guest Editor for that special issue is Professor H. Schenk and about 25 papers have been invited.

4.1.2. *Acta Crystallographica Section B (F. H. Allen, Editor)*. *Section B* published 1045 pages in 1997, comprising 109 Research Papers, 2 Topical Reviews and 2 Short Communications. The balance of papers was 43% inorganic, 19% metallo-organic and 37% organic. The authorship was spread amongst 21 countries. The rejection rate was 11%, and the withdrawal rate was 12%.

These statistics are healthily similar to those for 1995 and 1996. They confirm: (*a*) that the recovery from the lows of 1994 have been sustained over a three-year period, (*b*) that *Section B* does attract articles from the broad chemical spectrum that it aims to serve, and (*c*) that the journal is truly international. In terms of impact statistics, *Section B* lies fourth out of 17 current crystallographic journals, just behind three other IUCr publications. Citation analysis indicates also that papers in *Section B* are of lasting value, with a citation half-life of more than 10 years.

Once again, the quantity of review material published has been less than hoped. However, in 1997, this has been as much connected with ensuring the quality of such papers rather than their quantity.

On the positive side, publication times have been significantly reduced, by 1.4 and 1.0 months per paper over times experienced in 1995 and 1996, respectively. The publication time of 5.7 months in 1997 is the shortest for the past 5 years. Despite the fact that *Section B* appears only bi-monthly, the intention is further to reduce these times in 1998. A stricter regime has been introduced concerning revision times permitted to authors – a large component of earlier perceived delays. It is this regime that has led to a higher than normal withdrawal rate in 1997. Stricter adherence to CIF requirements and guidelines, where appropriate, has also been introduced during the year.

4.1.3. *Acta Crystallographica Section C (S. R. Hall, Editor)*. The number of pages printed for *Section C* in 1997 was 2004. This was a reduction of 1258 pages over that for 1996, partly as result of a decision by the Commission on Journals not to print the atomic coordinate tables unless they contained special positions, but mainly because the removal of Chester checking and editing backlogs in 1996 led to a much higher number of pages in that year. The number of structures published in 1997 was 1027 which was also less than the 1511 in 1996. This was because of a slightly lower throughput in Chester and the more stringent 1997 standards of acceptance meant that 145 submissions were rejected and 240 withdrawn in 1997, compared with 73 and 181, respectively, in 1996.

A number of important editorial and publication changes were made to *Section C* in 1997. First, a new publication format, the CIF-access mode, was offered. In this mode, the published paper was not printed in the journal but was listed in the Table of Contents and made available as a CIF by e-mail or *via* the IUCr web site. 32 papers were published by this mode in 1997. Second, new checking software was introduced in 1997 for the automatic validation of submitted data items in the CIF. These checking facilities are referred to as data validation tests and the algorithms for these tests are currently published on the web site (http://www.iucr.org/iucr-top/journals/acta/dv.html). The tests are being implemented as part of the checkcif e-mail services and this is expected to simplify the submission and review process.

4.1.4. *Acta Crystallographica Section D (J. P. Glusker, Editor)*. Thanks to the combined good efforts of the many reviewers of submitted articles, the Co-editors who oversee the

disposition of manuscripts, and the staff at Chester who ensure that the publication is correctly presented, this Section of *Acta* is progressing well. We are still trying to reduce the time between submission of a manuscript and its appearance in print, and an on-going dialogue on this subject is currently taking place. *Section D* accepts Research Papers, Lead Articles, Topical Reviews, Fast Communications, Short Communications, Crystallization Papers and Letters. Colour diagrams continue to be published free of charge to the author and this has helped attract some fine articles with diagrams that would be hard to interpret if they were published in black and white. This need for colour is a natural outcome of the inherent complexities of three-dimensional macromolecular structures. There are currently two vehicles for shorter style papers: (*a*) 'Crystallization Papers' which contain crystallization procedures and early attempts at structure determination; (*b*) 'Fast Communications' and 'Short Communications' which cover general items such as improvements in current crystallographic methods.

During 1997, *Section D* has published 130 articles and communications on various aspects of biological crystallography. Of these, 23 describe crystal structures of macromolecules, many of them well refined and include analyses of the biological relevance of their stereochemistries. In addition, 16 involve methods of phase determination and electron-density map interpretation. Articles were also published as follows: 8 on general aspects of crystallization, 6 on diffraction physics and experimental methods, 2 on neutron diffraction, 2 on crystallographic symmetry, 6 on structure refinement and 9 on interatomic interactions (such as the binding of ligands to macromolecules). Crystallization conditions and preliminary X-ray diffraction measurements were described in 58 articles.

Authors of all structural papers are required to deposit three-dimensional structural coordinates and structure factors with the Protein Data Bank before the article can be published. At present the author may request that deposited atomic coordinates be given a privileged status for one year and structure factors for four years, but these delays in availability of data are currently under review [see *Science* (1998), **279**, 306–307].

Future plans include the consideration of a macromolecular CIF approach to data submission, and more invitations for Lead Articles and Topical Reviews.

4.1.5. *Journal of Applied Crystallography (A. M. Glazer, Editor)*. In 1997, close to 1200 pages have been printed, including the Special Issue containing the Small-Angle Scattering Conference held in 1996 in Campinas, Brazil. The latter comprised 62 papers, and continues our tradition of serving the small-angle scattering community. Thanks are due to the Guest Editors of this special issue, A. Craievich, G. Kostorz and J. Teixeira, for their excellent efforts in putting this issue together. Readers will have noted that, as a result of this issue, the following December issue was larger than normal. This year, we have seen a large increase in the use of the Fast Communications section; and the Computer Abstracts section remains popular. A Lead Article written by E. F. Garman & T. R. Schneider dealing with the topic of Cryocrystallography appears to have been well received and has created interest in the readership of *JAC*. Indeed, a new section on Cryocrystallography (handled by Co-editor P. Weber) is beginning to flourish. The journal continues to attract a very wide range of research papers covering all aspects of crystallography.

4.1.6. *Journal of Synchrotron Radiation (S. S. Hasnain, J. R. Helliwell, H. Kamitsubo, Editors)*. This year saw the fifth anniversary of *JSR*. A total of 51 articles were published in 1997 (45 in 1996) and the total number of pages increased to 405 (326 in 1996). The median publication time of 2.9 months was unchanged, and represents the best performance of all of the IUCr journals. This year also saw the first entry of *JSR* into the citation ranking tables; on impact factor *JSR* was third out of 37 journals covering instruments and instrumentation, eighth out of 46 covering optics and eighteenth out of 60 covering applied physics. We acknowledge here the excellent papers submitted by authors, and thank the referees who have served the journal so well.

The biggest event of all in the year was SRI'97, and associated with it the Congress Proceedings. A total of approximately 1100 journal pages are now in proof for SRI'97. The refereeing was carried out to the standards expected of all *JSR* papers and these will be appearing in an excellent bumper issue of *JSR* in 1998.

4.2. *Commission on International Tables*

A summary of the information on all the volumes of *International Tables*, those which were published or are in the process of revision, or those which are being prepared or planned, has been collected in the form of a home page of the Commission on *International Tables*. The home page is accessible from the main IUCr home page (http://www.iucr.org/), and is maintained by the Editor of Volume B, U. Shmueli.

During ECM-17 at Lisbon in August, all Commission members present met with the IUCr's Managing Editor in order to discuss the future production and printing schedules of all *International Tables* volumes, in particular of those volumes ready for publication or for a new edition (Volumes A, B, C, E). The agreement reached was transmitted to all concerned later in the year.

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 space-group tables in this volume (Sections 6 and 7) will be transferred to LaTeX files by M. Aroyo and his colleagues in Sofia, Bulgaria. These files will be the basis for the printing of the Fifth Edition. The remaining text sections will be re-keyed in Chester. Completion of these two activities is expected for the end of 1998; publication of the Fifth Edition is envisaged for the summer of 1999.

4.2.2. *Volume B. Reciprocal Space; Editor U. Shmueli*. During the early part of 1997 the final editorial work on all the new and revised contributions to the Second Edition of Volume B was completed, and all the above material was transferred to the Technical Editor of the IUCr in Chester.

Various aspects of the preparation of the second edition, such as translation of the material to SGML (in preparation for an electronic version of this volume) were extensively discussed during ECM-17 in Lisbon, Portugal, with the Managing Editor and the majority of the members of the Commission. It is expected that the delays in publication that are due to this novel approach will result in a substantial time saving in the future.

4.2.3. *Volume C. Mathematical, Physical and Chemical Tables; Editor E. Prince*. During 1997 typesetting of the entire text of the revised edition of Volume C was completed, galley proofs were corrected by the authors, and Parts 1, 2 and

3 were in page proof. The typesetting, particularly of tabular material, was greatly facilitated by the existence of electronic files, which were successfully imported into the system used by the printers. The entire text now exists in electronic form, which should make future corrections and updates much easier. It is anticipated that the revised edition will be published early in 1998.

4.2.4. *Volume D. Physical Properties of Crystals; Editor A. Authier*. Most of the contributions still missing are expected to be delivered by May 1998 and the whole manuscript will be sent to Chester for technical editing in September 1998, even if one or two contributions are lacking by that time. These will be left for an eventual second edition. Update of the contributions already received is in progress and is expected to be completed by summer 1998. Publication is expected in 1999. Software packages will be included in a CD ROM which will accompany Volume D. The purpose of the first package (prepared in Nijmegen by T. Janssen and M. Ephraim) is (*a*) calculation of invariant tensors of any dimension and rank and with arbitrary permutation symmetry under the action of a chosen three-dimensional point group, and (*b*) representation of finite point groups; the second (prepared in Prague by V. Kopsky, V. Janovec and P. Bocek) presents (*a*) tables relevant to equitranslational phase transitions, and (*b*) tables relevant to group–subgroup phase transitions and symmetry analysis of domain structures. Progress of the two software packages is satisfactory.

4.2.5. *Volume E. Subperiodic Groups; Editors V. Kopsky and D. B. Litvin*. Volume E is scheduled for publication in the spring of 1999. The final draft of this volume is complete, except for minor modifications of the text of the last subsection, and has been sent to Chester.

4.2.6. *Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. A. Arnold*. Our goal in preparing this volume is to produce a comprehensive, yet relatively concise, reference work for macromolecular crystallography. This first *International Tables* volume devoted to macromolecular crystallography is intended to complement the existing volumes. This development recognizes the increasing size and vitality of the field of macromolecular crystallography. It is hoped that this volume will be particularly useful for 10–12 years; the projected timing should not interfere with other macromolecular crystallography review volumes that are currently in preparation.

Volume F will cover the theory and practice of macromolecular crystallography with an estimated total of 650 pages. In addition there will be surveys of the principles of macromolecular structure and of commonly used macromolecular crystallographic program systems. Approximately 100 authors have accepted invitations to write 95 articles in a total of 27 chapters. Two advisors and an International Advisory Board consisting of 27 members have assisted in the planning of the volume. A web site on the Internet at the IUCr Offices at Chester (http://www.iucr.org/~commit/itf/) has been set up to facilitate inter-author communication during the preparation of the volume. A CD ROM version will be produced to provide electronic access to the volume and accompanying materials.

As of January 1998, outlines have been received for 61 of the 95 (64%) articles, and seven manuscripts have been received. Assuming that most completed manuscripts will be received by the end of 1998, we plan to complete editing during 1999 and project publication in either 1999 or 2000.

4.2.7. *Volume G. Crystallographic Information; Editors B. McMahon and S. R. Hall*. A small number of contributions to Volume G have been received. The CIF dictionaries which the volume will document were formally approved by the IUCr Committee on the Maintenance for the CIF Standard (COMCIFS) during 1997, and some additional work by COMCIFS technical working groups needs to be completed before the interrelationship between the dictionaries can be finalized. The IUCr CIF web site at http://www.iucr.org/iucr-top/cif/home.html continues to be augmented with documentation that will be incorporated into the volume. Work on typesetting is expected to begin before the middle of 1998.

4.2.8. *Volume A1 (formerly H). Maximal Subgroups of Space and Plane Groups; Editor H. Wondratschek*. Volume A1 provides complete tables and diagrams of the maximal subgroups for each space and plane group; for the contents see the Report of the Executive Committee for 1995 [*Acta Cryst.* (1996), A**52**, 962].

The input of the data into the templates for the tables has been completed. All tables could be printed provisionally from the LaTeX manuscript in the style of *International Tables*, Volume A. At a meeting in Karlsruhe the homogenization of the data on isomorphic subgroups (derived by Y. Billiet in 1993/1994) and the data on non-isomorphic subgroups (derived in Karlsruhe before 1990) was put forward. There are still questions to be settled in 1998.

The main tasks in 1997 were the alignment of the style files for the tables to the style of the *International Tables* standard and the checking of the table contents. The alignment is almost finished as far as the authors are concerned. The checking has been performed by hand as well as by computer, using the *GAP* system of mathematical programs. In addition, the user's guide and the theoretical part have been tackled.

In 1998 the checking of the data, the homogenization of the data, and the text parts are to be completed. The manuscript is planned to be finished by the end of 1998.

4.3. *Commission on Aperiodic Crystals*

1997 was a very active year for the Commission. The Commission members were involved in the preparation and coordination of various conference programmes in which topics on aperiodic crystals were scheduled. These included ECM-17, Lisbon, Portugal, 24–28 August 1997, the ACA meeting in St Louis, Missouri, USA, 19–25 July 1997, preparation for ECM-18 which will take place in Prague, Czech Republic, August 1998, and the Fall Meeting of the Materials Research Society which is scheduled to be held in Boston, USA, 30 November–4 December 1998.

The most important activities of the Commission were related to the preparation of and participation in the Aperiodic '97 meeting in Alpe d'Huez, France, 27–31 August 1997. This series of conferences, held every three years under the aegis of the Commission on Aperiodic Crystals, brings together specialists from the fields of incommensurate compounds, polytypes, composite crystals and quasicrystals. The 1997 conference was characterized by the diversity and multidisciplinarity of the topics covered. In particular, new results in the fields of mathematical and theoretical studies, crystallography, diffuse scattering, growth and stability, phase transition, phonons, physical properties and interfaces were presented. Thus participants obtained a broad update on the most recent developments involving aperiodic crystals.

Some Commission members had the opportunity to meet in Tokyo, Japan, during the International Conference of Quasicrystals (ICQ6). Later, and with one exception, all the members met during the Aperiodic '97 conference. The Commission, together with the local conference organizers, selected the best poster and awarded a substantial prize to its author. The Commission members also discussed the organization of and coordination between the Aperiodic series of meetings and the ICQ conferences. The next Aperiodic meeting is scheduled for July 2000 and will take place in Nijmegen, The Netherlands; the next ICQ7 meeting will be held in Stuttgart, Germany, in September 1999.

The Commission has also undertaken some initiatives concerning the storage of structural information on aperiodic crystalline structures. The aim is not to create an independent database but rather to incorporate some additional and specific information into the existing databases. Contacts have been initiated with the authorities in charge of the organic and inorganic structural databases. This activity will be intensified further.

4.4. *Commission on Biological Macromolecules*

During 1997 and at the beginning of 1998, the Commission on Biological Macromolecules was engaged in three activities.

The Sixth International Conference on Biophysics and Synchrotron Radiation (BSR 98) will be organized by K. Moffatt at the Advanced Photon Source, Argonne National Laboratory, near Chicago, USA, 4–8 August 1998. The Commission has recommended that the IUCr supports this conference.

The issue of protein data deposition is still being discussed. Some journals require atomic coordinates and structure amplitudes to be deposited, others do not. Authors may also request that data deposited with the Protein Data Bank at Brookhaven be withheld for one year. The Commission is anxious to ensure that all data of published protein and nucleic acid structures should be deposited, including both coordinates and structure factors. The conditions governing deposition and release are being formally reviewed, in consultation with the crystallographic community.

The next IUCr conference will be held in Glasgow in 1999. The Commission is investigating the possibility of holding a minisymposium on Hydration of Biological Macromolecules at this meeting.

4.5. *Commission on Charge, Spin and Momentum Densities*

The Commission continued to promote the study of electron density distributions in both real and momentum space by bringing together physicists, chemists and crystallographers in conferences, workshops and schools and by initiating and carrying out projects.

Updated information is given on the web page (http://www.tuwien.ac.at/theochem/iucr/csmd.html) which is linked to the IUCr web page. This page contains the members of the Commission, their addresses (including e-mail) and their main activities. Reports and projects will be announced there.

With great sorrow, we learned of the passing away of member E. N. Maslen in February 1997.

4.5.1. *Meetings of the Commission*. The Commission met during the Sagamore XII conference in Canada. The following topics were discussed: the next Sagamore and Gordon Conferences and the progress of the projects.

4.5.2. *Conferences*. *Sagamore XII Conference.* This conference was held in Waskesiu, Saskatchewan, Canada, 27 July–1 August 1997, and was organized by B. Robertson. The main topics were Compton scattering, positron annihilation (for Fermi surfaces), X-ray and neutron diffraction or synchrotron radiation in studies of charge, spin and momentum densities. Orbital moments attracted much attention in the field of magnetism. Maximum entropy and multipole refinements were discussed extensively. The systems studied varied from solids (insulators, intermetallics, molecular crystals, transition-metal compounds) to (organic) molecules and proteins and peptides. The conference had traditionally a stronger emphasis on solids and physics than on molecules and chemistry.

DFT 97 Conference. This Conference was held in Vienna, Austria, 2–6 September 1997, and was organized by K. Schwarz and co-sponsored by the IUCr. It covered density functional theory from the fundamentals (with a key lecture given by W. Kohn), various forms of functionals to applications on large molecules, solids and materials sciences. Excited states, van der Waals interactions and software developments were further highlights.

Gordon Research Conference. For the first time the next Gordon Conference on Electron Distribution and Chemical Bonding will take place in Europe, at Queen's College in Oxford, UK, 30 August–4 September, 1998. K. Schwarz and C. Lecomte were selected as Chair and Vice-Chair. In this conference, chemistry and molecules will play the more important role, although the interdisciplinary nature of this topic will be stressed. The newly available area detectors are revolutionizing charge-density studies and their role in contrast to conventional schemes (image plates) will be discussed.

4.5.3. *Projects*. Five projects are currently being carried out by the Commission. Additional information can be found on the corresponding web page with continuously updated information.

1. *Density Matrix* (W. Weyrich). A progress report is expected at the Gordon Conference.

2. *Fermiology* (A. Bansil). This was extensively discussed at the last Sagamore XII meeting.

3. *Maximum Entropy* (M. Sakata). This is still a heavily discussed topic which will be taken up at the Gordon Conference.

4. *Mulitpole Refinement* (C. Lecomte). As an inorganic test case, Al_2O_3 (corundum) was chosen and first results were reported at Sagamore XII.

5. *Multipole Refinement Program* (T. Koritsansky). The program *XD* has been developed by T. Koritsansky and co-workers under the auspices of the IUCr. An *XD* User's Meeting was held in Berlin, Germany, 15–18 September 1997.

4.6. *Commission on Crystal Growth and Characterization of Materials*

In 1997, the Commission tried – with the help of its former Chair C. Paorici – to continue its tradition of holding International Schools on special topics of Crystal Growth and Characterization with the aim to enable the participation of young scientists from economically disadvantaged countries. The preparation of an International School on Epitaxy of Semiconductor Materials, to be held in November/December 1997 in Trieste, Italy, with the co-organization and main

financial support of the International Centre for Theoretical Physics (ICTP, an institution connected to UNESCO) was started and a lecturing programme was established. Such Schools, co-organized and co-sponsored by the ICTP, had been successfully arranged in previous years (*e.g.* Miramare, Trieste, Italy, 1992). Unfortunately, owing to drastic reduction of the ICTP budget, the plan to organize the above School had to be abandoned.

The Commission helped in the preparations of two other International Schools:

(i) The Tenth International Summer School on Crystal Growth (ISSCG-10), which is traditionally connected with the 12th International Congress on Crystal Growth (ICCG-12), is to be held 1–6 June 1998 in Rimini, Italy. Chairs of this School are C. Paorici (University of Parma, Italy) and R. Fornari (MASPEC-CNR Institute, Parma, Italy). Three present and two former members of the Commission are engaged in the lecturing programme.

(ii) The First International School on Crystal Growth Technology (ISCGT-1), which is to be held 5–16 September 1998 in Beatenberg, Switzerland. The Chair is H. J. Scheel, EPFL Lausanne, Switzerland. Three present and two former Commission members are engaged in the lecturing programme.

In addition, the Commission recommended IUCr sponsorship and financial support of both Schools and of the 12th International Congress of Crystal Growth (ICCG-12). ICCG-12 is to be held 26–31 July 1998 in Jerusalem, Israel.

4.7. *Commission on Crystallographic Computing*

The Commission's Web page (http://iucr.sdsc.edu/iucr-top/comm/ccom/index.html) has proved to be a popular form of access to the activities of the Commission. For example, since the page for the 1996 Computing School was officially announced in March of 1997 there have been 27 090 web hits on pages containing papers presented at the 1996 School. Towards the end of 1997, well after the announcement, there were 17 ftp downloads of PostScript versions of the papers per day. This form of accessibility to School Proceedings is clearly a success; however, there is still a need for producing the printed volume. Authors need to be able to cite a specific reference, libraries should be encouraged to stock the volume, and many crystallographers enjoy reading the complete volume in the form of a book rather than a series of printouts of web pages. The published Proceedings referred to as *Crystallographic Computing 7*, will appear as part of the IUCr/OUP Book Series in 1998.

A Computing School is planned as a satellite to the 1999 Glasgow Congress. The School is being organized by G. Bricogne and co-organized by J. Irwin, A. Bloomer, and D. Watkin (Commission member). The School (Frontiers in Computational Crystallography) will be held at the Hinxton Science Park near Cambridge, UK, 14–20 August 1999, following the main Congress. The School will be limited to 100 scientists and students who will receive lectures and hands-on teaching in the computational aspects of crystallography. Readers are referred to the Commission's web page given above to keep abreast of the latest developments for the School.

Current activities of the Commission are focused on the use of software and standard data in determining and improving the accuracy of crystallographic experiments, whether it be from powder diffraction, small molecules or macromolecules. The goal continues to be to provide a CD ROM of appropriate data sets with documentation to the community at the Glasgow Congress. The same material will be available from the Commission's web site. To complement these activities, an Open Meeting of the Commission will be held at the Glasgow Congress where key software developers will be invited to talk about codes they have developed relating to accuracy and validation.

4.8. *Commission on Crystallographic Nomenclature*

The work of the Commission in 1997 was concerned with three areas: the nomenclature of crystallography in n dimensions; the formulation of a clear and unambiguous nomenclature for each phase formed in a sequence of phase transitions; and active cooperation with COMCIFS on matters of nomenclature. The first two activities are in the hands of specialists, the last in that of a Commission Observer, see below. All communications within the Commission and its committees were by e-mail except for subgroups that met in July 1997 in Nijmegen, The Netherlands, in December 1997 in Paris, France, and in August 1997 in Geneva, Switzerland. The lack of new concerns brought before the Commission for consideration during the year probably reflects a current absence of nomenclature conflict in the crystallographic literature.

The Subcommittee on the Nomenclature of n-Dimensional Crystallography [see *Acta Cryst.* (1996), A**52**, 91–124 for membership] considered and improved several drafts of their first Report on point-group transformations, families, systems and geometric crystal classes during the year. Following vigorous discussion about such matters as the use of the overbar in the symbol for orthogonal transformations in n dimensions, the setting of lattices in 4, 5 and 6 dimensions, family ordering in these dimensions, and the distinction between the terms 'lattice system' and 'point-group system', a formal ballot showed the emergence of a rather high level of consensus. The Report is expected to be ready for submission to the Commission early in 1998. The nomenclature to be recommended for arithmetic crystal classes, centring symbols, Bravais classes and space groups in higher dimensions will be presented in a subsequent Report.

The primary concern of the Working Group on Phase Transition Nomenclature [see *Acta Cryst.* (1996), A**52**, 91–124, also (1997), A**53**, 822 for membership] is formulation of a unified, informative and unambiguous notation for each phase in the sequence that a material may form as a function of temperature and/or pressure. The resulting notation has to be clearly superior to the many ambiguous and uninformative notations that are widely used in the current literature. The innovative nomenclature that has evolved during discussions of the Working Group meets these objectives with a six-field notation, each field with a meaning that is intuitively clear while simultaneously presenting highly characteristic phase information. A first Report is expected to be submitted to the Commission for action early in 1998. Extension of this nomenclature to certain long-period or polytype structures, such as SiC or ZnS, and to quasicrystalline phases will be treated in a subsequent Report.

The Commission Observer [see *Acta Cryst.* (1997), A**53**, 822] has noted that COMCIFS continues to be very active, posting a slightly modified version of the Core CIF dictionary,

version 2.0.1, and the new Powder CIF dictionary, version 0.996, on the CIF web site. No issues concerning nomenclature have arisen.

In addition to a listing of all members on the Commission's attractive home page at http://www.iucr.org/iucr-top/comm/cnom/index.html, established through the efforts of B. McMahon, the page also provides general information about the Commission, the titles of all Commission reports, and a valuable group of sites presenting nomenclature resources. The page includes hypertext links to each member, to the full content online of six recent Commission reports and to nine major nomenclature resources.

4.9. *Commission on Crystallographic Teaching*

4.9.1. *Visiting Professorships*. In 1997, a grant of USD 3500 was provided through the ICSU grants programme by UNESCO to support IUCr Visiting Professors, especially in Africa.

4.9.2. *Contributions to Schools of Crystallography*. Professor K. El-Sayed was the main organizer of the Fifth International School and Workshop of Crystallography: Teaching and Applications, which was held in Suez, Egypt, 5–11 April 1997. Several members and consultants of the Commission participated as teachers.

Similarly, Professor M. Laing organized a School on Practical Applications of X-ray Powder Diffraction, in Durban, South Africa, 22–26 September 1997.

The Commission positively supported applications for IUCr sponsorships for two schools taking place in Erice, Italy, 22 May–2 June 1997, one on direct methods and one on electron crystallography.

4.9.3. *Other activities*. At ECM-17, in Lisbon, Portugal, 24–28 August 1997, a session on Computer-Based Teaching in Crystallography was organized and chaired by M. B. Hursthouse and E. Makovicky.

At ECM-18, which will be held in Prague, Czech Republic, 16–20 August 1998, there will be a session on Teaching Crystallography to be organized by A. Oskarsson.

4.10. *Commission on Electron Diffraction*

The Commission was involved in a NATO Advanced Study Institute School held in Erice, Italy, 22 May–2 June 1997. This meeting, which had partial support from the IUCr, was attended by more than 100 researchers from 25 countries. The School covered a wide range of aspects of electron crystallography with emphasis on its application to inorganic compounds. A particularly effective aspect of the meeting was the afternoon laboratories where first-hand experience was gained of image reconstruction, direct phase determination, calculation of dynamical scattering, and use of energy minimization procedures. Extensive computer facilities were available at two sites. The Proceedings were edited by D. L. Dorset, S. Hovmöller and D. Zou and published as *NATO ASI Series E: Applied Sciences*, Volume 347. The Applied Study Institute School was held concurrently with one on Direct Methods of Solving Macromolecular Structures, organized by S. Fortier, and there were shared speakers for common sessions.

Towards the latter part of the year, the Commission was involved in the organization of a School on Electron Crystallography to be held in Stockholm, Sweden, 14–19 June 1998.

4.11. *Commission on High Pressure*

This has been the first full year in the life of the Commission on High Pressure. The year has seen steady progress in establishing the framework of the Commission and clarifying the range of its responsibilities. It was created at the Congress in Seattle without prior preparation, and started out simply as the specialized High Pressure Group of the Commission on Crystallographic Apparatus, with the same membership and no specific new remit. It has seemed wise to take time to consider its new role carefully. Action has now been taken to repair two particularly evident gaps in the wider range of science it would be appropriate for the Commission to cover, by appointing consultants with special expertise in the areas of stress effects (A. K. Singh) and soft matter (S. M. Gruner). The Commission has a Secretary (J. B. Parise) and a Treasurer (W. F. Kuhs). A web page has been set up giving the names and contact addresses of all members and consultants, and details of future meetings.

The principal activity of the Commission has been to support and arrange regular workshops and other meetings. This is judged to be the most important and creative function the Commission can fulfil in a field that is experiencing a period of exceptionally rapid growth and development, particularly through the impact of third-generation synchrotron sources, improved neutron facilities, major improvements in detectors and high-pressure techniques, a steady widening of the range of experimental methods available for high-pressure studies, and a large increase in the capacity for complementary computational work.

The inaugural activity of the Commission was a one-day Symposium on Structural Study under High Pressure using X-rays and Neutrons, at the International Conference on High Pressure Science and Technology (AIRAPT-16) held in Kyoto, Japan, 25–29 August 1997. The organizer was O. Shimomura, who reports as follows. The Symposium was a full day of oral sessions, including also short talks on associated poster presentations. The programme aimed to provide an exchange of information on synchrotron and neutron facilities around the world, and the latest high-pressure results obtained using them. Reports on high-pressure research using synchrotron radiation in Europe, the USA and Japan showed that activities at so-called second-generation sources remain at a remarkably high level despite the impressive power and impact of the new third-generation sources. A review of the current status of neutron scattering under pressure underlined the importance of the continuing development of this complementary technique, and showed the unique contribution it can make. In talks on science topics, the latest results on the structural systematics of semiconductors emphasized the power of image-plate techniques in solving crystal structures; the growingly important experimental and theoretical topic of deviatoric stress was comprehensively reviewed; new techniques for the study of liquid structure, developed at the Photon Factory and ESRF, were presented, based on the combined use of XAFS and density measurements; the value of high-pressure neutron diffraction studies in probing the nature of hydrogen bonding was discussed; promising new applications of the Paris–Edinburgh pressure cell for neutron-scattering studies of phonons at high pressure were illustrated with recent results; and the effectiveness of high-pressure neutron diffraction for studying magnetism was illustrated with new work on rare-earth monopnictides. There was an excellent

attendance of some 50 participants throughout, despite the competition of eight other symposia for the overall 600 at the conference.

The Commission's first independent meeting was a three-day Workshop on Crystallography at High Pressure using Synchrotron Radiation: the Next Steps, held at the ESRF in Grenoble, France, 21–23 November 1997. The organizer was D. Häusermann, who reports as follows. The availability of very high brilliance radiation at the ESRF since 1993 has had a marked impact on high-pressure science – especially crystallography in extreme conditions of pressure and temperature. The time was right to organize a workshop focusing particularly on synchrotron-based research. 27 scientists representing the main groups active in synchrotron techniques and associated fields around the world gave invited talks on the latest results and developments. The first two sessions were concerned with non-structural techniques, and provided an overview of new work in magnetic dichroism, Mössbauer spectroscopy, inelastic scattering, X-ray absorption, EXAFS on single crystals, and combined spectroscopy and diffraction methods. Two lively sessions followed on the use of laser and resistive heating for work on iron and low-Z systems under extreme P–T conditions. After talks on liquids and large-volume presses, attention was turned to solving and refining structures – with an overview of the complementary use of neutron and X-ray techniques, a presentation of accurate work carried out recently at the ESRF on nitrogen, and a provocative comparison of the respective powers of angle-dispersive and energy-dispersive methods. After a stimulating session on strength, elasticity and kinetics – all 'hot' topics, as the extended accompanying discussion demonstrated – the last two sessions concentrated on data collection and analysis in 2D, developments in 2D detectors, and future prospects on third-generation sources. The latter session covered highlights of the ESRF programme, the promise of extra photon power at SPring-8, the high-pressure plans for APS, and a 'blue skies' forward look at the many new prospects now in view. There were over 80 participants from 18 countries. These included eleven young scientists, from nine different countries, who benefited from support provided by the IUCr. The workshop also benefited from generous financial support from the ESRF, for which the Commission records its gratitude.

During this workshop, the opportunity was taken for two meetings of the Commission. The main business covered included reports on the 1997 meetings, terms of reference, membership, web pages, an address list, and plans for future meetings and other activities. A long and careful discussion of the membership led to the recommendation to appoint two consultants, already reported above. It was agreed to develop and then maintain an up-to-date web page, and to establish as a project for the coming year the compilation of a comprehensive and accurate address list. Detailed discussion of possible plans for 1998 resulted in the choice of a workshop covering the whole breadth of the Commission's range, to be held in the USA late in the year. J. B. Parise and R. J. Hemley agreed to investigate various possibilities. Preliminary consideration of possible options for the 1999 Congress in Glasgow supported a bid for a number of coordinated microsymposia and keynote lectures, similar to the successful workshop within the 1996 Seattle Congress. A proposal from A. Katrusiak to promote high-pressure techniques and make them more widely accessible through a series of schools, starting with one in Erice, Italy, as soon as possible, was strongly supported. He undertook to make contact with the organizers of the Erice schools.

Subsequent developments have led to the choice of Argonne National Laboratory – with its twin facilities of the third-generation synchrotron source, APS, and pulsed neutron source, IPNS – as the venue for the 1998 workshop, to be held 14–17 November. First steps have been taken towards organizing a High-Pressure School at Erice in 2002 or 2003.

4.12. *Commission on Neutron Scattering*

The principal event for the Commission in 1997 was the International Conference on Neutron Scattering, organized by the Neutron Scattering Association of America, in Toronto, Canada, 16–20 August 1997. This meeting assembled about 200 scientists interested in neutron scattering and was most productive. It was extremely encouraging to see the breadth of neutron scattering applications developing in the USA, despite the set-backs which have occurred over the last few years in the construction of advanced neutron sources and the temporary shutdowns of the two major reactors at Brookhaven National Laboratory and Oak Ridge National Laboratory. Many participants from Europe and other parts of the world also attended.

The development in North America parallels the developments in Europe, where the European Neutron Scattering Association held a remarkably well attended and excellent meeting at Interlaken, Switzerland, in the previous year. About 800 scientists interested in neutron scattering attended that meeting and, once again, there were very innovative papers in new areas of science which show the health of neutron scattering as a widely used technique.

At the Toronto meeting, a closed meeting of the Commission was held. Four present members of the Commission were involved, as well as B. Lebech (Denmark), and S. Mason (France). In view of the success of the International Conference on Neutron Scattering meetings both in Europe and in the USA, a major item on the agenda for the Commission meeting was the way in which the IUCr General Assembly and Congress meeting (with its microsymposia) as well as the Neutron Scattering Satellite meeting, held in conjunction with the IUCr General Assembly, could be fitted into the world programme. As a number of members of the Commission were on the Organizing Committees for both the American and the European meetings, it was agreed that they would exert their influence to ensure that a regular cycle of meetings occurred. Scheduling should not disadvantage the neutron scattering component of the IUCr General Assembly and Congress. B. Lebech undertook to do this for the European meeting, and J. D. Jorgensen (who was one of the principal organizers of the Toronto meeting) was briefed to convey the information to the American Association. A phasing of the neutron scattering meetings in the two continents has been worked out and it is expected that, within the next three years, a programme could settle down which is of advantage to all.

Another matter raised at the closed Commission meeting was the formation of an Asia–Australasia Neutron Scattering Association, to complement the Neutron Scattering Associations in Europe and the USA. Various scenarios were discussed including combining the Asia–Australasia meeting with the USA meeting and having regular conferences in Hawaii, but it was finally resolved that if agreement could be obtained in the Asia–Pacific Region it was better that an Asia–

Pacific or Asia–Australasia Neutron Scattering Association should be formed. J. W. White and Y. Fujii, from Australia and Japan, undertook to take this matter further as J. W. White is Chair of the Australian National Committee and Y. Fujii is Chair of the Japanese Neutron Scattering Association.

4.12.1. *World-wide developments in neutron scattering*. At the OECD (Organization for Economic Cooperation and Development) Megascience Forum meetings, the question of provision of neutron scattering facilities world-wide was extensively discussed in 1997. One aspect of these discussions has been the suggestion that, for the period subsequent to the year 2000, there might be major new neutron sources in Europe, the USA and the Asia–Pacific Region. The suggestion went further to suggest that these might be sufficient to cover needs. Subsequent discussion has indicated that this is too narrow a view, and that high-quality medium-flux facilities existing in the various continents must be integrated into this scenario. These discussions are partly prompted by the fact that there may be a 'neutron drought' in the early part of the next century, owing to the expected close-down of a number of the medium-flux facilities world-wide. Given the growth indicated by the conferences referred to earlier, this drought is a serious matter, as neutron techniques become more widely used. In addition, it is clear that complementarity between neutron scattering techniques and X-ray scattering techniques, particularly using synchrotrons, remains a totally true concept, and that there will need to be co-existing X-ray and neutron facilities, of the highest quality, well into the next century.

In response to these types of discussion, the USA has now funded the first stage of the construction of a major spallation neutron source at Oak Ridge National Laboratory. This will be the leading facility of its kind in the USA and will possibly surpass the quality of the ISIS Neutron Scattering Source at the Rutherford Laboratory in the UK. That source is currently the world's leading neutron spallation source. Complementary developments in Europe also took a step forward with the publication of the full documentation for the European Spallation Source (ESS). A very clear case for a site-independent instrument has been made, and these proposals, coupled with the fullest use of the existing facilities in Europe, are supported by the document prepared in 1996 by the European Science Foundation (the so-called AUTRANS Report, May 1996). In the Asia–Pacific Region, there are also major developments in spallation neutron sources promised. In March 1997, there was a meeting at the KEK (Tsukuba, Japan) to discuss the possibilities of the Japanese Hadron Project (JHP). This is a USD 1 billion project aimed at producing powerful beams for particle physics projects, but also, as a component, a powerful spallation neutron source (power at target 0.5–1.0 MW). Such an instrument would surpass the Rutherford Laboratory performance at ISIS by factors of between 5 and 40, depending on the neutron wavelength and the application. J. W. White and a number of members of the Commission participated in this discussion and funding is being sought through the Japanese Education Ministry at present. In this context, it is also worth mentioning a very recent development announced by the Japanese Atomic Energy Institute (JAERI). That Institute held a workshop and an advisory meeting in March 1998 to discuss their proposal for the 'Japanese Neutron Project'. This project is to build an accelerator capable of delivering up to 5 MW of proton beam power on to a target. This greatly surpasses the power for even the Japanese Hadron Project and would give a neutron scattering facility of remarkable quality. The other aspect of this project, however, is that this beam could be used for prototype experiments on the spallation 'burning' of transuranic radioactive waste.

J. W. White was made Chair of the Advisory Group to draw up its recommendations to the Japanese Atomic Energy Institute. The conclusions of the working group were that the spallation burning project might be feasible given the technology that the Japanese are developing. It is apparent that Korea has an interest in this process as well, and that other countries in Europe and America might also be concerned.

Australia has also embarked on a new reactor project. This is to replace the 40-year-old HIFAR Reactor at Lucas Heights with a modern instrument capable of meeting Australia's medium-flux neutron demands at a quality which will endure into the middle of the next century. The reactor design and instrumentation conception are both now going ahead quickly with working parties drawn from the Academies and industry. The Australian government has decided to go ahead with the project. It is expected that this instrument will be complementary to the spallation neutron source developments in the Asia–Pacific Region.

4.12.2. *Workshops and outreach*. Members of the Commission have played a major part in organizing the international conferences referred to above, and preliminary submissions of microsymposia for the 1999 Glasgow Congress have been made. Plans are well developed for a Neutron Scattering Satellite Meeting in conjunction with the 1999 General Assembly and Congress.

As always, it is a pleasure to acknowledge the important contribution made to neutron scattering and the work of the Commission by *Neutron News*. The Commission wishes to thank G. Lander for his editorship and the lively way in which the magazine is presented.

4.13. *Commission on Powder Diffraction*

The Commission has made an excellent start to an ambitious programme of events and projects. The mailing list for the *CPD Newsletter* has now expanded to over 1200. The establishment of the European Crystallographic Association (ECA) and associated Special Interest Groups (SIGs) has raised interesting new ways of interacting with the European powder community that the CPD is investigating. The first round of the quantitative phase analysis project has begun and the CPD has a high profile in promoting a wide variety of workshops, tutorials and schools.

4.13.1. *Meetings/workshops/schools*. The largest meeting covering the areas of interest for the CPD in 1997 was the European Powder Diffraction Conference held in Parma, Italy. This was an excellent meeting organized by Professor G. Artioli covering: structure solution; refinement; QPA; *in situ* kinetics; catalysis; disordered structures; instruments; size/strain; accuracy; thin films; and general materials. The CPD held its business meeting in Parma and finally agreed that the main CPD-sponsored satellite would be fully integrated with the main IUCr Congress in Glasgow. The 46th Annual Denver meeting was held in Steamboat Springs, USA, covering a broad range of topics as usual. This was the last year that P. Predecki was master of ceremonies; in future the ICDD will be responsible for this meeting. There was CPD involvement in the 17th Conference on Applied Crystallography and 3rd Rietveld Summer School organized by D. Stroz and at the

workshop to discuss the possibly of a Spanish powder beamline at the ESRF.

4.13.2. *Projects*.

Quantitative phase analysis. An update was published in the *CPD Newsletter* in December 1997. Briefly, four samples of carefully constituted multiple composition are in the process of being distributed to those people who volunteered for the study. There was an excellent response to the original request for participants, 140 questionnaires have been distributed and to date 90 have been returned requesting material. 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. Madsen particularly but also to CPD consultant R. J. Hill, member D. K. Smith and a large number of co-workers. We expect some preliminary results for presentation at Budapest (EPDIC-6) and to be able to present the results of the study in full at the Glasgow Congress in 1999.

Rietveld guidelines. CPD member L. B. McCusker has submitted a paper to *Journal of Applied Crystallography* that contains advice and guidelines for Rietveld refinement. The paper has the endorsement of the CPD 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 CPD round robin were published by R. J. Hill and L. M. D. Cranswick [*J. Appl. Cryst.* (1994), **27**, 802–844].

Collaboration with other Commissions. This is proceeding well, especially with structure solution techniques using combinations of powder and electron diffraction; we hope that our collaborations will result in fruitful research with small-angle scattering, X-ray absorption spectroscopy, neutron scattering and high pressure, possibly leading to joint micro-symposia at the Glasgow Congress.

Industrial application notes. P. Scardi has begun research into the possibility of the CPD making further inroads towards industrial application notes. The aim would be to publish good practice in certain common industrial situations in a variety of languages.

Newsletters. There have been two *CPD Newsletters* published in this period, one edited by R. Delhez, the other by P. Scardi. Both editions have appeared on the web (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. We are investigating ways of mirroring this site to speed access.

ICDD. R. L. Snyder represented the ICDD at the CPD meetings, once again reporting on a wide range of activities, details of which can be found at http://www.icdd.com/.

4.14. *Commission on Small-Angle Scattering*

Members of the Commission participated in a number of activities of broad interest to the world-wide small-angle scattering (SAS) community during the last year. Additional activities planned for July and August of 1998 will also be described.

On the technical side, there has been considerable activity with regard to standardization of data formats. Commission member D. Svergun is in charge of a project to develop a suitable format for one-dimensional SAS data. It is anticipated that the outcome will be along the lines of the powder diffraction CIF.

Workers at the ILL and the ESRF convened a meeting devoted to data-handling matters in Grenoble, France, 4–6 February 1998. The meeting was labelled 'canSAS', which stands for Collective Aid to Nomadic Small-Angle Scatterers. The web site for this activity can be found at http://www.ill.fr/lss/canSAS/main.html. The 25 experts present at the meeting mapped out a series of tasks that can be expected to serve as a strong focus for wide-ranging efforts to improve the lot of the users of scattering facilities all over the world. These 'nomads' are thought to number upwards of 1000 scientists. Representatives of the Commission participated in this meeting and it is anticipated that the Commission will continue to support the resulting activities in the future.

A workshop on Data Handling for Small-Angle Scattering is scheduled to be held in conjunction with the 1998 ACA Annual Meeting in Washington, DC, USA, 18 July 1998. This workshop has been organized on behalf of the Commission by the Commission Chair. It is designed to provide a broad overview of the problems associated with the acquisition, reduction, transport, and modelling of SAS data. Leading experts in these areas have been recruited as discussion leaders of the workshop. The complete programme is available on the ACA's web pages at http://www.hwi.buffalo.edu/ACA. Look for the details on the 1998 annual meeting.

Education is another component of the Commission's agenda. Examples of this include a special session on Small-Angle Scattering in the Industrial Plastic Laboratory as part of the ANTEC meeting of the Society of Plastics Engineers to be held in Atlanta, Georgia, USA, 27 April 1998. A tutorial workshop on Small-Angle Scattering in Polymers is scheduled as part of the August 1998 meeting of the American Chemical Society's Division of Polymeric Materials Science and Engineering, to be held in Boston, Massachusetts, USA. The workshop will take place on 22 August 1998. A major symposium on SAS in Polymers will have sessions on 23–27 August.

The publication of the Proceedings from the ongoing series of International SAS Congresses is always a milestone for the community. The Proceedings of the X Congress, held in Campinas, Brazil, July 1996, appeared in a special issue of the *Journal of Applied Crystallography* (Volume 30, Part 5, Number 2, 1 October 1997). A. Craievich (who was the Conference Chair), G. Kostorz and J. Teixeira served as Guest Editors of the special issue. The issue has 320 pages, with 62 articles. The table of contents and synopses of the articles can be accessed at http://www.iucr.org/iucr-top/journals/jac/jac.html and its mirror sites. Additional articles based on presentations at Campinas can be found in the subsequent issue of *Journal of Applied Crystallography*.

Planning for SAS XI is under way, with the event scheduled to take place in May 1999 at Brookhaven, USA. This series of Congresses started in 1965 in Syracuse, USA, and it is a core institution in the community. A number of the early organizers remain active in SAS research. Continuity has been assured through the experience inherited through a strongly motivated International Committee integrating past organizers with enthusiastic local organizers. The published proceedings of the Congresses are an invaluable resource for both experienced and beginning workers in the field of SAS.

The SAS web pages are now well established and continue to attract new subscribers to the associated list server. These

web pages feature the latest news on meetings and other activities of interest to small-angle scatterers. The URL is http://www.nist.gov/sas. Any scientist with an interest in this area of research is encouraged to visit the site, subscribe to its list server, and post questions or discussion topics. Most of this material is mirrored on the various IUCr continental servers. Just look for the Commission on Small-Angle Scattering in the site index.

4.15. *Commission on Structural Chemistry*

As in 1995, the Commission was involved in a second major workshop called Indaba II held in the Kruger National Park, South Africa, August 1997. The general title was Intermolecular Interactions, and the meeting was organized again by J. C. A. Boeyens and his co-workers. Proceedings are being edited, as for Indaba I, by W. Gans and published by Plenum. The meeting was divided into three general areas: practical aspects of inter- and intramolecular interactions; new developments in hardware and software; and theoretical aspects of intermolecular interactions. There were 31 full lectures and more than 25 poster presentations. The latter were presented mainly by local young scientists. The meeting was excellently organized and the location with its natural attractions well chosen.

A workshop entitled Predictability of Crystal Structures on Inorganic Solids organized by the German Crystallographic Society (DGK) together with the German Chemical Society (GDCh) (about 50 participants with 15 lecturers from most European countries), held 27–30 October 1997, was also supported by the Commission. The workshop which was organized by H. Burzlaff was divided into three topics: (1) classification and prediction of crystal structures, (2) empirical and (3) *ab initio* structure predictions. Among the lecturers were H. Burzlaff (Germany), W. E. Klee (Germany), I. D. Brown (Canada), G. Bergherhoff (Germany; ICSD), U. Müller (Germany), J. M. Perez-Mato (Spain), E. Parthé (Switzerland), E. Makovicky (Denmark), H. Bärnighausen (Germany), M. Jansen (Germany), J. Schoen (Germany), J. D. Gale (UK), K. Wright (UK), V. Urusov (Russia), K. Schwarz (Austria) and B. Winkler (Germany).

Support was also approved for the 10th International Symposium on Organic Crystal Chemistry which was held 17–21 August 1997 in Poznan-Rydzyna, Poland. This series of symposia started in 1977 with topics such as determination and interpretation of crystal structures. This year the topic was production and design of crystals with desired properties. There were more than 100 participants from 13 countries. The Programme Committee of this four-day meeting was chaired by J. Bernstein. A special plenary lecture was delivered by J. Karle as Honorary Chair of the symposium. Other speakers included M. Hollingsworth, C. Eckhardt, W. D. S. Motherwell, Yu. Antipin, M. Nieuwenhuyzen, C. P. Brock, K. Roberts, R. Davey, I. Karle, W. L. Duax and A. Katrusiak and about 20 other speakers, mainly from Europe including Poland.

At the ACA meeting in St Louis, USA, there were four sessions plus a poster preview session. The sessions highlighted: intermolecular interactions and hydrogen bonding; contemporary small-molecule work which included discussions of problems, programs and current journal policies; powder diffraction methods; and state-of-the-art charge density analysis. All sessions were well attended and lively discussions followed most of the presentations.

The 1998 Spring BCA Meeting will include sessions on disorder and supramolecular assemblies as well as a workshop on twinning. A four-day Workshop and Symposium on Advanced Methods of Structure Determination by Diffraction and Related Methods will be held at the spring national meeting of the American Chemical Society in March 1988. This workshop was organized by A. Clearfield (current Vice-President of the ACA) and the opening speaker at the workshop will be P. Coppens (Immediate Past-President of the IUCr). It is an example of efforts being made by the small-molecule community to 'expose' a broad-based chemical audience to the benefits of X-ray crystallography.

Programme input for the Glasgow Congress was provided directly to the Programme Chair at a meeting of the Commission during the Seattle Congress. The structural chemistry community will have continuing input to the Glasgow Congress through Programme Committee members C. Kruger (Chair of the Commission on Structural Chemistry) and C. P. Brock.

Of major concern to the members of the Commission and the structural chemistry community in general is the shrinking presence of 'small-molecule' crystallography at crystallographic meetings. It is ironic that this area of crystallography, which has become an indispensable part of so many research programmes, is being pushed into the background as a 'black-box' analytical tool. Crystallography is being taught at fewer and fewer universities and the unfortunate results can already be seen in the increasing number of errors appearing in published crystallographic results. What the Commission and the IUCr can do to reverse this trend, or at least to ensure the accuracy of reported results, will be topics on the Commission's agenda when it meets in Glasgow.

4.16. *Commission on Synchrotron Radiation*

The Commission has continued its work over the broad field of crystallography with the use of synchrotron radiation (SR).

The Commission organized a scientific meeting on the crystallographic application of synchrotron radiation (1–2 August 1997) at the Photon Factory as a satellite meeting of the Sixth International Conference on Synchrotron Radiation Instrumentation (4–8 August 1997), which was held at Himeji, Japan. Professor Y. Amemiya (University of Tokyo) and Professor T. Matsushita (Photon Factory) co-chaired the satellite meeting. At the meeting, particular attention focused on 'time-resolved X-ray experiments'. The satellite meeting consisted of the following six oral sessions: (1) New opportunities for time-resolved experiments (I): third-generation SR sources; (2) New opportunities for time-resolved experiments (II): new methods; (3) Time-resolved small-angle X-ray scattering; (4) Mössbauer spectroscopy in time domain; (5) Time-resolved XAFS; and (6) Detectors for time-resolved measurements. About sixty people from ten countries participated in the satellite meeting. Advanced techniques and new methods as to time-resolved measurements were discussed in detail over a broad range. The role of second-generation sources was discussed in relation to the new third-generation sources in order to broaden experimental opportunities available and to activate further the field of synchrotron-radiation research. The collaboration of the Photon Factory staff in the organization of the satellite was greatly appreciated. The Proceedings of the satellite meeting were issued as

a KEK Proceedings (74–14, November 1997, M), which is available from the KEK library.

The Committee also started to discuss the satellite meeting of the Glasgow Congress in 1999. The venue will be at Daresbury Laboratory and the dates will be 2–3 August 1999, with a bus to take delegates to Glasgow on 4 August. The suggested title for the meeting is 'From source to science' and it will cover those topics that will be suggested in the coming year. The initial ideas are for a small (~200 people) well focused friendly meeting with a single set of sessions. We would like to invite four or five well known figures in the field to give keynote talks and to cover a wide range of topics in SR crystallography.

4.17. *Commission on XAFS*

No report has been received from the Chair.

5. Sub-committee on the Union Calendar

The Sub-committee receives and considers requests for IUCr sponsorship and nominal financial support and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-committee, during 1997 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1997 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1998, but approved in 1997, are listed below:

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. 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.

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

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, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands (e-mail: schenk@chem.uva.nl).

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

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

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

The Committee has expended considerable effort during 1997 on the implementation and deployment of a web pan-crystallography information system which may be viewed at the URL http://www.iucr.org/iucr-top/index.html and its mirror sites. The distributed sources of information for this system come from IUCr Commissions and Committees, IUCr conference organizers, IUCr in-house secretarial and journal editors, and the Sincris and CWW news resources. The web pages are given a unified appearance. Further contributions from sources of information of concern to the IUCr and of interest to crystallographers are always most welcome. Information can be obtained from the Chair of this Committee. During its meeting in Lisbon in August 1997, the IUCr Executive Committee delegated editorial powers for IUCr web services to this Committee.

To ensure a ready access world-wide to the pan-crystallography service, the Committee has elaborated a strategy of IUCr-accredited mirror sites. This policy was approved by the IUCr Executive Committee at its meeting in Lisbon in August 1997. The deployment of the mirror-site system depends on the good will and involvement of the IUCr members (*i.e.* the National Committees for Crystallography) in providing equipment with network connectivity to act as mirror sites for their country or region. Some regions of the world are inadequately covered at the moment depriving crystallographers of a very important resource. Administrative and technical information on forming and running an IUCr-accredited mirror site is available from the IUCr Executive Secretary. As part of this strategy for mirror sites, the IUCr has acquired the Internet second-level domain name iucr.org, permitting a unified naming of Chester and the mirror sites; *e.g.* the web sites have the Internet names: www.iucr.org (IUCr offices, Chester, UK), www.fr.iucr.org (France), www.se.iucr.org (Sweden), www.us.iucr.org (USA), www.za.iucr.org (South Africa) and www.ch.iucr.org (Switzerland).

The Committee identified a need within the community for discussion forums operated by means of an e-mail list server. To this end, the IUCr R&D group has sought out, implemented and tested software to meet this demand. The system offers web interfaces for dealing with administrative affairs and for viewing each list's archive. A policy document for online discussion groups has been formulated and submitted to the IUCr Executive Committee for approval. Full details may be obtained from URL http://www.iucr.org/iucr-top/lists/ for those wishing to avail themselves of this service.

The electronic online distribution of the IUCr's six journals will require an infrastructure that the Chester office is probably not in a position to provide itself, indeed in the same way that the printing, mailing and subscription administration for the printed journals is subcontracted. It may be that there is a distinct advantage in being associated with an electronic distribution service giving access to other related scientific journals. The Committee is active in surveying the market of

service providers in this field. Work is continuing at the Managing Editor's office to develop the editorial processes involved in full-text SGML markup of the IUCr journals and other publications. This is an essential prerequisite for the supply of content to electronic online distribution processes. It is also a key to the database-driven integration of manuscript handling and refereeing. The Committee advises on and monitors this strategy.

The Tenth Edition of the *World Directory of Crystallographers* (*WDC*) has been published and is available in printed form. Individuals can purchase the directory from Kluwer Academic Publishers (price NLG 50); group purchases are also possible by contacting the IUCr Promotions Representative (as@iucr.org). For the online version of the *WDC*, tests have been undertaken using LDAP servers in order to benefit from the LDAP functionality now available in the most popular internet communication systems or web browsers. The Committee is currently involved in the elaboration of policy and technical documentation for the future development of the *WDC* to cover needs that have been identified.

A project has begun for the production of CD ROMs containing crystallographic information. This support is primarily intended for those scientists lacking suitable internet connection to avail themselves of the on-line services.

The Chair of the Committee visited the IUCr Chester offices in November 1997.

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

Since its founding, COMCIFS has been working to bring three dictionaries to approval. Even before the founding of COMCIFS, *Acta Crystallographica Section C* had committed itself to the use of CIFs for the submission of papers describing crystal structure determinations and in recent years all papers have been submitted as electronic CIFs. As a result of this experience, a number of changes were required to the core dictionary. These were approved on 12 November 1996 as version 2.0 of the core dictionary (coreCIF.dic 2.0). This was followed by the approval of the first versions of the macromolecular dictionary (mmCIF.dic 1.0) on 8 June 1997 and the powder dictionary (pdCIF.dic 1.0) on 9 July 1997. The International Centre for Diffraction Data is committed to using pdCIF for the Powder Data File, and both the Protein Databank and the Nucleic Acid Databank are committed to using mmCIF. Modifications are being proposed to these approved CIF dictionaries and we expect new versions to appear in the next year or two. In addition, work is in progress for dictionaries covering area detectors (raising problems of how to store large arrays of primary data), electron densities, modulated structures, symmetry and diffuse scattering. Technical discussions are under way on how best to represent images, how to combine binary data with CIFs and how to link different CIF dictionaries.

Current dictionaries and drafts of dictionaries under development are available on the IUCr web pages, and all approved dictionaries will appear in hard copy in Volume G of *International Tables for Crystallography*.

The membership of this Committee follows. Full members: I. D. Brown (Canada; Chair), S. R. Hall (Australia), P. R. Edgington (UK), P. M. D. Fitzgerald (USA), B. H. Toby (USA), G. Madariaga (Spain), M. Spackman (Australia), B. McMahon (IUCr R&D Officer). Consultants: A. Authier (France; Commission on Crystallographic Nomenclature), G. M. Sheldrick (Germany), P. Murray-Rust (UK), P. E. Bourne (USA), E. Ulrich (USA; NMR Databank), O. Ritter (USA; Protein Data Bank), H. Berman (USA; Committee on Crystallographic Databases). In addition, there are a number of people who have requested to receive the mailings of COMCIFS. We consider these as auditors and welcome any comments they have on the business of the Committee.

8. Committee on Crystallographic Databases

The members of the Committee have been concerned with two major issues: the future of the non-organic databases and the support of CIF-related activities.

ICSD has been run by Fachinformationszentrum Karlsruhe (FIZ). Since FIZ will move from the public domain into the private sector, there are concerns about how this will affect the future of the inorganic database. The metals database (CRYSTMET) was formerly run by NRC Canada and is now run by TOTH. Funding for this project is not certain. Several parties have expressed interest in stewarding these data and it has been recommended that these individuals be brought together so as to ensure that access to these data is not jeopardized.

The mmCIF software developers workshop held at Rutgers, USA, in October 1997 spurred several new efforts. There is now serious work being carried out to create macromolecular CIF (mmCIF) output from key crystallographic programs. K. Henrick from the European Bioinformatics Institute (EBI) has sent a letter co-signed by H. Berman, J. Sussman and P. Fitzgerald to all software developers urging their cooperation. Another meeting, planned in the fall of 1998 and hosted by EBI, will bring together crystallographic software developers, database curators and mmCIF experts.

At the same time, the process of extending the dictionary has been brought into an orderly framework. A board of editors has been created to help review new definitions. The process works well and it is expected that version 2.0 will be released before the ACA meeting in July 1998. In addition to the work on mmCIF, the image CIF (imgCIF) effort continues to evolve.

9. Promotion Committee

The most important matter dealt with so far regarding promotions activity has been the appointment of the Promotions Representative (PR), A. J. Sharpe. It will be the duty of the PR to increase revenue to the IUCr through various promotional activities, including obtaining advertising revenue and through the sales of IUCr products. Following her appointment, the first task will be to locate advertisers for the special issue of *Journal of Synchrotron Radiation*. Other activities will include administering further advertising, producing and distributing promotional leaflets for ICCBM-7 (*Acta D*), *Acta Crystallographica* in general and the *IUCr Newsletter*. Travel/registration/promotional campaigns for the following meetings will also need to be planned: Computers in Structural Chemistry and Molecular Biology, Manchester, 16–17 June 1998; American Crystallographic Association, Arlington, USA, 12–20 July 1998; XAFS X, Chicago, USA, 8–12 August 1998; ECM-18, Prague, Czech Republic, 15–19

August 1998; and American Chemical Society, Boston, USA, 22–26 August 1998.

10. Regional Associates and Scientific Associates

10.1. *American Crystallographic Association (ACA)*

The yearly ACA meetings continue to be highly successful. Though many aspects of crystallography continue to be represented, the emphasis on the life sciences is evident from the distribution of the contributed papers. The ACA membership increased by about 5% in 1997 as compared with the previous year, an increase not unrelated to the attractiveness of the annual ACA meetings. ACA council made additional funding available for student travel, and established the Elizabeth A. Wood Science Writing Award, designed to recognize those who communicate science to a general audience. The Warren, Buerger and Patterson Awards were presented to D. L. Price, C. K. Johnson and C. E. Nordman, respectively. A call for nominations was issued for the Fankuchen Award, to be presented at the 1998 meeting in Washington, DC. The ACA, which includes both US and Canadian crystallographers, continues to be a very strong Regional Associate of the IUCr.

10.2. *Asian Crystallographic Association (AsCA)*

The next Triennial Conference of the AsCA will be held in Hotel Equatorial Bangi, Selangor, Malaysia, 13–15 October 1998. Professor S. L. Chang is the Chair of the International Organizing Committee, Professor A. H. Othman the Chair of the Local Organizing Committee and Professor T. Yamanaka is the Chair of the International Programme Committee. The first circular of AsCA '98 has been distributed to all the societies concerned. The conference is intended as a forum of all the fields of crystallography in Asia. A special symposium on the celebration of the 50th Anniversary of the IUCr will be included. The homepage address of the Conference is http://gandalf.otago.ac.nz:800/rweavers/ASCA/asca98.htm. The AsCA has developed its own e-mail version of the *AsCA Newsletter* to improve communication within its member countries. The editor is Professor J. Simpson.

10.3. *European Crystallographic Committee (ECC)/European Crystallographic Association (ECA)*

The ECC met in Lisbon, Portugal, 25–27 August 1997, during the Seventeenth European Crystallographic Meeting (ECM-17). ECM-17 was highly successful with more than 800 participants. The contributions ranged from biocrystallography to mineral science with a large proportion of molecular biology and molecular crystals.

Prior to the central discussion on the creation of a more formal association, during the ECC session the organizers of ECM-18 to be held in Prague, Czech Republic, in 1998 reported on the timetable of the meeting and the proposed satellites. Nancy, France, has been chosen to welcome ECM-19 in 2000. A preliminary vote for 2001 in favour of Cracow, Poland, was registered.

As agreed during the Seattle Congress, a working group had elaborated statutes and by-laws of a European Crystallographic Association. These documents had been circulated among the delegates. These statutes were extensively discussed, partially amended and finally adopted by those present. The Chair of the ECC, H. Fuess, declared the ECC as dissolved and the ECA to exist. A new Executive Committee was elected on the basis of the new statutes. Those elected are: C. Giacovazzo (President), J. Bernstein (Vice-President), P. Beurskens (Secretary), S. Harkema (Treasurer) and A. Carrondo, P. Paufler, F. H. Allen (members). The legal domicile of the Association is Nijmegen, The Netherlands. The membership shall consist of National Members (adhering bodies), Affiliate Members (legally constituted bodies) and Individual Members. The ECA is the Regional Associate of the IUCr for Europe and some neighbouring countries.

10.4. *International Organization of Crystal Growth*

The main acitivities of the IOCG in 1997 involved preparations for the following International School and International Congresses:

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

The 12th International Congress on Crystal Growth (ICCG-12), Jerusalem, Israel, 26–31 July 1998; Chair A. Horowitz.

The 10th International Congress on Vapour Growth (ICVGE-10), Jerusalem, Israel (to be held in connection with ICCG-12), 26–31 July 1998; Chair M. Roth.

Moreover, the IOCG Executive Committee collected suggestions for candidates for the Frank Prize (fundamental aspects of crystal growth) and the Laudise Prize (technological aspects of crystal growth). Both prizes will be awarded during ICCG-12 in Jerusalem.

10.5. *International Centre for Diffraction Data*

No report has been received from the IUCr Representative.

11. Representatives on Other Bodies

11.1. *IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS)*

The annual meeting of IDCNS was held 27–28 August 1997, during the 39th IUPAC General Assembly. Members of IDCNS have been very active since their last annual meeting, having reviewed 18 new nomenclature reports – several in multiple parts – prior to publication in *Pure & Applied Chemistry*. Members also reviewed many other reports originating in the various Commissions of IUPAC. Quality control of all IUPAC nomenclature documents before publication, and resolution of any interdivisional nomenclature conflict that might arise in this process, are the primary purposes of these reviews. The number of reports directly of interest to crystallographers varies considerably; most were somewhat marginal this past year. Two of interest are concerned with the nomenclature of chemical kinetics and with X-ray emission spectrochemical analysis. A revised list of atomic weights through atomic number 111 (symbol Uuu, name unununium, atomic weight ~272) has been published in *Pure Appl. Chem.* (1997), **69**, 2471–2473. (Uuu and the element with atomic number 110, symbol Uun, name ununnilium, atomic weight ~269, are the only elements with three-letter symbols.)

Many IUPAC nomenclature reports are now mounted on the web. The largest collection of reports, including that with the revised list of atomic weights, may be found at: http://www.chem.qmw.ac.uk/iupac/. The decision by the Conférence Générale des Poids et Mesures to abolish the class of SI supplementary units (the radian and the steradian) has

reached the Draft International Standard stage. Publication of a new edition of The SI Brochure was expected by December 1997. The International Organization for Standardization (ISO) is also drafting a new International Standard on the presentation of quantities and units in tables and diagrams.

The IUPAC Secretariat has now moved from Oxford, UK, to Research Triangle Park, North Carolina, USA, where the next meeting of IDCNS is tentatively scheduled to be held 21–22 August 1998. Dr V. Metanomski of *Chemical Abstracts* becomes the new Secretary of IDCNS on 1 January 1998. Professor T. Cvitas of Zagreb, Croatia, will succeed Professor I. Mills as Chair in January 2000.

11.2. *International Council for Scientific and Technical information (ICSTI)*

This report has been prepared by H. D. Flack who assumed responsibility as the IUCr Representative to ICSTI in mid-July 1997, a post left vacant following the untimely death of E. N. Maslen on 2 February 1997. As a consequence, the IUCr was not represented at the ICSTI Annual General Assembly in Philadelphia, USA, in early June 1997. General information on ICSTI and its current projects are available on its web site (http://www.icsti.nrc.ca/icsti/).

Of the points treated at the Annual General Meeting and at the Technical Activities Coordinating Committee, one sees that ICSTI has been active with and completed a Networking Survey, has set up a permanent Web Advisory Committee, has continued its project with UNESCO aid to give access to telematics facilities in the Eastern Caribbean, has continued with its International Classification Scheme for Physics, has made a comparative study of access to journals through subscriptions and document delivery, has completed a multilingual thesaurus in geosciences, has established links between Archive and Information (A&I) services and the ISSN register, and has selected the virtual library topic for special treatment at the 1998 General Assembly since it englobes many of the topics such as metadata and encryption of current concern. During the General Assembly, the President laid particular stress on the need for ICSTI to collaborate with other related organizations such as ICSU and its group on Data and Information, STM, CODATA, AAP, and others. ICSTI set up a new Information Policy Committee to be active in the field of international standards, laws and regulations in order to maximize the use of, and access to, scientific and technical information.

A one-day discussion session was held during the meeting in Philadelphia on the electronic scientific archive, a subject of preoccupation to the IUCr. ICSTI will draw up a clear plan of action concerning this as a follow-up to the ICSU Press Conference on Electronic Publishing in Science held in Paris, France, February 1996. A further session dealt with legal aspects of information transfer.

The ICSTI graphics project established by E. N. Maslen to measure the efficiency of encoding techniques for different sorts of graphics information has been curtailed for lack of a leader.

ICSTI produces a newsletter (*ICSTI Forum*) in print form which is also available on the web. This publication provides useful current information prepared by experts on topics concerning scientific and technical information. Articles of interest to the IUCr dealt with Information Security on the World-Wide Web, Issues of Global Access to Scientific Data, The Role of A&I Services in Facilitating Access to the E-Archive of Science, and Archiving the On-line Journals. Other Committee documents of use were the annual report of the Committee on Legal Issues, a report on the DOI (Digital Object Identifier) and a document containing a bibliography and web sites produced by the Information Policy Committee.

ICSTI was concerned in 1997 with the issue of Copyright Rights in Databases. This matter came to a head due to newly introduced legislation in the European Union which would severely limit an individual's rights to access databases and considerably increase the rights of the database producer. The dividing line between database generation and publication having become exceedingly fuzzy, ICSTI feels its mandate touches this area. However, CODATA has formed an ICSU/CODATA Group on Data and Information which produced a long position paper on access to databases for presentation at a conference of the World Intellectual Property Organization in Geneva, Switzerland, in September 1997.

11.3. *International Council of Scientific Unions (ICSU)*

The International Council of Scientific Unions has proposed a change in its structure and its name. According to the proposal, the General Committee, on which the Scientific Unions are represented, is to be abandoned, and many of its functions are to be taken over by the Executive Committee, including the nomination for new members of the Executive Committee. The Scientific Unions will continue to be represented in the General Assembly of ICSU. In connection with this change the name of the organization is to become ICSU: International Council for Science (note the mismatch between the acronym and the name). The changes are to be voted on in an Extraordinary General Assembly, to be held in Vienna, Austria, 25 April 1998, at which the IUCr will be represented by P. Coppens. The few Unions that have expressed an opinion on the proposed changes have come out mostly in the negative. It is not clear at the time of writing whether all of the changes will be approved by the General Assembly.

During 1997, J. Marton-Lefèvre stepped down as the Executive Director of ICSU. She was replaced by J.-F. Stuyck-Taillandier. ICSU has a large number of Committees and Groups dealing with issues that impact science. A Group on Data and Information was established to deal with the potential adverse effects of the new international property laws on the conduct of science and education. One of the aims of the Group is to induce national organizations to alert policy makers and legislators of the importance of the issue and its potential negative impact. The ICSU Press Committee was charged with the follow up of the Conference on Electronic Publishing, which took place in Paris in 1996. A workshop on the costs and benefits of electronic publishing is to be held in Oxford early in April 1998. The publishing programme of ICSU Press has been discontinued with the transfer of the last journal to a commercial publisher. Among the activities of ICSU's programme on Capacity Building in Science are enhancement of communication between scientists and the general public, and promotion of teacher training and education. A conference is to be organized in Brazil in September 1998. World Climate Research and the environment are among the other important concerns of ICSU.

11.4. *ICSU Committee on Capacity Building in Science (CCBS)*

No significant meetings occurred in 1997 but the IUCr's Visiting Professorship Programme, which receives support from the ICSU/UNESCO subvention, continues.

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

No report has been received from the IUCr Representative.

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

COSTED–IBN continued its activities to strengthen science in small states and developing countries. A conference and workshop took place in Mozambique in July 1997. Recommendations were made for sustainable agriculture, and a working group of regional experts was established.

11.7. *ICSU Committee on Space Research (COSPAR)*

The main formal activities were directed to the preparations of the 32nd COSPAR Scientific Assembly and Associated Events which will be held 12–19 July 1998 at the Solar–Terrestrial Environment Laboratory, Nagoya University, Japan, with Professor Y. Kamide as Chair. This meeting is connected with the 40th Anniversary of COSPAR, which was established by the International Council of Scientific Unions in October 1958 to continue the cooperative programmes and satellite research successfully undertaken during the International Geophysical Year of 1957–1958. Moreover, in Nagoya new members of the COSPAR Council and COSPAR Bureau for the term 1998–2002 will be elected. The COSPAR Secretariat has collected nominations for the slate. Following a decision of the COSPAR Council during the 31st Assembly in Birmingham in 1996, the Secretariat has worked out modifications of the COSPAR Charter and By-Laws in order to create a new category of affiliate for organizations or individuals that would support financially the activities of the Organization. The proposed changes of the Charter and By-Laws were discussed by the COSPAR Bureau and are subject to voting by the Council members.

In 1997, the Panel on Space Research in Developing Countries (PSRDC–COSPAR) continued its efforts to initiate, encourage and promote the participation of scientists from developing countries in space research and its application for national development. For this purpose, a compendium on information on typical ground-based instruments complementary to space-based observations and data for pursuing research in space science and applications will be prepared. A questionnaire for collecting information on this matter has been prepared and distributed among National and International COSPAR Scientific Unions by the Indian Space Research Organization (ISRO) Headquarters, Bangalore. Finally, COSPAR edited in April 1997 its Directory of Organizations and Associates (160 pages). A limited number of copies of this edition is available for FF 75 each (or the equivalent in USD) and may be obtained by writing to the COSPAR Secretariat, 51 bd de Montmorency, F-75015 Paris, France (e-mail: cospar@paris7.jussieu.fr. The COSPAR web address is http://cospar.itodys.jussieu.fr/).

12. Finances

The audited accounts of the year 1997 are given at the end of this Report. For comparison, the figures for 1996 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 1997 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 gain has arisen on the assets of the IUCr, in terms of CHF, amounting to CHF 737 989. The gain attributable to investment activities has been assigned to the General Fund and the gain attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1997. It should be noted that this gain in CHF is not a real gain of money, but rather a gain on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 1997. The total of CHF 296 902 with the banks at the end of the year was represented by USD 97 658 with Merrill Lynch, GBP 53 493 with National Westminster Bank and CHF 39 160 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the IUCr, including the gain of CHF 737 989 resulting from fluctuations in rates of exchange, have increased during the year, from CHF 6 089 600 to CHF 7 151 105.

A transfer of CHF 50 000 was made to the Publication and Journals Development Fund from the *Acta Crystallographica* Fund. Transfers of CHF 50 000 and CHF 50 000 were made to the Research and Education Fund from the General Fund and the *Journal of Applied Crystallography* Fund. A transfer of CHF 50 000 was made to the Ewald Fund from the *Journal of Applied Crystallography* Fund. A transfer of CHF 75 000 was made to the *Newsletter* Fund from the *Acta Crystallographica* Fund. A transfer of CHF 50 000 was made to the *Journal of Synchrotron Radiation* Fund from the *Journal of Applied Crystallography* Fund.

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

The General Fund account shows a surplus of CHF 39 834 before the transfers totalling CHF 50 000 to the Research and Education Fund, as compared with a deficit in 1996 of CHF 68 921 before transfers totalling CHF 150 000 to the Publication and Journals Development Fund and the Ewald Fund. The administrative expenses were CHF 313 338 in 1997 as compared with CHF 220 091 in 1996. Of this amount, CHF 81 619 was charged to the publications of the IUCr. The administrative expenses are incurred in GBP and the significant increase in 1997 can be attributed to exchange-rate fluctuations.

CHF 27 705 was spent on the Eighteenth General Assembly and Congress and CHF 2 945 in assisting the work of the non-publishing Commissions. The expenses of the IUCr Representatives on other bodies were CHF 1 958. The cost of the Finance Committee meetings held in 1997 was CHF 22 763, while the Executive Committee meeting cost CHF 38 219. The income from the IUCr/Fachinformationszentrum Agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 4 569. The IUCr received CHF 23 200 from the UNESCO subvention to ICSU. The subscriptions from Adhering Bodies were CHF 151 562. Interest on bank accounts and investments credited to the General Fund was CHF 212 865.

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 2 210. Grants totalling CHF 7 558 were paid from the fund.

The *Acta Crystallographica* account for 1997 shows a surplus of CHF 269 302 before the transfer of CHF 125 000 to other fund accounts, as compared with a surplus of CHF 77 363 in 1996 before transfers of CHF 250 000.

The subscription rates were increased for 1997. In 1997, the number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 54 (63) personal subscriptions, was 638 (687) (values for 1996 are given in parentheses). The number of paid subscriptions to *Sections A+B+C*, including 15 (12) personal subscriptions, was 137 (133). The number of paid subscriptions to the separate sections of the journal were: *Section A* 258 (255 for 1996), *Section B* 204 (202), *Section C* 151 (147) and *Section D* 186 (174). 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 878 571 (for 4733 published pages) as compared with CHF 756 672 in 1996 (6596 pages published). The technical editing costs are incurred in GBP and the significant increase in 1997 can be attributed to exchange-rate fluctuations. 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 15 583 before transfers of CHF 150 000 to other fund accounts, as compared with a surplus of CHF 79 664 in 1996 before transfers of CHF 50 000. The deficit in 1997 can be attributed to the publication of a Special Issue. In 1997, the number of paid subscriptions, including 102 (108 in 1996) personal subscriptions, was 820 (868 in 1996).

The *Journal of Synchrotron Radiation* account shows a deficit of CHF 142 541 before receiving a transfer of CHF 50 000 from the *Journal of Applied Crystallography* Fund, as compared with a deficit of CHF 33 600 in 1996 before receiving a transfer of CHF 90 000. In 1997, the number of paid subscriptions, including 120 (129 in 1996) personal subscriptions, was 269 (253 in 1996).

The *International Tables* account shows a surplus of CHF 8 095, as compared with a surplus of CHF 78 172 in 1996 before transfers of CHF 60 000 to the Research and Education Fund and CHF 90 000 to the Publications and Journals Development Fund. The net sales income was CHF 146 020 in 1997 as compared with CHF 120 666 in 1996.

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

The *Newsletter* Fund account received transfers of CHF 75 000 from the *Acta Crystallographica* Fund in both 1997 and 1996. The cost to the IUCr of producing the *Newsletter* in 1997 was CHF 84 574 (CHF 66 950 in 1996).

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 256 908 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 IUCr's journals, promotional costs and web input costs are also charged to the Publication and Journals Development Fund account. CHF 91 816 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the IUCr, and CHF 16 661 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.

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

We have audited the financial statements on pages 584 to 600 which have been prepared under the accounting policies set out on page 587.

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 1997 and of the result for the year then ended.

Deloitte & Touche
Chartered Accountants and Registered Auditors
3 June 1998

Income and Expenditure Account for the year ended 31 December 1997

	Note	1997		*1996*	
			Swiss Francs		
Income					
Membership subscriptions			151,562		*148,822*
Sales					
Journals		2,740,553		*2,372,961*	
Books		196,741		*166,962*	
Back numbers and single issues		36,798	2,974,092	*32,859*	*2,572,782*
Investment income					
Income from investments	14.7	280,164		*221,774*	
Bank interest	14.8	32,148		*29,739*	
Profit on sale of investments	14.9	15,566	327,878	*6,009*	*257,522*
Other income					
Grants		23,200		*22,359*	
Royalties and copyright fees		12,136		*9,446*	
Advertising income		87,957		*72,259*	
General Assembly refund		7,150	130,443	–	*104,064*
TOTAL INCOME			3,583,975		*3,083,190*
Expenditure					
Journals					
Publication costs		1,297,065		*1,217,659*	
Editorial expenses		143,523		*102,709*	
Technical editing		1,052,692	2,493,280	*877,301*	*2,197,669*
Books					
Publication costs		105,969		*63,666*	
Editorial expenses		46,198	152,167	*22,641*	*86,307*
Newsletter					
Publication costs		118,790		*95,776*	
Editorial expenses		48,032	166,822	*35,695*	*131,471*
President's Fund					
Grants and Young Scientists' support			99,374		*71,543*
General Assembly costs			27,705		*65,549*
Ewald Prize			–		*36,000*
Committee meetings and expenses			60,982		*91,883*
Publications and journals development					
General		231,464		*192,602*	
Electronic Publishing Committee/Section Editors meeting expenses		1,343		*1,573*	
Electronic publishing project		27,545	260,352	*46,546*	*240,721*
Subscriptions paid			8,661		*7,127*
Visiting Professorship programme			16,661		*1,290*
Administration expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		9,365		*7,740*	
Secretarial assistance		346		*542*	
Audit and accountancy charges		39,721		*32,228*	
Legal and professional fees		2,293		*2,415*	
Postage and sundries		206		–	
Travelling expenses		2,940		*2,685*	
Bank charges		3,156	58,027	*1,307*	*46,917*

	Note	1997		*1996*	
		Swiss Francs			
Expenditure (*cont.*)					
Executive Secretary's office:					
Salaries and expenses		242,130		*172,634*	
Travel expenses of IUCr representatives on other bodies		1,958		*3,784*	
Star/CIF		22,656		*4,646*	
Commission expenses		2,945		*28,842*	
Sponsorship of meetings		10,525		*40,169*	
President's secretary		1,206		*14,322*	
IUCr/FIZ agreement		(4,569)		*16,225*	
Bad debts – subscriptions		(6,000)	270,851	*6,000*	*286,622*
Depreciation			57,719		*36,894*
Total Ependiture			3,672,601		*3,299,993*
Deficit of income over expenditure (carried forward)			(88,626)		(*216,803*)
Movement in market value of investments in year	14.5		412,142		*266,072*
			323,516		*49,269*
Fluctuation in rates of exchange					
Trading activities	14.2	49,454		*78,851*	
Investment activities	14.2	688,535	737,989	*736,790*	*815,641*
Total recognized gains and losses relating to the year			1,061,505		*864,910*
Opening fund accounts at 1 January			6,089,600		*5,224,690*
Closing fund accounts at 31 December			7,151,105		*6,089,600*

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 14.9. 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.

Balance sheet as at 31 December 1997

	Note	Swiss Francs 1997		*1996*	
FIXED ASSETS					
Tangible fixed assets	14.4		167,852		*173,002*
CURRENT ASSETS					
Stock			38,180		*59,274*
Cash at bank					
Current accounts		55,310		*40,093*	
Deposit and savings accounts		241,592		*309,080*	
Cash with Union officials		26,243	323,145	*19,685*	*368,858*
Investments at market value	14.5		6,627,615		*5,513,221*
Debtors, accrued income and payments in advance			262,437		*236,689*
Subscriptions from Adhering Bodies			29,192		*27,220*
TOTAL CURRENT ASSETS			7,280,569		*6,205,262*
Creditors: amounts falling due within one year	14.6		(297,316)		(*288,664*)
NET CURRENT ASSETS			6,983,253		*5,916,598*
TOTAL FUNDS			7,151,105		*6,089,600*

Cash Flow statement for the year ended 31 December 1997

	Note	Swiss Francs 1997		*1996*	
Net cash outflow from operating activities (see below)			(374,526)		(*654,874*)
Returns on investments					
Interest received		32,148		*29,739*	
Investment income (net of notional dividends)		116,598		*85,042*	
Net cash inflow from returns on investments			148,746		*114,781*
Investing activities					
Purchase of fixed assets		(52,569)		(*88,569*)	
Purchase of investments	14.5	(1,389,353)		(*588,677*)	
Disposal of investments	14.9	1,554,768		*1,103,757*	
Net cash inflow/(outflow) from investing activities			112,846		*426,511*
Decrease in cash	14.11		(112,934)		(*113,582*)

Reconciliation of (Deficit)/Excess of Income over Expenditure to Net Cash Outflow from Operating Activities

(Deficit)/excess of income over expenditure		(88,626)	(*216,803*)
Exchange rate fluctuations attributable to operating activities	14.10	(17,767)	(*3,552*)
Interest received	14.8	(32,148)	(*29,739*)
Investment income	14.7	(280,164)	(*221,774*)
Profit on disposal of investments	14.9	(15,566)	(*6,009*)
Depreciation charges		57,719	*36,894*
Decrease/increase in stock		21,094	(*59,274*)
Increase in debtors		(27,720)	(*33,860*)
Increase/(decrease) in creditors		8,652	(*120,757*)
Net cash outflow from operating activities (see above)		(374,526)	(*654,874*)

14. Notes to the Accounts

14.1. *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.

14.2. *Rates of exchange*

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

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

	1997	*1996*
Netherland Guilders (NLG)	1.3908	*1.3333*
Danish Crowns (DKK)	4.5501	*4.5581*
Pounds Sterling (GBP)	0.4219	*0.4605*
US Dollars (USD)	0.7042	*0.7752*

The net assets of the Union at 1 January 1997 (CHF 6,089,600) would have had the value of US D 4,720,658 or GBP 2,804,261 if expressed in those currencies.

At 31 December 1997, the net assets (CHF 7,151,105) would have had the value of USD 5,035,808 or GBP 3,017,051, respectively, being an increase of USD 315,150 or a increase of GBP 212,790 from the previous year.

14.3. *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.

14.4. *Tangible fixed assets*

	Leasehold property improvements CHF	Office equipment CHF	Computer equipment CHF	Total CHF
Cost				
As at 1 January 1997	126,188	47,895	46,449	220,532
Additions	–	14,800	60,970	75,770
VAT adjustment	(23,201)	–	–	(23,201)
As at 31 December 1997	102,987	62,695	107,419	273,101
Accumulated depreciation				
As at 1 January 1997	12,637	19,410	15,483	47,530
Charge for the year	10,299	11,614	35,806	57,719
As at 31 December 1997	22,936	31,024	51,289	105,249
Net book value 31 December 1997	80,051	31,671	56,130	167,852
31 December 1996	113,551	28,485	30,966	173,002

14.5. *Investments*

	Swiss Francs								
	Holding at market value 1 January 1997	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 1997	Holding at revalued cost 31 December 1997	Holding at revalued cost 31 December 1996
Held by Merrill Lynch									
GNM P146535-2016 (USD) 2,445 Units	4,812	–	–	(1,669)	584	157	3,884	3,444	4,336
GNM P169332-2016 (USD) 19,973 Units	26,948	–	–	(4,068)	2,661	1,878	27,419	28,694	24,261
Haussmann Holdings (USD) 122 Units	333,905	–	–	(209,147)	57,684	16,771	199,213	84,176	156,621
British Gas Finance (USD) 75,000 Units	99,587	–	–	–	12,897	(2,441)	110,043	112,511	99,470
Global Allocation Portfolio Class A (USD) 5,700 Units	103,310	–	–	–	14,045	8,305	125,660	87,737	77,574
Meridian Funds Global 11,448 Units Government Fund (USD) 9,503 Units	150,657	–	7,927	–	19,725	(8,122)	170,187	193,357	163,520
Meridian Charter Income Fund (USD) 12,234 Units	171,575	–	11,395	–	23,421	3,956	210,347	211,158	176,005
Lehman Brothers Holdings (USD) 80,000 Units	103,272	–	–	–	13,538	142	116,952	115,399	102,032
Permal Investment Holdings NV (USD) 53 Units	175,534	–	–	(59,766)	27,633	23,501	166,902	102,106	131,161
Repsol International Capital Limited 2000 Units	–	72,448	–	–	1,968	(921)	73,495	74,438	–
Santander Finance Limited 1900 Units	–	72,649	–	–	1,925	(3,022)	71,552	74,644	–
Aetna Emerging Europe FD 3125 Units	–	60,561	–	–	(1,302)	(6,651)	52,608	59,301	–
Lord Abbett Developing 2648 Units	–	58,031	4,460	–	435	(7,990)	54,936	63,125	–
ML ECS Capital Portfolio CLB 20764 Units	322,229	–	–	–	45,338	50,802	418,369	302,946	267,856
ML Global Alloc A (Offshore) 3286 Units	–	74,861	446	–	2,373	(5,718)	71,962	77,808	–
Altos Hornos DE MEX 200,000 units	–	289,823	–	(279,830)	13,180	(23,173)	–	–	–
Pacific Equity 3,000 units	173,905	–	–	(195,383)	38,738	(17,260)	–	–	174,956
Held by Foreign & Colonial									
Reserve Asset Fund Class D (USD) 16,887 Units	900,998	–	27,614	(357,249)	114,061	(9,737)	675,687	663,483	525,604
Reserve Asset Fund Class L(GBP) 21,581 Units	874,276	138,220	25,880	–	93,291	227,465	1,359,132	876,835	771,228
Reserve Asset Fund Class X (GBP) 9,581 Units	329,399	622,760	57,826	–	14,496	(12,186)	1,012,295	1,034,637	397,896
Reserve Asset Fund Class M (USD) 11,080 Units	438,880	–	3,525	(260,977)	54,574	57,283	293,285	68,140	277,248
Reserve Asset Fund Class E (GBP) 7,937 Units	340,072	–	24,493	–	38,566	25,618	428,749	415,135	413,124
Reserve Asset Fund Class N (JPYn) 17,828.27 Units	148,588	–	–	(171,113)	8,294	14,231	–	–	131,682
Treasury Stock									
Treasury stock UK Treasury 2006	815,274	–	–	–	90,410	79,254	984,938	953,369	862,004
	5,513,223	1,389,353	163,566	(1,539,202)	688,535	412,142	6,627,615	5,603,637	4,756,578

14.6. *Creditors: amounts falling due within one year*

	Swiss Francs 1997	*1996*
Trade Creditors	53,859	*73,562*
Accruals	174,731	*167,423*
Lease creditor relating to property	4,067	*7,812*
Payroll creditor including tax and social security	52,179	*35,841*
Other creditors	12,480	*4,026*
	297,316	*288,664*

14.7. *Investment income*

	Swiss Francs 1997	*1996*
ML Global Allocation A (offshore)	446	–
GNM P146535 - 2016	404	*424*
GNM P169332 - 2016	2,417	*1,281*
ML Capital Fund/CLB	3,450	*2,596*
Haussmann Holdings	342	*738*
Meridian Funds Global – Government Fund	7,927	*7,648*
Meridian Charter – Income Fund	11,395	*9,624*
British Gas Finance	9,745	*7,809*
GEC	–	*3,632*
US Treasury Note 6.875% 31.10.1996	–	*8,353*
Global Allocation	1,295	*884*
Foreign and Colonial – Reserve Asset Fund Class D	27,614	*34,366*
Foreign and Colonial – Reserve Asset Fund Class L	25,880	*30,020*
Foreign and Colonial – Reserve Asset Fund Class X	57,826	*14,362*
Foreign and Colonial – Reserve Asset Fund Class M	3,525	*14,015*
Foreign and Colonial – Reserve Asset Fund Class E	24,493	*20,062*
Foreign and Colonial – Reserve Asset Fund Class N	–	*132*
Lehman Brothers	7,217	*6,503*
UK Treasury 7.75% 22.9.2006	73,371	*59,325*
Lord Abbett Developing	4,460	–
Altos Hornos Demex	15,944	–
Repsol International Capital Ltd	1,043	–
Santander Finance Ltd	1,370	–
	280,164	*221,774*
Allocated to:		
President's Fund	2,210	*2,476*
Ewald Fund	19,580	*15,335*
Publication and Journals Development Fund	33,986	*20,313*
Research and Education Fund	43,671	*40,416*
Balance left in General Fund	180,717	*143,234*
	280,164	*221,774*

14.8. *Bank interest*

	Swiss Francs 1997		*1996*	
National Westminster Bank Plc				
Manchester Business Reserve Account	7,480		*6,465*	
Manchester Capital Reserve Account	2,747		*3,977*	
		10,227		*10,442*
Merrill Lynch CMA Account		6,033		5,775
Foreign & Colonial				
Cash balance	580		*474*	
Petty cash accounts	–		–	
Interest from Munksgaard	15,308		*13,048*	
		15,888		*13,522*
Allocated to General Fund		32,148		*29,739*

14.9. *Profit on disposal/redemption of investments*

	Swiss Francs 1997	*1996*
Proceeds	1,554,768	*1,103,757*
Book value	1,539,202	*1,097,748*
Profit allocated to General Fund	15,566	*6,009*

Book value represents market value at 1 January 1997. The profit on disposal based on historic cost was CHF 378,338 (1996: CHF 81,179). Therefore historic cost results would be as follows:

	Swiss Francs 1997	*1996*
Excess/(deficit) of income over expenditure	289,712	(*141,633*)

14.10. *Exchange rate fluctuations attributable to operating activities*

	Swiss Francs 1997	*1996*
Total fluctuations in exchange rates dealt with in Fund accounts	737,989	*815,641*
Adjustments for exchange differences attributable to:		
Investments (note 14.5)	(688,535)	(*736,790*)
Cash and bank balances	(67,221)	(*82,403*)
	(17,767)	(*3,552*)

14.11. *Analysis of changes in cash during the year*

	Swiss Francs	
	1997	*1996*
Balance at 1 January 1997	368,858	*400,037*
Net cash (outflow)/inflow	(112,934)	(*113,582*)
Fluctuations in rates of exchange on cash and bank balances	67,221	*82,403*
	(45,713)	(*31,179*)
Balance at 31 December 1997	323,145	*368,858*

14.12. *Analysis of balances of cash as shown in the balance sheet*

	Swiss Francs			
	1997	*1996*	Change 1997	*Change 1996*
Cash at bank and in hand	323,145	*368,858*	(45,713)	(*31,179*)

14.13. *Capital commitment*

	Swiss Francs	
	1997	*1996*
Contracted for but not provided	–	*7,280*
Authorized but not yet contracted for	35,016	*25,606*

14.14. *Operating lease commitments*

At 31 December 1997, the Union was committed to making the following payments during the next year in respect of operating leases.

	Land and buildings	Other
	Swiss Francs	
	1997	1997
Leases which expire:		
within two to five years	28,739	6,719
after five years	62,400	78,120
	91,139	84,839

14.15. *Sponsorship commitments*

At 31 December 1997 the Union had authorized, but not contracted for, sponsorship grants of CHF 57,631 (1996: CHF 47,916)

14.16. *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.

Fund Accounts as at 31 December 1997

				Swiss Francs			
					Fluctuations in exchange rates (Note 14.2)		
	As at 1 January 1997	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Gain on market value of investments	Trading	Investments	Balance at 31 December 1997
FUND ACCOUNTS							
General Fund	1,992,999	(50,000)	39,834	412,142	18,468	688,535	3,101,978
President's Fund	44,391	–	(5,348)	–	301	–	39,344
Acta Crystallographica	1,392,573	(125,000)	269,302	–	11,851	–	1,548,726
Journal of Applied Crystallography	377,785	(150,000)	(15,583)	–	1,636	–	213,838
International Tables	195,091	–	8,095	–	1,567	–	204,753
Book Fund	17,065	–	3,495	–	159	–	20,719
Publications and Journals Development Fund	716,497	50,000	(116,080)	–	5,016	–	655,433
Research and Education Fund	836,332	100,000	(64,806)	–	6,721	–	878,247
Ewald Fund	326,335	50,000	19,580	–	3,053	–	398,968
Newsletter Fund	60,685	75,000	(84,574)	–	394	–	51,505
Journal of Synchrotron Radiation	129,847	50,000	(142,541)	–	288	–	37,594
	6,089,600	–	(88,626)	412,142	49,454	688,535	7,151,105

General Fund Account for the year ended 31 December 1997

	Note	1997		*1996*	
			Swiss Francs		
Income					
Grant received from UNESCO subvention to ICSU			23,200		*22,359*
Subscriptions from Adhering Bodies			151,562		*148,822*
Income from investments	14.7		180,717		*143,234*
Interest on bank accounts	14.8		32,148		*29,739*
Profit on disposal/redemption of investments	14.9		15,566		*6,009*
General Assembly refund			7,150		–
Amounts charged to the following journals and publications:					
Acta Crystallographica		60,398		*66,248*	
Journal of Applied Crystallography		15,508		*7,703*	
Journal of Synchrotron Radiation		5,713	81,619	*3,081*	*77,032*
Total Income			491,962		*427,195*
Expenditure					
Subscriptions to ICSU and ICSU bodies			8,661		*7,127*
Administrative expenses:					
General Secretary and Treasurer:					
Honorarium to Treasurer		9,365		*7,740*	
Secretarial assistance		346		*542*	
Audit and accountancy charges		39,721		*32,228*	
Legal and professional fees		2,293		*2,415*	
Postage and sundries		206		–	
Travelling expenses		2,940		*2,685*	
Bank charges		3,156		*1,306*	
Executive Secretary's office:					
Salaries and expenses		242,130		*172,634*	
Depreciation of office equipment		2,882		*541*	
Depreciation of freehold property		10,299	313,338	–	*220,091*
Seventeenth General Assembly and Congress expenses		27,705		*63,028*	
Meeting of the Executive Committee		38,219		*75,374*	
Finance Committee expenses		22,763		*16,508*	
Travel expenses of IUCr Representatives on other bodies		1,958		*3,784*	
Star/CIF		22,656		*4,646*	
Commission expenses		2,945		*28,842*	
Sponsorship of meetings		10,525		*40,169*	
President's secretary		1,206		*14,322*	
IUCr/FIZ agreement		(4,569)		*16,225*	
Bad debts – subscriptions		(6,000)		*6,000*	
Programming and development costs		12,721	130,129	–	*268,898*
Total Expenditure			452,128		*496,116*
Excess/(deficit) of income over expenditure			39,834		(*68,921*)
Reconciliation of movements					
Balance at 1 January			1,992,999		*1,190,554*
Transfers to other Funds:					
Research and Education Fund		50,000		–	
Publications and Journals Development Fund		–		*100,000*	
Ewald Fund		–	(50,000)	*50,000*	(*150,000*)
Excess/(deficit) of income over expenditure		39,834		(*68,921*)	
Movement in market value of investments in the year	14.5	412,142	451,976	*266,072*	*197,151*
Fluctuations in rates of exchange			707,003		*755,294*
Balance at 31 December			3,101,978		*1,992,999*

President's Fund Account for the year ended 31 December 1997

	Note	1997	*1996*
Income			
Investment income	14.7	2,210	*2,476*
TOTAL INCOME		2,210	*2,476*
Expenditure			
Grants		7,558	*7,125*
Deficit of income over expenditure		(5,348)	(*4,649*)
Reconciliation of movements			
Balance at 1 January		44,391	*48,386*
Deficit of income over expenditure		(5,348)	(*4,649*)
Fluctuations in rates of exchange		301	*654*
Balance at 31 December		39,344	*44,391*

Acta Crystallographica Account for the year ended 31 December 1997

	Note	Swiss Francs 1997		*1996*	
Income					
Subscriptions to Volume 53 (*1996 Volume 52*)		2,229,054		*1,910,033*	
Sale of back numbers and single copies		29,327		*28,369*	
Airfreight charged to subscribers		52,914		*53,691*	
Royalties and copyright fees		8,531		*5,852*	
		2,319,826		*1,997,945*	
Less Publisher's commission on sales		158,087	2,161,739	*135,688*	*1,862,257*
Income from advertisements (net)			1,459		*683*
TOTAL INCOME			2,163,198		*1,862,940*
Expenditure					
Publication expenses:					
Printing and binding Volume 53 (*1996 Volume 52*)		559,821		*686,225*	
Distribution and postage		90,611		*108,129*	
Airfreight costs		18,531		*25,072*	
		668,963		*819,426*	
Net loss on reprints		1,313		*12,039*	
Index to Volume 52 (*1996 Volume 51*)		2,046		*459*	
Supplement to Volume 52		–	672,322	*37,415*	*869,339*
Editorial expenses:					
Editorial honoraria		75,110		*73,474*	
Secretarial assistance		11,145		*6,080*	
Postage, travel and sundries		27,603		*13,764*	
Technical Editing:					
Salaries and expenses		809,494		*708,502*	
Computer expenses		36,119		*27,774*	
Depreciation of office equipment		32,958	992,429	*20,396*	*849,990*
Programming and development			168,747		–
Administration expenses recharged from General Fund			60,398		*66,248*
TOTAL EXPENDITURE			1,893,896		*1,785,577*
Excess of income over expenditure			269,302		*77,363*
Reconciliation of movements					
Balance at 1 January			1,392,573		*1,544,696*
Transfers to other Funds					
Publications and Journals Development Fund		50,000		*175,000*	
Newsletter Fund		75,000	(125,000)	*75,000*	(*250,000*)
Excess of income over expenditure			269,302		*77,363*
Fluctuations in rates of exchange			11,851		*20,514*
Balance at 31 December			1,548,726		*1,392,573*

Journal of Applied Crystallography Account for the year ended 31 December 1997

	Note	Swiss Francs 1997		*1996*	
Income					
Subscriptions to Volume 30 (1996 Volume 29)		333,119		*320,069*	
Sale of back numbers and single copies		3,589		*2,805*	
Airfreight charged to subscribers		7,604		*7,958*	
Royalties and copyright fees		2,328		*2,406*	
Special issue income		21,885		–	
		368,525		*333,238*	
Less Publisher's commission on sales		23,570	344,955	*22,601*	*310,637*
Recharge for special issue			96,488		–
TOTAL INCOME			441,443		*310,637*
Expenditure					
Publication expenses:					
Printing and binding Volume 30 (1996 Volume 29)		82,601		*88,512*	
Distribution and postage		15,181		*14,262*	
Airfreight costs		2,193		*3,157*	
		99,975		*105,931*	
Net (profit)/loss on reprints		(1,894)	98,081	*10,987*	*116,918*
Editorial expenses:					
Special issue costs		118,373	–		
Editorial honoraria		12,224		*6,784*	
Secretarial assistance		6,029		*2,140*	
Postage, travel and sundries		3,727		*2,444*	
Technical Editing:					
Salaries and expenses		164,660		*89,383*	
Computer expenses		6,788		*3,229*	
Depreciation of office equipment		6,194	317,995	*2,372*	*106,352*
Programming and development costs			25,442		–
Administration expenses recharged from General Fund			15,508		*7,703*
TOTAL EXPENDITURE			457,026		*230,973*
(Deficit)/excess of income over expenditure			(15,583)		*79,664*
Reconciliation of movements					
Balance at 1 January			377,785		*342,556*
Transfers to other Funds					
Ewald Fund		50,000		–	
Research and Education Fund		50,000		*50,000*	
Journal of Synchrotron Radiation		50,000	(150,000)	–	(*50,000*)
Excess of income over expenditure			(15,583)		*79,664*
Fluctuations in rates of exchange			1,636		*5,565*
Balance at 31 December			213,838		*377,785*

Journal of Synchrotron Radiation Account for the year ended 31 December 1997

	Note	Swiss Francs 1997		*1996*	
Income					
Subscriptions to Volume 4 (*1996 Volume 3*)		93,282		*77,945*	
Sales of back numbers and single issues		3,408		*1,684*	
Airfreight charged to subscribers		2,695		*2,393*	
		99,475		*82,022*	
Less publisher's commission on sales		6,775	92,700	*5,574*	*76,448*
Income from advertisements			2,356		*6,055*
Income from copyright fees			187		*30*
TOTAL INCOME			95,243		*82,533*
Expenditure					
Publication expenses:					
Printing and binding Volume 4 (*1996 Volume 3*)		70,300		60,164	
Distribution and postage		8,213		4,276	
Airfreight costs		437		760	
		78,950		*65,200*	
Net loss on reprints		10,655	89,605	*1,427*	*66,627*
Editorial expenses:					
Editorial honoraria		16,181		*3,827*	
Secretarial assistance		5,929		*3,784*	
Postage, travel and sundries		5,504		*821*	
Technical Editing:					
Salaries and expenses		82,875		*35,753*	
Computer expenses		3,417		*1,292*	
Depreciation of office equipment		3,118	117,024	*948*	*46,425*
Programming and development costs			25,442		–
Administration expenses recharged from General Fund			5,713		*3,081*
TOTAL EXPENDITURE			237,784		*116,133*
Deficit of income over expenditure			(142,541)		(*33,600*)
Reconciliation of movements					
Balance at 1 January			129,847		*71,534*
Transfers from other Funds					
Journal of Applied Crystallography			50,000		–
International Tables			–		*90,000*
Deficit of income over expenditure			(142,541)		(*33,600*)
Fluctuations in rates of exchange			288		*1,913*
Balance at 31 December			37,594		*129,847*

International Tables Account for the year ended 31 December 1997

	Note	Swiss Francs 1997		*1996*	
Income					
Sales of copies					
Volume A		69,461		*60,078*	
Volume B		33,918		*53,349*	
Teaching Edition of Volume A		5,556		*3,562*	
Volumes II, III and IV		–		*55*	
Volume C		77,726		*46,016*	
		186,661		*163,060*	
Less publisher's commission on sales		40,641		*42,394*	
TOTAL INCOME			146,020		*120,666*
Expenditure					
Publication expenses:					
Printing and typesetting Volume A		16,426		*11,646*	
Printing and typesetting Volume C		32,288		*7,779*	
Printing and typesetting Volume B		47,209		(*5,379*)	
Printing and typesetting Teaching Edition of Volume A		1,987	97,910	*6,296*	*20,342*
Editorial expenses:					
Editorial honoraria		11,345		*10,449*	
Secretarial assistance, postage and office equipment		5,557		*11,703*	
Technical editing		214	17,117	–	*22,152*
Programming and development			22,898		–
TOTAL EXPENDITURE			137,925		*42,494*
Excess of income over expenditure			8,095		*78,172*
Reconciliation of movements					
Balance at 1 January			195,091		*264,045*
Transfers to other Funds					
Research and Education Fund		–		*60,000*	
Journal of Synchrotron Radiation		–		*90,000*	(*150,000*)
Excess of income over expenditure			8,095		*78,172*
Fluctuations in rates of exchange			1,567		*2,874*
Balance at 31 December			204,753		*195,091*

Book Fund Account for the year ended 31 December 1997

	Note	Swiss Francs 1997	*1996*
Income			
Sales of copies, net of Publisher's commission on sales			
Historical Atlas of Crystallography		436	*332*
World Directory of Crystallographers 10th Edition		8,468	*1,267*
Escher *Kaleidozyklen*		83	–
Sundry publications		1,093	*182*
Structure Reports		384	*2,120*
Royalties			
IUCr/OUP Book series		1,090	*1,158*
TOTAL INCOME		11,554	*5,059*
Expenditure			
Publication expenses:			
World Directory of Crystallographers 10th Edition		8,059	*1,419*
TOTAL EXPENDITURE		8,059	*1,419*
Excess of income over expenditure		3,495	*3,640*
Reconciliation of movements			
Balance at 1 January		17,065	*12,522*
Transfers between Funds			
To Ewald Fund		–	(*615*)
Excess of income over expenditure		3,495	*3,640*
Fluctuations in rates of exchange		159	*1,518*
Balance at 31 December		20,719	*17,065*

Publications and Journals Development Fund Account for the year ended 31 December 1997

	Note	Swiss Francs 1997		*1996*	
Income					
Investment income	14.7		33,986		*20,313*
Expenses					
Computer expenses:					
Purchase of computer equipment and software		2,485		*17,722*	
Programming and development		254,423		*174,880*	
Recharged to other Funds		(254,423)	2,485	–	*192,602*
Electronic Publishing Committee/Section Editors' Meeting			1,344		*1,573*
Special issue costs			96,488		–
Electronic Publishing Project			27,545		*46,546*
Promotions Representative			17,334		*12,637*
Advertising costs			1,194		–
Web input			3,676		–
TOTAL EXPENDITURE			150,066		*253,358*
Deficit of income over expenditure			(116,080)		*(233,045)*
Reconciliation of movements					
Balance at 1 January			716,497		*579,275*
Transfers from other Funds					
Structure Reports		–		*85,979*	
General Fund		–		*100,000*	
Acta Crystallographica		50,000	50,000	*175,000*	*360,979*
Deficit of income over expenditure			(116,080)		*(233,045)*
Fluctuations in rates of exchange			5,016		*9,288*
Balance at 31 December			655,433		*716,497*

Research and Education Fund Account for the year ended 1997

	Note	Swiss Francs 1997		*1996*	
Income					
Investment income	14.7		43,671		*40,416*
Expenditure					
Young Scientists' Support		91,816		*64,409*	
Moscow ECM Funds		–		*9*	
Visiting Professorship Programme		16,661		*1,290*	
TOTAL EXPENDITURE			108,477		*65,708*
Deficit of income over expenditure			(64,806)		(*25,292*)
Reconciliation of movements					
Balance at 1 January			836,332		*739,304*
Transfers from other Funds					
General Fund		50,000		–	
Journal of Applied Crystallography		50,000		*50,000*	
International Tables		–	100,000	*60,000*	*110,000*
Deficit of income over expenditure			(64,806)		(*25,292*)
Fluctuations in rates of exchange			6,721		*12,320*
Balance at 31 December			878,247		*836,332*

Ewald Fund Account for the year ended 1997

	Note	Swiss Francs 1997	*1996*
Income			
Investment income	14.7	19,580	*15,335*
Expenditure			
Selection Committee and expenses		–	*2,520*
Ewald Prize		–	*36,000*
Excess/(deficit) of income over expenditure		19,580	*(23,185)*
Reconciliation of movements			
Balance at 1 January		326,335	*294,098*
Transfers from other Funds			
Book Fund		–	*615*
General Fund		–	*50,000*
Journal of Applied Crystallography		50,000	50,000 – 50,615
Excess/(deficit) of income over expenditure		19,580	*(23,185)*
Fluctuations in rates of exchange		3,053	*4,807*
Balance at 31 December		398,968	*326,335*

Newsletter Fund Account for the year ended 1997

	Note	Swiss Francs 1997	*1996*
Income			
Income from advertisements		82,248	*65,521*
TOTAL INCOME		82,248	*65,521*
Expenditure			
Editorial Honoraria		5,600	*4,585*
Editorial expenses		42,432	*32,110*
Newsletter printing and distribution		98,228	*79,396*
Advertising costs		20,562	*16,380*
TOTAL EXPENDITURE		166,822	*132,471*
Deficit of income over expenditure		(84,574)	*(66,950)*
Reconciliation of movements			
Balance at 1 January		60,685	*51,741*
Transfers from other Funds			
Acta Crystallographica		75,000	*75,000*
Deficit of income over expenditure		(84,574)	*(66,950)*
Fluctuation in rates of exchange		394	*894*
Balance at 31 December		51,505	*60,685*