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International Union of Crystallography

Report of the Executive Committee for 1992

Meetings

The IUCr sponsored the following meetings held during 1992:

1. Direct Methods of Phasing in Macromolecular Crystallography, Panama City Beach, Florida, USA, 24–27 April 1992.
2. Accuracy in Powder Diffraction II, Gaithersburg, Maryland, USA, 26–29 May 1992.
3. Diffraction at High Pressure, Washington, DC, USA, 29–31 May 1992.
4. 4th International Conference on Quasicrystals, St Louis, Missouri, USA, 31 May–5 June 1992.
5. School on Crystallographic Computing, Balatonfüred, Hungary, 31 May–6 June 1992.
6. Gordon Research Conference on Electron Distribution and Chemical Bonding, Plymouth, New Hampshire, USA, 20–24 July 1992.
7. Symposium on Organic Crystal Chemistry, Poznań, Poland, 26–30 July 1992.
8. European Powder Diffraction Conference, Enschede, The Netherlands, 30 July–1 August 1992.
9. Fourteenth European Crystallographic Meeting, Enschede, The Netherlands, 2–7 August 1992.
10. American Crystallographic Association Meeting, Pittsburgh, Pennsylvania, USA, 9–14 August 1992.
11. Eighth International Summer School on Crystal Growth and Tenth International Conference on Crystal Growth, Palm Springs and San Diego, California, USA, 9–14 August 1992 and 16–21 August 1992.
12. Rietveld Summer School, Cieszyn, Poland, 13–15 August 1992.
13. International Conference on Anomalous Scattering of X-rays and Neutrons, Hamburg, Germany, 17–21 August 1992.
14. XII Congreso Iberoamericano de Cristalografía and II Escuela Iberoamericana de Cristalografía, Toledo and Madrid, Spain, 7–11 September 1992 and 14–18 September 1992.
15. Inaugural Conference of the Asian Crystallographic Association, Singapore, 13–16 November 1992.

The Executive Committee met in Pittsburgh, USA, in August. The Finance Committee met twice, in Chester, England, in March and then in August in Pittsburgh 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, Section Editors for *Acta Crystallographica* and other matters concerning the IUCr journals;
- (2) publication of a new Section (Section D) of *Acta Crystallographica* on Biological Crystallography;

(3) consideration of the possible publication of a new journal, the *Journal of Synchrotron Radiation*;

(4) appointment of new staff in the IUCr office in Chester;

(5) upgrading of office technology in the IUCr office in Chester;

(6) future of *Structure Reports* and cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and the International Centre for Diffraction Data;

(7) the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* papers and other uses of CIF, patent application and adoption of the STAR file and CIF by other bodies;

(8) progress with Volumes B, C, D and E of *International Tables for Crystallography* and consideration of possible further volumes;

(9) establishment of an international crystallographic newsletter, the *IUCr Newsletter*;

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

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

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

(13) investment policy;

(14) UK taxation considerations;

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

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

(17) discussion of the arrangements for the Beijing General Assembly and Congress and consideration of the Programme Committee proposals;

(18) review of the activities of the Commissions.

Publications

Volume 48 of *Acta Crystallographica*, Volume 25 of the *Journal of Applied Crystallography*, the third, revised edition of Volume A and Volume C of *International Tables for Crystallography* and Volumes 51B and 57A of *Structure Reports* were published.

Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Annex IV to the Report of the Fifteenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (1992), **A48**, 402–403].

Table 1. *Survey of the contents of the Union Journals**Acta Crystallographica*

Vol.	Year	Number of Pages*	Number of Papers	Full Articles		Short Format Papers†		Short Communications		Fast Communications	
				Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length
A44	1988	1104	159	150	6.3	—	—	9	1.1	24	0.6
B44		680	104	100	6.4	—	—	4	0.3		
C44		2240	897	712	2.5	174	1.5	11	0.3		
A45	1989	920	143	122	6.6	—	—	14	0.9	35	0.8
B45		600	94	90	6.6	—	—	4	0.5		
C45		2030	806	550	2.8	239	1.9	17	0.8		
A46‡	1990	998	150	126	7.0	—	—	19	1.2	39	0.9
B46		864	123	120	6.7	—	—	3	0.8		
C46		2500	980	693	2.6	270	1.8	17	0.6		
A47	1991	860	123	104	7.2	—	—	15	1.2	28	1.0
B47		1030	137	130	7.4	—	—	6	1.0		
C47		2740	1076	678	2.7	391	1.8	7	0.6		
A48	1992	954	117	106	7.9	—	—	10	2.2	28	1.5
B48		856	125	113	7.4	—	—	10	1.8		
C48		2280	914	499	2.9	407	2.0	8	0.6		

Journal of Applied Crystallography

Vol.	Year	Number of Pages*	Number of Papers	Full Articles		Short Communications		Fast Communications (from 1990) Crystal Data (1988–1989)		Computer Programs		Short Items§	
				Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length
21¶	1988	996	169	139	5.7	6	1.5	1	0.4	10	2.7	13	0.6
22	1989	642	125	81	6.7	18	1.6	—	—	12	4.3	14	0.8
23	1990	560	105	72	5.6	13	1.7	1	2.0	11	2.3	9	0.8
24**	1991	1102	176	138	5.7	20	1.7	5	2.6	13	2.9	13	0.8
25	1992	812	127	94	7.0	9	1.5	2	3.5	12	4.6	10	1.4

* Excluding indexes.

† Including Regular Structural Papers.

‡ Volume A46 includes, in addition, 540 pages of abstracts communicated to the Bordeaux Congress.

§ Excluding Union Announcements, Crystallographers, New Commercial Products and Book Reviews.

¶ Volume 21 includes 303 pages of 43 papers presented at the International Conference on Applications and Techniques of Small-Angle Scattering, Argonne, 1987.

** Volume 24 includes 464 pages of 68 papers presented at the International Conference of Small-Angle Scattering, Leuven, Belgium, 1990.

Work of the Commissions*Commission on Journals*

Volume 48 of *Acta Crystallographica (Acta)* was published in 1992, and included a total of 1156 papers (a decrease from 1336 in 1991) received from 50 countries, with an overall total of 4090 pages. The decrease in published papers from 1991 is primarily due to the new publication requirements and submission procedures for *Acta C* papers. Manuscripts received by Co-editors in 1992 numbered 1265 and included 54 papers for the new *Acta D* to be initiated in January 1993. Following the appointment at mid-year of a new Book-Review Editor, 13 Book Reviews were received.

The average lengths of Full Articles in *Acta A* and *Acta B* in 1992 increased to 7.9 and 7.4 pages, respectively, while *Acta C*'s Full Articles and Short-Format papers showed slight increases at 2.9 and 2.0 pages. The new Regular Structural Papers averaged 2.3 pages. Median publication

times for Full Articles, the average elapsed time between the published acceptance and nominal publication dates, were up slightly to 5.9 months for *Acta A*, but were little changed for *Acta B* at 5.9 months and *Acta C* at 6.8 months. The overall median publication time in 1992 for Fast Communications was 2.4 months.

A total of 37 inorganic, 14 organometallic and 62 organic papers appeared in Section B in 1992 compared with 53, 13 and 62, respectively, in 1991. The distribution of papers in Section C was 90 inorganic, 267 organometallic and 540 organic in 1992, compared with 115 inorganic, 358 organometallic and 603 organic articles in 1991.

The number of papers for Volume 25 of the *Journal of Applied Crystallography (JAC)* in 1992 was 94, compared with 138 for 1991. The 1991 figures reflect papers received for the Small-Angle Scattering special issue. The number of pages published was 812 (1102 in 1991) and the median publication time for Full Articles was 5.8 months

(7.0 months in 1991). Manuscripts received by Co-editors increased to 192 in 1992 from 166 in 1991.

The average length of Full Articles in *JAC* was 7.0 pages in 1992, compared with 5.7 pages in 1991. The average length for Short Communications and Computer Programs was 1.5 and 4.6 pages in 1992, compared with 1.7 and 2.9 pages in 1991. Papers were received from 26 countries.

New procedures for the submission and publication of *Acta C* papers were instituted in early 1992. These procedures were designed to facilitate the direct transfer of text and numerical data from authors' computers to the typesetting programs in the Technical Editor's office, by use of the Crystallographic Information File (CIF). About 25% of *Acta C* papers were submitted in the CIF format during the year, and it is expected that this number will increase as authors become more familiar with the streamlined procedures that have now been implemented in Chester.

The Executive Committee approved the appointment of individual editors for the separate sections of *Acta*, with the Chairman of the Commission on Journals to serve as Editor-in-Chief. Jenny P. Glusker is in place as Editor of *Acta D*; the individual editors for *Acta A*, *B* and *C* will be nominated to the Executive Committee prior to the 1993 Congress in Beijing.

Hiroshi Iwasaki and Bruno Morosin retired as *JAC* Co-editors during the year. New Co-editors appointed were Jean Vicat, Ting C. Huang and Hiroo Hashizume for *JAC* and Dieter Schwarzenbach, Margaret J. Adams, Elinor T. Adman, T. Alwyn Jones and M. Vijayan for *Acta*. Robert F. Bryan was appointed as the new Book-Review Editor.

Commission on Structure Reports

Volume 57A (Metals and Inorganic Compounds for 1990) and Volume 51B (Organic Compounds for 1984) were published in 1992. The Multi-Year Index for the Organic Compounds to 1980 (Volume 47B) has been completed, is with the publisher and will appear in 1993. Co-editorial work has been completed for Volume 50B (Organic Compounds for 1983) and final assembly of the camera-ready pages and indexes is in progress. Co-editorial work is near completion for Volume 52B (Organic Compounds for 1985) and is in progress for the 1913–1990 Metals and Inorganic Indices (Volume 58A) – the final *Structure Report* Volumes. The Volumes on which work is in progress (50B, 52B and 58A) should be with the publisher before the 1993 Beijing IUCr Congress.

Commission on International Tables

A. J. C. Wilson has resigned as Chairman of the Commission with effect from 1 July 1993. He will be succeeded by Professor Theo Hahn. Detailed reports on the individual Volumes are given below.

Volume A. Space-Group Symmetry; Editor T. Hahn

The third, revised, edition of *International Tables for Crystallography*, Volume A: *Space-Group Symmetry* (1992) was published by Kluwer Academic Publishers in November 1992. The main feature of the third edition is the incorporation of new diagrams for the tetragonal and,

in particular, for the cubic space groups. With these additions, this volume contains new diagrams for the plane groups and for all tetragonal, trigonal, hexagonal and cubic space groups.

The cubic diagrams have been thoroughly redesigned. They contain, among other improvements, new symbols for the 'inclined' two- and threefold axes, explicit graphical indication of the horizontal $\bar{4}$ axes (rather than their twofold 'subaxes'), complete sets of 'heights' (fractions) for the horizontal fourfold axes and for the $\bar{4}$ -inversion points, as well as for the symmetries $4_2/m$ and $6_3/m$ in cubic, tetragonal and hexagonal space groups. These changes have required substantial modifications in Section 1.4. This section and its footnotes should be helpful for a better understanding of the complexities of the cubic diagrams. Table 5.1 has been extended by one page. Work on the preparation of the remaining triclinic, monoclinic and orthorhombic space-group diagrams has continued throughout the year, as have the efforts towards a more detailed and improved presentation of the subgroups of space groups.

A list of errata to the second edition (1987, 1989) will appear early in 1993 [*Acta Cryst.* (1993), **A49**, 592–593]. These errata have been corrected in the third edition.

Volume B. Reciprocal Space; Editor U. Shmueli

During 1992, all the remaining corrected page proofs reached the Editor's office; they were reviewed, uniformly marked for indexing purposes and submitted to the Technical Editor's office. The main editorial work was concluded in 1992 with the submission of a preface to the Volume to the Technical Editor. All this was accompanied by usual correspondence between Editor, authors and Technical Editor, which became much more efficient due to the availability of electronic mail to all those concerned.

The structure of Volume B is the same as was announced during the Bordeaux meeting in 1990. The planned Chapters on *Particle Size and Texture*, *Diffraction by Polymers* and *Dynamical Theory of Neutron Diffraction* were not included because of author withdrawal or lack of willing contributors.

Volume C. Mathematical, Physical and Chemical Tables; Editor A. J. C. Wilson

The first edition of Volume C of *International Tables for Crystallography* was published in March 1992; it is intended to supersede Volumes II, III and IV of the previous series *International Tables for X-ray Crystallography*. Since Volume C contains many sections contributed by many authors, it has been necessary to make the indexes more extensive than in any previous volume; an author index is included for the first time.

A second printing is likely to be required in 1994 and authors and other users are requested to notify the Editor of misprints and other errors so that corrections can be made.

Volume D. Physical Properties of Crystals; Editor A. Authier

The potential authors of papers for Volume D who had been suggested by the Working Party that met in Paris in

June 1991 and who had been approved by the Executive Committee in August 1991 have been invited to participate. Some did not answer immediately, some refused and others resigned after having first accepted. About three-quarters have accepted and have started work on their manuscripts. New persons are being approached for the remaining parts. It had been proposed that the volume be accompanied by software to read the *Tables*, based on test software made in Czechoslovakia. It turned out however, that, owing to the situation in that country, the firm that was to develop the software was no longer in a position to do so and another solution will have to be found. It is hoped that the manuscript of Volume D can be completed in 1994.

Volume E. Subperiodic Symmetry Groups; Editors V. Kopsky and D. B. Litvin

Volume E consists of three parts. Part 1 consists of a guide to the subperiodic group tables and the tables for the frieze groups, rod groups and layer groups. This has been read by Professor Theo Hahn, whose comments have been incorporated into the material. The diagrams are now to be redrawn professionally and a final section comparing the numerous sets of symbols of subperiodic groups is being written.

A document entitled *Nomenclature, Symbols and Classification of the Subperiodic Groups*, containing the standards for the nomenclature, symbols and classifications used in Volume E, was written by the Editors. This was submitted to and approved by the Commission on Crystallographic Nomenclature [Abstract in *Acta Cryst.* (1993). A49, 594].

Parts 2 and 3 deal with the relationship between subperiodic groups and space groups. Subperiodic groups are considered as factor groups of space groups in Part 2 and as subgroups of space groups in Part 3. A draft of Part 2 has been written and of Part 3 partially done. It is expected that all parts will be completed in 1993.

Volume 'F'. Multidimensional Crystallography; no Editor appointed

No direct progress has been made with planning a volume on *N*-dimensional crystallography. Cooperation with the Commission on Crystallographic Nomenclature has resulted in clarification and improvements of existing systems of symbols and classification. Further discussion of this volume is included in the report for the triennium.

Commission on Biological Macromolecules

The last year has seen continued growth in crystallographic studies on biological macromolecules in both academic and industrial laboratories. This follows further increases in the number of crystallographic research groups and the growing effectiveness and power of the experimental and computational techniques available.

One major concern of the Commission is with the further development of the structural databases, which are now faced with almost overwhelming volumes of submitted structures. There is also recognition that validation of the data is needed. The European Commission is supporting an initiative to establish a coordinated programme with Brookhaven and interested groups in the USA to

provide agreed procedures by which observed amplitudes and the atomic parameters can be assessed and validated. The Commission wishes to see these developments available for structural laboratories throughout the world and is investigating mechanisms for this.

As usual, there have been numerous conferences and meetings in which current structural results and new techniques have been reviewed. The tradition in which students and post-doctorates receive intensive training in specific workshops is still very much in practice and is providing a valuable and efficient means to disseminate crystallographic and related skills.

The growth of X-ray structural analysis (and the growth of nuclear magnetic resonance studies) has stimulated the arrival of *Acta Cryst* Section D. This volume will publish macromolecular structures and will encourage biologically related discussion. A number of other journals with a strong commitment to the structure of biological molecules are now well established, providing the community with a variety of publishing possibilities.

Amongst a number of important structure determinations this year is that of the reverse transcriptase molecule from the human immunodeficiency virus (HIV) reported by the group at Yale. Many structural details of the enzyme still remain to be established but analyses on other crystal forms of the enzyme, progressing rapidly in other laboratories, will help to provide these details, essential for understanding the molecule's catalytic and binding interactions. The research should also provide structural explanations for the drug binding and the resistance conferred on the enzyme by various mutations, illustrating the increasing relevance of structural studies in medical and pharmaceutical research.

Commission on Charge, Spin and Momentum Densities

The Commission has promoted worldwide efforts related to the field of accurate determination of density distributions in real and momentum space both among the crystallographic community and among those physicists and chemists whose interest in ground-state properties of condensed matter is connected with electron densities.

In 1992, members of the Commission actively contributed to the Gordon Conference on Electron Distribution and Chemical Bonding, 20–24 July. These Conferences are mainly devoted to the chemical aspect of electron-density studies and are therefore to some extent complementary to the Sagamore Conferences.

During the Gordon Conference in 1992, a new Commission project on Multipole Refinement and Properties: a Program Package for Analysing Electron Densities from Diffraction Data was initiated by P. Coppens, N. K. Hansen, T. Koritsanszky and P. Mallinson. The purpose of this project is to produce a unified version of *MOLLY* for analysing electron-charge-density distributions by including features of other currently used programs and by adding programs for derivation of properties and for topological studies. This project was finally approved by the Commission at the end of December 1992.

Another Commission project, Fermiology of High-*T_c* Superconductors via High-Resolution Synchrotron-Based Compton Scattering Spectroscopy, initiated at the 1991 Sagamore Conference and finally approved at the Gordon

Conference, was the reason for a number of small meetings during 1992 at different locations between A. Bansil, J. R. Schneider, W. Schülke, N. Shiotani and L. Dobrzynski. The result of these meetings is a project description detailing the way to proceed in order to reach the rather ambitious goal. It was also found necessary to have a meeting among those who want to contribute to the project. This meeting will be held 2–4 July in Kraków, Poland.

In preparing for the IUCr Congress in 1993 in Beijing, the Commission has proposed an Open Commission Meeting where the status and progress of all Commission projects will be reported. Speakers and topics for this meeting, as selected during 1992, have been approved by the Beijing Programme Committee.

During the Gordon Conference, there was a closed Commission meeting, where Commission projects were discussed and approved and the nomination of new Commission members and a new Commission chairman was decided.

Commission on Crystal Growth and Characterization of Materials

The main activities of the Commission in 1992 were centred on the organizational work for the International School on Advanced Electronic Materials to be held in Madras, India, at the Crystal Growth Centre of Anna University at the end of 1993. This school, which will be jointly programmed and steered by the Commission and the ICS of Trieste, Italy (ICS is an institution related to UNESCO), will be open to young scientists from all over the world, though emphasis will be placed on attracting attendees from the South-East-Asia region. As this school is scheduled to be held within three months of the Beijing Congress, the Commission is grateful to the Chairman of the Beijing Congress Programme Committee, who approved sponsorship by the IUCr.

In order to continue the successful series of schools for the benefit of young scientists, a series that started more than a decade ago, the Commission is now considering the possibility of an International Summer School on Growth and Characterization, to be held in the period August/September 1994 in Kraków, Poland. An application for this school, presently under examination by the Commission, has been advanced by the Polish Association for Crystal Growth.

Commission on Crystallographic Apparatus

The past year has seen the completion of a number of initiatives undertaken by this Commission. Successful outcomes have been achieved in the fields of X-ray scattering and XAFS. A survey of the status projects in which the Commission is involved is given below.

1. *The X-ray Attenuation Project* (D. C. Creagh). With the publication of *International Tables for Crystallography*, Volume C, a decade of work on the parameters used by crystallographers (the attenuation coefficients and dispersion corrections) has come to a successful conclusion. Detailed comparison of experiments and theory for the dispersion corrections have been given at recent conferences [the International Conference on Anomalous Scattering, Malente (1992), and the National Seminar on Recent Trends in Photon-Atom Interactions, Karnataka

(1992)]. At present, work is proceeding on producing parameterized fits to the X-ray attenuation data to aid the handling of the data by crystallographers.

2. *The Single-Crystal Lattice Parameter Project* (G. De Titta). Progress on this project has been slower than expected in 1992. With all the specimen crystals prepared and mounted in 1993, it is anticipated that this project will be brought to a satisfactory conclusion.

3. *The Accuracy in XAFS Project* (D. C. Creagh, H. Oyanagi and R. Frahm). The dialogue between the XAFS body and members of the Commission has continued with a view to determining whether the XAFS body wishes to become part of the IUCr on the one hand and to improving the standards of experimentation, data interpretation and reporting of XAFS experiments on the other.

The XAFS body has finally become a formal entity and is now the International XAFS Society (IXS) with Professor Dale Sayers as President and discussions have been held between Professor Sayers and the President of the IUCr concerning links that could be made between the IXS and the IUCr.

Because it is believed that the best way to improve the standards of experimentation, data interpretation and reporting is through education, a Workshop was held in Chicago to develop an International Short Course on XAFS. The aim is to provide a course of three days' duration using a variety of educational media. All aspects of XAFS usage was included in the discussions. The X-ray optics section for this short course was written by D. C. Creagh.

4. *The Evaluation of Two-Dimensional Detectors*. Some progress was made in gathering information that could lead to establishing criteria for area-detector performance. Whether or not this can proceed as a project depends on the response of the crystallographers to papers to be given at the Open Commission Meeting at the forthcoming IUCr Congress at Beijing.

5. *The Absolute Structure Determination of Light-Atom-Compounds Project* (L. Malakhova). Professor Malakhova has established that sufficient laboratories interested in pursuing this project exist to make this a viable project. Commission members have formally agreed that the project should proceed in the forthcoming triennium.

6. *The High-Pressure-Group Committee* (R. Nelmes). The high-pressure group has once again completed a busy and successful year. It held a meeting in collaboration with the Commission on Powder Diffraction in Washington in May 1992. It has also been busy planning for its Micro-symposium at the forthcoming IUCr Congress in Beijing.

The high-pressure group was formed from the remnants of membership of the High-Pressure Commission, which was disbanded at the Perth Congress. Since its formation it has acted with great vigour and its membership has increased substantially. If it continues to grow during the forthcoming triennium, it will have established a case for readmission as a Commission of the IUCr.

Other matters. The Commission is at present investigating the possibility of becoming involved in a project to measure X-ray wavelengths, which has been proposed by Dr Richard Deslattes (NIST). Crystallographers have long been aware of deficiencies in the tables of X-ray wavelengths in *International Tables for X-ray Crystallography*, Vol. III, and which have been reprinted in *International*

Tables for Crystallography, Vol. C. The resolution of discrepancies in the wavelength tables is of great importance to crystallographers. Our Commission considers this to be a project of great significance to crystallographers and will do all in its power to assist its progress.

Commission on Crystallographic Computing

The following list gives the main occupations of the Commission during 1992.

1. Refereeing the section Computer Program Abstracts in *J. Appl. Cryst.* by A. Olson and G. Reck.

2. The Veszprém School on Crystallographic Computing held at Balatonfüred, Hungary, from 31 May to 6 June 1992 was the 13th such school organized since 1960 under the auspices of the IUCr Commission on Crystallographic Computing. The school was attended by 85 participants from 20 countries. The school had initially been planned to take place in the old-town area of the city of Veszprém. However, for organizational reasons, it finally took place in a hotel on the northern shore of Lake Balaton. There were 20 invited lectures and *ca* 12 contributed posters. The school provided a balanced programme of lectures, tutorials in small groups and demonstrations of crystallographic computer programs on a plentiful array of modern computer equipment, both PCs and workstations. A noteworthy aspect of the work presented at the school was the presentation of systems using modern windowing techniques and object-oriented programming. The organization of the school was the work of two committees: (a) a Programme Committee, comprised of H. D. Flack (Chair), F. H. Allen, H.-F. Fan, K. Huml, N. W. Isaacs, C. Kratky, A. J. Olson, L. Párkányi, G. Reck, H. Schenk, M. I. Sirota, I. Vickovic, D. Viterbo and K. Watenpaugh; and (b) a Local Organizing Committee, comprised of K. Simon (Chair), Gy. Argay (Secretary), Zs. Böcskei, M. Czugler, G. Csonka, G. Náray-Szabó, I. Sajó and G. Speier. M. Hanusz provided much technical help before and during the meeting.

3. The invited lectures and contributed posters of the Veszprém School have been prepared for publication in the IUCr series of monographs published by Oxford University Press. The editorial work on this book was undertaken by H. D. Flack, L. Párkányi and K. Simon. M. Hanusz also participated actively in the editorial work necessary to prepare this book. At the time of writing this report (March 1993), the manuscripts and figures have all been formatted and delivered to OUP.

4. The local organization of a School on Crystallographic Computing to be held in Hefei, Anhui Province, People's Republic of China, as a satellite meeting to the IUCr Congress ran into considerable difficulties. Most regrettably, the Chairman of the Commission, after consultation with the IUCr Executive Committee, decided to cancel the school. Preliminary negotiations are under way to find a site for a school in the Asian area in 1994/1995.

5. The organization and programme of an Open Commission Meeting with the title Crystallographic Computing for the IUCr Congress in Beijing is being undertaken by H. D. Flack.

6. In conjunction with the European Crystallographic Committee, crystallographic news on conferences, meetings, IUCr circulars and journals have been installed on

the information server CONCISE of the RARE project COSINE. This server is available for consultation by e-mail, interactive session or file transfer. Connection details have been circulated by e-mail and by announcements in the *IUCr Newsletter*. The IUCr editorial office in Chester kindly provides computerized versions of the Tables of Contents of *Acta Crystallographica* and the *Journal of Applied Crystallography* for CONCISE. Considerable experience has been gained in the use of such computerized information systems.

Commission on Crystallographic Data

This year has seen the consolidation of the Crystallographic Information File (CIF) as a standard format for the interchange of crystallographic data and as a medium for the machine-readable submission of manuscripts to *Acta Crystallographica*. The development of extensions to the CIF Core Dictionary [*Acta Cryst.* (1991), A47, 655–685] to cover macromolecules and powder diffraction data are now well advanced and should be finalized within this triennium. Software for CIF generation is now becoming available in a number of computer packages for structure determination or is available as a stand-alone routine in individual laboratories. This activity has resulted in a steady increase in CIF submissions to the *Acta* Editorial Office, rising to about 25% of input by the end of 1992. The use of keyboarded CIF input at the Editorial Office has enhanced the checking and evaluation of data prior to publication. Both forms of CIF input are passed routinely to the crystallographic databases as an enhancement to their data-capture activities.

Members of the Commission have been involved in planning some of the technical aspects for the new edition of the *World Directory of Crystallographers*, which will begin information collection in 1993. The crystallographic data activities of the IUCr were represented at the CODATA International General Assembly held in Beijing in October 1992.

Discussions with the Chemical Structure Association and other related bodies concerning the incorporation of the standard molecular data format (SMD) within STAR/CIF have continued during 1992. A detailed proposal for a companion molecular information file (MIF) has now been tabled for discussion early in 1993. Such a file would encode, in a standard manner, the 2D chemical connectivity data required for a full description and representation of molecular structure.

If the CIF is to be a continuing standard in our subject area, one which will develop and expand over time, then that standard must be continuously and carefully maintained. To this end, a Committee for the Maintenance of CIF Standards (ComCIFs) was formed towards the end of 1992 at the request of the IUCr Executive Committee. This Committee will be independent of any Commission and will report directly to the IUCr Executive Committee. ComCIFs has a purely technical role and its initial membership will be announced in a suitable IUCr publication in 1993. The new Committee will also be responsible for the dissemination of information concerning the development and availability of software for CIF creation and manipulation. This is seen as an area of considerable and continuing importance.

The crystallographic databases continue to develop and expand and software activities associated with the databases is now an increasingly important area. Close to 200 000 structure determinations are now recorded in the four structural databases. The Cambridge Structural Database passed 100 000 entries during 1992, whilst dramatic increases in protein structural output presage a period of rapid development for the Protein Data Bank.

Commission on Crystallographic Nomenclature

A major part of the Commission's work was accomplished in 1992, as in previous years, through the devoted efforts of its committees and subcommittees. The final Report of the IUCr *Ad Hoc* Committee on the Nomenclature of Symmetry, under the chairmanship of P. M. de Wolff, was approved by the Commission and the Executive Committee; the Report, entitled *Symbols for Symmetry Elements and Symmetry Operations*, was published in *Acta Cryst.* (1992), **A48**, 727–732. In addition to redefining printed symbols for symmetry elements, the Report recommends use of the letters *e* and *k* for certain glide planes that previously were without either a unique or a specific symbol.

A Working Group of the Commission, consisting of the editors (V. Kopsky & D. B. Litvin) for Volume E of *International Tables for Crystallography*, completed a report entitled *Nomenclature, Symbols and Classification of the Subperiodic Groups*. The Commission accepted the final Report, which will be published in Volume E in due course, and agreed that an Abstract of the Report should be published in *Acta Cryst.* [(1993), **A49**, 594] as a form of advance notice to the crystallographic community. Preprints of the Report are available from D. B. Litvin. The report recommends symbols for the 7 frieze groups, 80 rod groups, and 75 layer groups together with symmetry tables and a classification of the subperiodic groups.

The Working Group of the Commission's Subcommittee on the Nomenclature of *N*-Dimensional Crystallography, under the chairmanship of A. J. C. Wilson, has not found it possible to resolve differences between several widely divergent naming and notation proposals in this area. These problems have led to the perception that it is premature to try to reach a solution fully acceptable to all proponents at present. Accordingly, it has been suggested that the Subcommittee allow time for further nomenclature proposals to develop before resuming its charge to recommend a unified nomenclature and symbolism for use in *N*-dimensional crystallography. It may be useful to recall that the primary purpose of this Commission is to provide an effective means for settling crystallographic nomenclature disputes. The mechanism of choice in reaching the best nomenclature decisions lies in the appointment of expert subcommittees charged with presenting recommendations to the Commission for possible revision and subsequent approval. It is customary to appoint a small number of Commission members with appropriate backgrounds to most subcommittees, to assist in maintaining a well balanced point of view. The *ex officio* membership of the editors of the primary IUCr publications on the Commission, together with the chairs of other selected IUCr bodies, is designed to ensure maximum sensitivity to the appearance of nomenclature obscurities or disputes in the

publications for which they have primary responsibility while simultaneously providing an impartial forum for settling them satisfactorily. Readers of this Annual Report are encouraged to bring potential nomenclature problems directly to the attention of the Commission.

Consideration is being given to the establishment of a Working Group that will examine the recently issued ISO *Guide to the Expression of Uncertainty in Measurement* for its possible impact on the nomenclature of statistical techniques used in crystallography, and that will be charged with making such recommendations as are appropriate.

Commission on Crystallographic Teaching

1. *Visiting Professorships*. Dr Ward T. Robinson of the University of Canterbury, New Zealand, was a Visiting Professor and organized a course in December 1992 at the Institute of Theoretical Chemistry, Jilin University, Changchun, People's Republic of China.

Dr C. H. L. Kennard gave a course, as a Visiting Professor, at the Technical University of Hanoi, Vietnam, 9–19 December 1992. The organizers were very happy with the course and hope to arrange another such visit in the near future. Ten 90-minute lectures and five two-hour tutorials, together with detailed tutorial notes, were presented. Dr Kennard reported on the lack of equipment and facilities that the international crystallographic community may be able to help with. For example, no diffraction equipment was in working order.

A School on the Rietveld Method was held in conjunction with the XVI National Meeting of the Brazilian Association of Crystallography at the University of São Paulo, San Carlos, Brazil, 14–16 December 1992 and the Rietveld Summer School at the National University of La Plata, Argentina, 8–10 December 1992, immediately before the Brazil Meeting. The IUCr sponsored and underwrote these schools at which Professors R. A. Young, A. K. Cheetham and R. Von Dreele were the Visiting Professors.

2. *Pamphlet Project*. The Pamphlet Project has been reinstated and an arrangement has been made for Polycrystal Book Service to print and distribute the pamphlets. A set of notes for authors of pamphlets has been prepared and the IUCr technical editing staff will assist with technical editing when requested. The previous set of 19 pamphlets is still available from Polycrystal Book Service (PO Box 3439, Dayton, OH 45401, USA). Several letters of invitation have been sent out and several crystallographers have each promised to write a new pamphlet.

Commission on Electron Diffraction

The project of the Commission to produce a multi-author publication on electron diffraction techniques has been completed with the publication of two volumes by Oxford University Press as part of the IUCr Monographs on Crystallography series. Volume 1 was published towards the end of 1992 and Volume 2 will appear early in 1993. The original plan to produce a single volume of about 500 pages in 1989 was modified as a result of difficulties experienced by various authors in meeting their deadlines and in confining themselves to the specified number of pages. It is hoped that the resulting 1000 pages in two volumes will provide a comprehensive, although not

completely contemporary, account of most of the significant areas of current interest in the theory, techniques and methods of analysis for electron diffraction using high-energy (greater than about 20 keV) electrons for the study of the structures of solids and gases.

The Commission has organized a Summer School on Electron Crystallography – Theory and Techniques as a Satellite Meeting of the IUCr Congress in Beijing in August 1993. The School will be held at the University of Peking, Beijing, in the week immediately preceding the Congress. An international panel of instructors will lead discussions on the various methods for deriving structural information on crystals, amorphous materials and gases using high-energy electrons. Topics will include recent developments in the crystal structure analysis of biological and non-biological organic and inorganic thin crystals and the high-precision determination of structure factors by convergent-beam electron diffraction and allied techniques.

Because of the difficulty that may be experienced by many students in meeting the costs of travel to China from other parts of the world, tentative plans have been made to hold a similar Summer School in Europe; possibly at Halle in 1994.

The Commission was again active in making proposals for the programme of the forthcoming Congress of the IUCr. The Commission is pleased to note that the programme will contain a number of special talks and special sessions which will make the Congress a valuable forum for the electron-diffraction community.

Commission on Neutron Diffraction

Many of the Commission's activities are continuing ones, and often informal, involving communication of information, encouraging exchanges, involvement of members in organizing meetings *etc.* It was particularly pleasing to see publication in 1992 of Volume C of *International Tables for Crystallography*, which includes a wealth of pertinent information for neutron scatterers. Many of our colleagues contributed, but the efforts of Terry Willis are particularly noted. As another example, members of the Commission and of that on Powder Diffraction have helped to organize IAEA Training Courses in China and Grenoble. These courses promote the use of neutrons for, for example, materials development and characterization, particularly in countries new to neutron-beam research. They bring together scientists needing to use neutron beams and experienced lecturers, for both in-depth course work and hands-on experience in running experiments. Typical techniques are powder diffraction, small-angle neutron scattering and radiography. The IAEA will propose further courses where required.

The Commission continues to promote *Neutron News*, edited by Gerry Lander (with John Axe and Commission member Yasuo Endoh), in every possible way. It has since 1990 been a powerful means of communication between all neutron scatterers – not only diffractionists – and this wide readership is a source of strength to the neutron diffraction community. The dynamism of *Neutron News* was earlier shown once again, with publication in Vol. 3, No. 3 (1992) of not only the Koester, Rauch & Seymann table of experimental values of neutron scattering lengths as a handy wall chart, but also of the latest V. F. Sears

rationalized values of neutron scattering lengths and cross sections.

The next edition of the *World Directory of Crystallographers* is in preparation – the last dates from 1990 – and for the first time it will be prepared from a database maintained at the IUCr office in Chester. It is important to note that the *Directory* is open to anybody working in crystallography and related topics. See the *IUCr Newsletter*, Vol. 1, No. 1 and *Acta Cryst* (1993), A49, 222–225 for details. All those using neutron diffraction, even occasionally, are urged to see that they are entered into the database, as this will help the Commission to fulfil its role. Eventually, the IUCr database should replace other less well maintained databases as the primary source for address lists for special-interest groups, conference organizers, seekers of technical information *etc.*

As the mandate of the present Commission nears its end, its attention turns increasingly to the Beijing Congress. The Commission proposed a number of microsymbiosia as well as a list of suggested plenary lecturers. We thank those inside and outside the Commission who helped us in the preliminary stages by contacting potential contributors. The severe selection from the very large number of propositions meant that not all of our suggestions were accepted but it was pleasing to see that the subjects chosen emphasized the complementarity of neutron scattering with other techniques. There will also be an Open Commission Meeting of the Commission on Neutron Diffraction devoted to the complementarity of neutron sources. And, of course, many of the other sessions will have contributions involving neutrons: area detectors, superconducting materials *etc.*

Every three years, the membership of IUCr Commissions is modified at the time of the IUCr Congress and General Assembly. This is also an appropriate time, for anyone who wishes to do so, to suggest new directions or new projects or simply to offer constructive remarks about the work of the Commission. This can be done through any Commission member.

Commission on Powder Diffraction

During 1992, the CPD was actively involved in various projects, meetings and workshops/schools and in planning for future ones.

1. *Publications.* The results of the first phase of the Rietveld Refinement Round Robin (RRRR) were published [*J. Appl. Cryst.* **25**, 589–611].

The Proceedings of the International Conference on Accuracy in Powder Diffraction II (see below), held 26–29 May 1992, were published as *NIST Special Publication* No. 846 at the end of the year. Copies are available from: Superintendent of Documents, Government Printing Office, Washington, DC 20402, USA for \$14.00 per copy. The stock No. SN 003-003-03186-1 should be included in the request.

The intended two-per-year schedule for producing CPD Newsletters was kept. No. 8 was edited by Dr D. Louër (France) and appeared in March; No. 9 was edited by Dr D. E. Cox (USA) and was dated November. More than 1000 copies of each were distributed. A conscious effort to increase the mailing list of interested persons has met with some success. A check of the mailing list against the

current *World Directory of Crystallographers (WDC)* verified that our newsletters reach a community not well represented in mainline crystallography: approximately one half of the names on our mailing list are not in the current *WDC*.

A mechanism for significant further extension of the Newsletter's distribution has been agreed with Professor Lin of Nankai University, Tianjin, China. He will translate the newsletters into Chinese and his university will distribute them periodically along with about 300 Chinese-language copies of *Powder Diffraction*, which they will prepare.

All author and scientific-editor work on the multi-author book *The Rietveld Method* was finished during the year. (The book came off the presses of the Oxford University Press in February of 1993.)

2. *Meetings/Workshops/Schools*. A major inter-congress meeting was held 26–29 May 1992 at the National Institute of Standards and Technology in Gaithersburg, MD, USA, with the title Accuracy in Powder Diffraction II (APD-II). There were 175 registered participants from 18 countries. The meeting was organized by the CPD and was sponsored by the ICDD, the IUCr and NIST. Generous financial support for speakers and young scientists was received from the ICDD and the IUCr, respectively. Excellent local arrangements were made under the Co-chairmanship of Dr E. Prince and Dr J. Stalick of the NIST. The Programme Chairman was Dr R. J. Hill (Australia), who is also the Secretary of the CPD. The participants seemed very satisfied with the meeting.

Because so many CPD members were attending the APD-II meeting anyway, a successful CPD business meeting was held, at several times, before and during the APD-II period.

Three 3-day Rietveld Summer Schools featuring hands-on practice on PC-type computers were organized by the CPD in 1992. The one in Cieszyn, Poland, held 13–15 August, was attended by 42 students from several European countries. Financial support was provided by the IUCr for the travel expenses of the main lecturers (Professors A. K. Cheetham, R. B. Von Dreele and R. A. Young) and for registration and living-costs grants for 20 students.

The other two Rietveld Summer Schools were held in December with the same three main lecturers. The first was in La Plata, Argentina, 8–10 December 1992 with Professor Graciela Punte (National University of La Plata) as chair of the local organizing committee. The second was held in São Paulo, Brazil, 14–16 December with Professors Yvonne Mascarenhas and Lia Amaral (University of São Paulo at San Carlos and at São Paulo) in charge of the local organization. 30 students, out of 50 applicants, were accommodated for the La Plata School. In the São Paulo School, 42 students were accommodated. Co-organized by the host groups, the Schools received financial sponsorship from CONICET (Argentina) and CNPQ (Brazil). The full travel expenses of the three lecturers from the northern hemisphere were funded by the Cooperative Science programmes of the US NSF with CONICET and CNPQ. The schools were also sponsored in name and underwritten by the IUCr through its Visiting Professorship Programme and Commission on Teaching. The underwriting by the IUCr was crucial, as the NSF funding actually came

through only after all plans and local arrangements, including local financial commitments, had been made and travel tickets had been bought.

Carried out during this year was much of the CPD's work as co-organizer of the International Workshop of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis to be held in Aswan, Egypt, 16–26 January 1993. Three CPD members served on the Programme Committee, one as Chairman. The IUCr's Visiting Professorship Programme came to the rescue by providing travel funds for Professor D. K. Smith (Consultant to the CPD) to give an intensive 5-day course on Mineralogical Crystallography at Ain Shams University in Cairo after the Workshop. This made it possible for him to organize and conduct one of the most important teaching sections of the Workshop, that on quantitative phase analysis by diffraction means. Also on the teaching programme were F. Ahmed (NRC, Ottawa), A. Authier (IUCr President, Paris), S. Gorter (Delft), R. Jenkins (ICDD), S. E. Rasmussen (Aarhus), J. Schneider (Munich), H. Toraya, (Nagoya), G. Will (Bonn), A. Wright (Reading) and CPD members J. I. Langford and D. Louër, who also served on the Programme Committee.

The Satellite Meeting on Powder Diffraction to be held in Hangzhou, China, 31 August – 3 September 1993 was initiated and is being co-organized by the CPD. The Programme Committee, under the able chairmanship of CPD member J. I. Langford, performed most of its work during 1992.

3. *Other projects*. A Task Group on Crystallite Size and Microstrain Determination has been set up jointly with the ICDD. Dr J. Fiala (CPD) and Professor R. L. Snyder (ICDD) are the Co-chairs. The first focus is to be a round robin that will illuminate the current methodologies and data-interpretation models used by the participants, including strengths and weaknesses of the methods and models.

The CIF/STAR format, previously recommended by the CPD to be extended for use with powder data, has now been accepted by the ICDD. J. I. Langford chairs the CPD's development efforts and coordinates with B. Toby who chairs the ICDD's.

Phase two of the Round Robin on Rietveld Refinement is nearing completion. In mid-1993, the results will be submitted for publication in the *Journal of Applied Crystallography*. This large project is being coordinated by Dr R. J. Hill (CPD Secretary). It is an intercomparison of 41 X-ray and neutron powder diffraction data sets collected on a standard sample of monoclinic zirconia using 31 different instruments in 18 countries. The results should prove to be even more interesting than those arising from Part I of the project. Dr Hill is scheduled to present a short summary of them at the 1993 Satellite Meeting on Powder Diffraction in Hangzhou.

The JCPDS-ICDD's Hanawalt award was presented to CPD member Dr D. Louër during the opening ceremonies of the EPDIC-2 meeting in Enschede, The Netherlands. It is given for excellence in the field of powder diffraction.

Commission on Small Molecules

The principal activities of the Commission in 1992 concerned the organization and planning of the Satellite Sym-

posium on Molecular Structure to be held in Fuzhou, China, 31 August – 1 September 1993, immediately following the IUCr Congress and a Symposium on New Trends in Small-Molecule Crystallography to be held in Atlanta, Georgia, 26 June – 1 July 1994 in conjunction with the 1994 ACA meeting.

William Duax and Judith Howard visited the site of the Fuzhou meeting to discuss its organization with Professor Jing-Ling Huang and Jin-Xi Liu in April of 1992. Details of the programme, which include four main topics (Systematic Analysis of Molecular Geometry, Conformation and Thermal Motion; Molecular Interaction and Recognition in Crystals; Structure and Activity of Biological Molecules; Phase Relation and Transformation in Some Small Moiety Systems), were included in the first issue of the *IUCr Newsletter*. The International Programme Committee is composed of Judith A. K. Howard, William L. Duax, Hans-Beat Bürgi, Maureen Mackay, Gaston Gilli, Luigi Nassimbeni, Shi-Xiong Liu and Jing-Ling Huang.

The programme Frank Herbstein has organized for New Trends in Small Moiety Crystallography will emphasize the tremendous qualitative and quantitative changes to be expected in the nature of the next century's structural information because of the anticipated advances in experimental and computational diffraction techniques. Speakers will be asked to look critically at how their topics have developed and to dare to peer some way into the future. Invited speakers will be: S. Amelinckx (The Netherlands), J. Burdett (USA), H. B. Bürgi (Switzerland), P. Coppens (USA), R. Destro (Italy), J. D. Dunitz (Switzerland), J. L. Finney (UK), F. Frey (Germany), A. F. Garito (USA), D. M. Grant (USA), M. M. Harding (UK), M. Hart (UK), H. Hauptman (USA), D. N. Hendrickson (USA), J. Karle (USA), F. K. Larsen (Denmark), C. N. R. Rao (India), J. A. Ripmeester (Canada), H. G. von Schnering (Germany), G. A. Somorjai (USA) and A. Weiss (Germany). The proceedings will be published.

The Eighth Crystal Chemistry Symposium organized by Roland Boese, Josef Garbaczyp, Zygmunt Kaluski and Derry Jones was held in Rydzyna, Poland, 26–30 July 1992. Topics of the meeting included crystal engineering and the design of crystals with specific properties, information on crystal chemistry derived from databases and low-temperature crystal chemistry. A report from the meeting appeared in the first issue of the *IUCr Newsletter*.

A slate of candidates for the membership of the Commission in the next triennium has been developed with input sought from the entire current membership.

Commission on Synchrotron Radiation

A major activity throughout the year has been in leading the discussions on the proposal for a *Journal of Synchrotron Radiation*. Potential co-editors of the journal were contacted and their views solicited. Open discussions were held at a variety of conferences, both national and international, in Europe, the USA and Japan. Representative organizations and the directors of SR laboratories have also been contacted.

Planning of the Satellite Meeting on Applications of Synchrotron Radiation in Crystallography in Beijing, immediately following the IUCr Congress, has continued. The host laboratory of the Meeting is the Institute of High

Energy Physics of Academia Sinica and the site of the Chinese Synchrotron X-radiation Source. There has been a very good response to the first circular.

1992 has seen the commissioning of the first of the next generation of high-brilliance high-energy synchrotron-radiation sources in Grenoble, namely the European Synchrotron Radiation Facility (ESRF). This is indeed a milestone for the field of synchrotron radiation.

Ad Interim Commission on Aperiodic Crystals

The Commission project of elaborating a set of guidelines for the items to be included in structural reports of incommensurately modulated structures progressed during 1992. After producing a first draft, other specialists outside the Commission were consulted. The discussion of their suggestions and additional proposals that emerged during the process have led to a careful transformation of the initial draft. A final version is expected to be approved by the Commission before the next Congress in Beijing. The elaboration of a similar list for incommensurate composite structures has been postponed until this subfield further develops and some standards become commonly accepted.

A fluid mail contact with the Subcommittee on the Nomenclature of *N*-Dimensional Crystallography of the IUCr Commission on Crystallographic Nomenclature has been maintained. At the ACA meeting in Pittsburg, some of the members of the present Commission met and organized an informal short meeting to obtain the opinion of interested people on the nomenclature of *N*-dimensional crystallography. A general agreement could be ascertained that the adoption by the IUCr of a standard nomenclature and notation for higher-dimensional space groups at this time is premature. This opinion is shared by this Commission and was communicated in a formal letter to the Subcommittee on the Nomenclature of *N*-Dimensional Crystallography.

Under the support of this Commission and the sponsorship of the IUCr, the fourth International Conference on Quasicrystals took place in St Louis in June. A coordination of the frequency of these meetings with the more general International Conferences on Aperiodic Crystals that the present Commission organizes on a triennial basis could be achieved. Thus, in 1994 (18–22 September), an International Conference on Aperiodic Crystals (Aperiodic '94) will take place in Lausanne (Switzerland) while, in 1995, Avignon will be the site of the fifth International Conference on Quasicrystals. The organization of Aperiodic '94 is under way and the first announcement will be distributed in March 1993.

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 1992 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1992 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1993, but approved in 1992, are listed below:

1. 4th International School of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis, Aswan, Egypt, 16–26 January 1993.
2. Workshop on Optoelectronic Materials and their Applications, La Habana, Cuba, 18–25 February 1993.
3. Fourth Intensive Course in X-ray Structure Analysis of Small and Medium Sized Molecules, Birmingham, England, 22–28 March 1993.
4. Third European Workshop on Crystallography of Biological Macromolecules, Como, Italy, 24–28 May 1993.
5. Summer School on Electron Crystallography – Theory and Techniques, Beijing, China, 16–20 August 1993 (satellite meeting of Beijing Congress).
6. Neutron Scattering, Beidaihe, China, 17–19 August 1993 (satellite meeting of Beijing Congress).
7. Symposium on Molecular Structure, Fuzhou, China, 31 August – 3 September 1993 (satellite meeting of Beijing Congress).
8. Application of Synchrotron Radiation in Crystallography, Beijing, China, 31 August – 3 September 1993 (satellite meeting of Beijing Congress).
9. Powder Diffraction, Hangzhou, China, 31 August – 3 September 1993 (satellite meeting of Beijing Congress).
10. International School on Advanced Electronic Materials, Madras, India, 23 November – 5 December 1993.

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 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 date of the meeting, writing to the Chairman of the Sub-Committee. The present Chairman is Professor P. Coppens. A new Chairman will be appointed at Beijing.

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

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

Regional Associates and Scientific Associates

American Crystallographic Association (ACA)

The ACA held its annual meeting jointly with the golden anniversary of the Pittsburgh Diffraction Conference in

Pittsburgh, PA, 9–14 August. The ACA honored Dr Donald L. D. Caspar of Brandeis University with the Frankuchen Award and the Pittsburgh Diffraction Society honored Raymond Stevens of Harvard University with the Sidhu Award. This highly successful meeting had several novel sessions including a poster preview session and an opening mixer for the young scientists group. The meeting was preceded by a Summer School for Crystallography, which provided an intensive training period involving hands-on use of diffractometers and computers for 32 students. The Summer School was successful and will be repeated in subsequent years.

The ACA has taken a leadership role in raising funds to support crystallographic colleagues in the former Soviet Union. These efforts are coordinated with those of the USNCCr and the American Association for the Advancement of Science. The 1993 meeting of the ACA is scheduled for Albuquerque, New Mexico, 23–28 May and the 1994 meeting will be held in Atlanta, Georgia, in June.

The officers for 1993 are Richard Marsh, President; Elinor T. Adman, Vice-President; Keith Watenpugh, Past-President; Vivian Cody, Secretary; S. N. Rao, Treasurer; I. David Brown, Canadian Representative.

Asian Crystallographic Association (AsCA)

The main event of AsCA activities in 1992 was the Inaugural Conference of the Asian Crystallographic Association, AsCA '92, which was held at the Regional English Language Centre (RELC), Singapore, 14–16 November 1992. Professor André Authier, President of the IUCr, and Professor H. H. Huang, Deputy Vice-Chancellor, National University of Singapore, accepted invitations to attend the opening ceremony of AsCA '92. The total registration was 320 with 240 full participants and 80 students, excluding 30 accompanied persons. This was 60% more participants than initially estimated. Several difficulties that were encountered owing to the unexpectedly large attendance (the ideal capacity of the venue was 250–275) were solved by the kind cooperation of the executive members of the Organizing Committee with the staff at the RELC. The national distribution of participants and scientific presentations are shown below.

	Participants	Presentations
Japan	180	134
Australia	57	53
China	14	11
India	14	23
Taiwan	14	12
Singapore	12	8
Europe	8	6
Thailand	5	1
Malaysia	3	
Bangladesh	2	1
New Zealand	1	1
Sri Lanka	1	1
Vietnam	1	2
USA	5	5
Israel	1	1
Russia	1	2
Venezuela	1	2
Total	320	264

The scientific program consisted of 16 oral sessions with 73 papers and 22 poster topics with 190 papers.

The success of AsCA '92 was a tribute to the organizers, to the sponsors and to the participants but it is noted that the success is partly because the Society of Crystallographers in Australia and The Crystallographic Society of Japan decided to hold their joint annual meetings under the auspices of the AsCA in order to promote the Inaugural Conference of the AsCA.

European Crystallographic Committee (ECC)

Instead of the expected 600–700 participants at ECM-14 (Enschede, The Netherlands, 2–7 August), there were only 450, which can be attributed to the problems with hotels, dormitories *etc.* There were last-minute (entry/exit) visa problems for scientists from Croatia, Slovenia, Russia and Serbia. Considerable support was given to scientists from Eastern/Central Europe. For young scientists, 22 IUCr scholarships were offered, of which 18 were used and 2 were switched to other beneficiaries. Of 26 Senior Scientist supports administered by the ECC executive (given by the IUCr), 22 were used by the applicants, 4 were used only in the last minute. Other sources from The Netherlands allowed 11 more scientists to attend the meeting. 500 abstracts were received but *ca* 25–30% of the submitting authors were not present in Enschede. Since EPDIC-2 preceded ECM-14, it was felt that this specialized conference had drained off many of the people interested in powder diffraction. The Vice-Chairman expressed his concern about the increasing (negative) influence of special meetings on the future of general conferences.

The ECM-14 meeting took place on the Campus of the University of Twente. Since the IUCr Executive Committee convened in Pittsburgh, only the Vice-President, Professor A. Kálmán, attended the opening ceremony and welcomed the participants on behalf of the President and the EC. The Conference Lecture, presented by Professor M. Hart (Manchester), with the title Anomalous Scattering in Structure Determination, was dedicated to the memory of the famous Dutch crystallographer J. M. Bijvoet born a century ago.

At the request of the IUCr representative, the ECC met on the evening of the first conference day. The meeting started with a dinner at 20.30 and lasted until midnight. After the approval of the agenda and the minutes of the previous ECC meeting (28 August 1991, Trieste), the Chairman gave a brief report on the year's activities. The principal theme of his address was that the time was not suitable for the formation (although many delegates are in favour of it) of a European Crystallographic Association, owing to the unstable political situation in Europe. However, the formation of an ECA should be included in the agenda of the next ECC meeting.

Reviewing the membership status of the new independent European countries, it was first decided unanimously that the membership of USSR and Yugoslavia to the ECC should be cancelled. After discussion and the presentation of their accreditations, Latvia, Croatia, Slovenia and Ukraine were admitted by vote as members of the ECC. The approved membership of Russia should be confirmed by a letter from the President of the Academy of Sciences

of Russia, while the applications of Moldavia and Estonia are expected about the fall of 1992.

Finally, reports were presented on the forthcoming ECMs.

It was decided that, instead of Leipzig, ECM-15 will be held in Dresden, the capital of Saxony in 1994 (28 August – 2 September). The participation fee is DM 300. It was suggested that there should be a special registration fee for students.

ECM-16 will be held in Lund in 1995 (about the second week of August). 400–800 participants are expected and can be catered for. The accommodation for the participants seems to be available with a reliable price of about DM 50–60 per night.

Preliminary consideration of ECM-17: oral invitations were received from Egypt (Cairo) and Portugal (Lisbon, 1997) and a written invitation from the President of the Associations of Scientific Societies of the Czechoslovak Academy of Sciences (Prague, but no date is specified). The discussion on this topic will be held over until the next ECC meeting or even 1994.

Despite the usual plan to renew ECC officers in Beijing during the IUCr Congress in 1993, the unexpected decision is, as disclosed recently by the ECC Secretary Dr H. Flack, that there will be no ECC meeting in Beijing. The new officers will be elected in 1994 in Dresden.

International Centre for Diffraction Data (ICDD)

ICDD activities. The ICDD continues to be a dynamic, strong and growing organization. The growth is partly in size but also, notably, in the scientific content of the projects that the ICDD undertakes.

As most readers of this report probably know, the ICDD operates with a staff of about 25 full-time employees plus several part-time (*e.g.* the editors) and well over 100 well organized volunteer members plus many volunteer non-members. (There are about 120 ICDD active members, none of whom may receive any compensation from the ICDD.) The volunteers do much of the work. They are organized in Sub-committees, which further divide into Task Groups. There is a Technical Committee that consists of all Sub-committee Chairs plus other *ex-officio* members. The Sub-committees meet during the twice-a-year ICDD meetings, receive and discuss reports of Task Groups, take appropriate actions including identification of and prioritizing additional work needed and prepare necessary motions for the Technical Committee (TC) to consider. If the TC approves, they pass on the motions, perhaps with changes, to the BoD (ICDD Board of Directors) for action.

In continuation of the ICDD's efforts to increase international participation, the BoD has appointed to leadership positions Daniel Louër (France), Herbert Göbel (Germany), Walter Eysel (Germany) and Larry Calvert (Australia).

After nearly two years of misunderstandings and two special meetings of representatives to clear them up, at its October 1992 meetings the BoD passed a motion that the ICDD adopt the CIF/STAR format as standard for the interchange and archiving of PDF-3 and future databases. The major of the two special meetings was that of several members of the IUCr EC meeting with the ICDD Chair-

man and other BoD members in Pittsburgh in August prior to the ACA meeting. Much was accomplished there to dispel any mistrust and to establish a base of mutual understanding of the good intentions of each organization.

Elections of ICDD officers were held in March 1992 with the following results: Professor G. G. Johnson (Penn State) is the new Chairman; Jan Visser (The Netherlands) continues as Vice-Chairman; Dr Gerhard Fischer is the new Treasurer; Dr Tom Blanton (Eastman Kodak) was elected a BoD member at large; and Dr. Ting C. Huang (IBM, San Jose) is the Chairman of the Technical Committee.

Of very special interest to the IUCr is that CPD member Dr Daniel Louër was selected to receive the 1992 Hanawalt Award. It was presented to him at EPDIC-2 by Dr Ludo Frevel, the immediate Past Chairman, a previous winner of the Award and the representative to the CPD.

An ICDD Task Group was set up, with Professor R. Snyder as Chair, to conduct a project jointly with the CPD on Crystallite Size and Microstrain. One aspect of the work is expected to be a Round Robin on Crystallite Size and Microstrain (Dr Fiala chairs the CPD's Task Group on this).

The ICDD had several other round robins in progress in 1992, mostly from the Data Collection and Analysis Subcommittee: (i) instrument parameters (Jenkins, ICDD); (ii) automated peak finding (Ryba, Penn State University); (iii) statistical process control (Blanton, Eastman Kodak); (iv) profile fitting (Cline, NIST); (v) preferred orientation (Diffraction Problems Subcommittee).

A project investigating a suitable standard sample for small-angle (Bragg) scattering (large d values) under Tom Blanton has found that silver behemate (first d at ~ 58.3 Å) has many good properties for the purpose. The project is not yet finished, but a first paper will be published [*J. Appl. Cryst.* (1993), **26**, 180–184].

In 1992, the ICDD again operated the 'clinics' on X-ray fluorescence and X-ray diffraction, this year at Swarthmore College. These are clinics that were established and have been operated by Henry Chessin at SUNY-Albany for more than 20 years.

Grants. The ICDD Crystallography Scholarship Awards are being continued at the rate of two per year. The two awarded in 1992 went to graduate students in the UK.

In keeping with the ICDD's international character, the BoD approved a small grant to be administered by the Organizing Committee of EPDIC-2 to assist scientists from the former Eastern bloc countries to attend the meeting.

The ICDD contributed \$15 000 in support of the Accuracy in Powder Diffraction II meeting organized by the CPD in May 1992 at NIST. The money was to be used primarily for the travel expenses of lecturers who would also provide good manuscripts in a timely manner for the Proceedings. Since the Proceedings were published within about 6 months, it appears that the money was well spent.

The ICDD is contributing \$5000 in support of the Satellite Meeting on Powder Diffraction to take place 31 August – 2 September 1993 in Hangzhou.

The ICDD paid the travel costs for one teacher/lecturer (R. Jenkins) in the 16–26 January 1993 International Workshop of Crystallography: Computational Methods in Powder Diffraction co-organized by the IUCr's Commission on Powder Diffraction.

The Grants-in-Aid program continues at an annual rate of more than \$300 000. Many of these grants go to persons outside the USA.

Other. PDF-3 is to be based on fully digitized patterns. A few hundred are now in hand and are coming in at a rate of about 500–600 per year. There is a growing and spreading recognition that a great many analyses formerly undertaken with the 'd & I' type of database can be done much better with digitized full patterns. Included are quantitative phase analysis, phase identification in complex mixtures and extracting useful information from the 'pathologies' of the patterns, such as various effects characteristic of different clays. Such patterns might also be used for *ab initio* structure determinations.

At the end of 1992, the ICDD were making plans to move into their new building early in 1993. It is a 25 000 ft² building located at the Newton Square Corporate Campus, 12 Campus Blvd, Newton Square, PA 19073-3273, USA.

International Organization for Crystal Growth (IOCG)

The main activities of the IOCG during 1992 were the organization of the Tenth International Conference on Crystal Growth (ICCG-10) and the Eighth International Summer School on Crystal Growth (ISSCG-8). Both events were hosted in the USA by the American Association for Crystal Growth (AACG).

ICCG-10 was held in San Diego, CA, 16–21 August 1992. It was attended by 64 delegates (less than in the previous ICCG-9, held in Japan in 1989) from 33 countries. 264 delegates were from the USA, 138 from Japan, 41 from Germany and more than 20 delegates each from China, CIS and the UK. Out of 32 sections, nine were devoted to semiconductors (80 communications), three to superconductors (26 communications), three to non-linear optical materials (25 communications) and the others were on various materials including biomaterials and solution-grown industrial crystals.

ISSCG-8, held in Palm Springs, CA, 9–15 August 1992, was well attended by about 150 participants, with an increase of about 20% compared to the previous ISSCG-7 in Japan. The school provided a high-level programme of lectures that covered a wide range of topics, including both fundamentals, such as morphological stability, surfaces and interfaces, heat and mass transport *etc.*, and advanced technological aspects.

During the IOCG General Assembly in San Diego, the membership of the IOCG Executive Council was renewed for the coming triennium 1992–1995. The slate of officials elected by the Council and formally approved by the General Assembly is as follows. Officers: President: B. Cockayne (UK); Vice-Presidents: T. Nishinaga (Japan) and R. F. Sekerka (USA); Secretary: M. Schieber (Israel); Treasurer: E. Kaldis (Switzerland); Past President: R. Kern (France). Executive Committee: K. W. Benz (Germany), A. A. Chernov (CIS), R. Feigelson (USA), D. T. J. Hurle (UK), P. Ramasamy (India), R. Rodriguez-Clemente (Spain), G. M. van Rosmalen (The Netherlands), I. Sunagawa (Japan). *Ex officio* Members: W. Bonner (USA), J. F. Wenkus (USA), C. F. Woensdregt (The Netherlands), P. Dauday (The Netherlands), R. A. Laudise (USA), V. V. Osiko (CIS) (Representative to IUCr), C. Paorici (Italy) (Representative of IUCr).

During the General Assembly of San Diego, it was decided that ICCG-11 will be held in The Hague, The Netherlands in June 1995, preceded or followed by ISSCG-9. It was also recommended that ICCG-12 should be held in 1998 in Israel and that ISSCG-10 should be held in Italy.

Representatives on Other Bodies

The Condensed Matter Division of the European Physical Society (EPS)

The Board of this body met on 7 April in Prague, Czechoslovakia, and on 14 November in Geneva, Switzerland. Both meetings were attended by the IUCr representative, who received progress reports on future meetings in Regensburg (1993) and Madrid (1994).

Among topics discussed were: the future of European conferences on condensed matter which are becoming increasingly more expensive and less efficient (a task force has been nominated to analyse all aspects of the problem); relations with EEC divisions; contacts with EEC representatives. The problem of how to publish CMD Proceedings was again addressed.

Interdivisional Committee on Nomenclature and Symbols (IDCNS)

The annual meeting of IDCNS was held 4–5 September 1992 in Oxford, England, and was attended by the alternate to the IUCr representative in order to reduce travel costs for the IUCr. IDCNS acts on all nomenclature proposals originating in the various divisions of IUPAC before they are allowed to proceed to publication; about 35 documents were received in 1992 for review by the representative. Documents of potential interest to the IUCr included nomenclature standards relating to chemical thermodynamics, inorganic chain and monocyclic compounds, organic chemistry and polymers, all of which will be published in *Pure Appl. Chem.* Two other documents with greater potential impact on IUCr publications were entitled *Definitions of Terms Relating to Phase Transitions of the Solid State* and the *ISO Guide to the Expression of Uncertainty in Measurement*. The former, which provides definitions for a broad range of phase transitions involving the solid state, will probably be published next year. The latter (ISO/TAG 4/WG 3), which was published June 1992 by the International Organization for Standardization, provides procedures to be followed in evaluating and expressing the uncertainty of the result of a measurement. The basis of this *Guide* is an International Committee for Weights and Measures recommendation (CI-1981) and is the only recommendation concerning the expression of uncertainty in measurement endorsed by an inter-governmental organization. Consideration is being given (see the Report of the Commission on Crystallographic Nomenclature above) to undertaking a formal study of this *Guide* in order to determine the possible impact it may have on current crystallographic statistical nomenclature.

International Council for Scientific and Technical Information (ICSTI)

The Draft Strategic Plan, prepared by the ICSTI Planning Group, includes the following:

ICSTI *aims* to enhance delivery of and access to information for all constituencies in business, industry, academia and the public through the exchange of information and the sharing of experience among international peers.

ICSTI *must* benefit its members, truly reflect an international composition, be able to react swiftly and with expertise to important events occurring in the world of scientific and technical information.

ICSTI *goals* include: to provide the benefits of an organized society to all classes of members under the sponsorship of ICSU; to promote awareness of the value and economic significance of scientific and technical information; with an understanding of user needs, to assist in the development of mechanisms to satisfy the requirements of the world community of generators and consumers of scientific and technical information. To advocate and support international standards, laws and regulations that will maximize the use of and access to appropriate information by diverse constituencies.

ICSTI programme *targets* include: to improve collectively the relations among the different communities involved in the information chain between generator and user; to define the present and future needs of the user and to monitor the progress being made in meeting them; to keep under review the impact, costs and acceptability of new technologies and to provide for the exchange of information on related developments in member organizations; to develop common approaches to such matters as standards and legal aspects of information management, including copyright.

As shown by these extracts from its draft strategic plan, ICSTI objectives are closely aligned with those of the IUCr. If achieved, they would overcome many difficulties encountered by crystallographers in accessing crystallographic information.

ICSTI's accomplishments fall short of its objectives. Its main activities reflect commercial publishing management's concern to ensure the survival of their constituent organizations through the upheaval in publishing generated by new technology. That is compounded by failure, in the commercial sense, of most ICSTI publications. Currently, ICSTI does not have the financial and organizational strength necessary to achieve its laudable objectives. However, one would be pressed to identify how an alternative organization could do better. As pointed out when the IUCr representative raised this question at the ICSTI Council Berlin meeting in 1992, 'at least the main players in the publishing industry are here'. I regret that other commitments preclude the attendance of the IUCr representative at the 1993 Council meeting in Williamsburg.

The IUCr representative recommends that the IUCr persist with its membership of ICSTI, while recognizing its shortcomings. As a matter of policy, the Union should foster links between ICSTI and CODATA, with the ultimate objective that those two organizations merge.

International Council of Scientific Unions (ICSU)

The IUCr representative attended the 30th General Committee Meeting of ICSU and the associated meetings of the Working Group of Earth, Space, Physical and Mathematical Sciences held at the Israel Academy of

Sciences and Humanities in Jerusalem, 5–7 November 1992.

Many general problems and the activities of the Scientific Committees were discussed. At a round table presentation of important news of the Unions, held during the meeting, the IUCr representative illustrated the structure of the IUCr based on the Commissions and its publishing activities, pointing out the improvements in automation in Chester. He also announced the publication of the new Section D of *Acta Crystallographica* that will start in 1993, and mentioned the strong request for a journal on synchrotron radiation by the crystallographers who used this kind of radiation.

At the general meeting, reports were given on a number of Committees and activities in which ICSU is involved. One afternoon was devoted to the reports of a number of Union representatives who illustrated the new scientific developments in the fields covered by their Unions, following a custom started at the Oslo meeting (1991). These reports were very interesting, giving a picture of what is going on at the frontiers of modern science in the world.

Other general topics discussed at the general meetings were: free circulation of scientists (there are still cases of problems regarding entry visas); ethics (ICSU might contribute to solving the general problem of ethics in science); cooperation with scientists in developing countries (the IUCr representative illustrated the IUCr policy for helping young scientists, particularly from developing countries, to attend international IUCr-sponsored meetings and the Visiting Professorship Programme); cooperation with scientists in Central and Eastern Europe (coordination is missing).

The Standing Committee on Structure and Statutes proposed some amendments of the Statutes to ensure equality of votes for the two categories of membership (National Scientific Members and Scientific Union Members). Financial aspects concerning the annual dues of the members were also considered and some proposals were made to be submitted for approval to the 24th General Assembly (Santiago, Chile, October 1993). The scientific programme associated with this General Assembly was also discussed.

ICSU Committee on Data for Science and Technology (CODATA)

The 13th International CODATA Conference took place in October 1992 in Beijing, China. The theme of the Conference was New Data Challenges in Our Information Age. A novel feature was the opportunity to hold joint sessions with the ICSU Panel on World Data Centres, a group that was meeting concurrently with CODATA. The main CODATA Conference comprised 21 sessions covering materials science, the geosciences, biology, chemistry, industrial physics and environmental issues. Various Commissions and Task Groups organized three other meetings and workshops on various topics in 1992. Of most interest to crystallographers was the Materials Regularities Workshop held in Como, Italy, in April 1992. CODATA supports the work of a variety of Commissions that address interdisciplinary issues associated with scientific and technical data. These include Commissions on Artificial Intelligence and Computer Graphics and on Biological Macromolecules. Particular attention is paid to

data needs, accessibility and activities in developing countries, to whom many CODATA publications and data sources are supplied freely.

ICSU Committee on Science and Technology in Developing Countries (COSTED)

The IUCr representative informed the Chairman of the Committee about the success of the Union policy for supporting young scientists, particularly those from developing countries, to attend international crystallographic meetings and schools. Also the Visiting Professorship Programme, coordinated by the IUCr Commission on Crystallographic Teaching, was illustrated.

As became apparent at the ICSU General Committee Meeting in Jerusalem, it seems that there is not enough communication between COSTED and the Unions.

ICSU Committee on Space Research (COSPAR)

The most important activity of COSPAR in 1992 was the World Space Congress – I, jointly organized by COSPAR and IAF by merging the Plenary Meeting of COSPAR and the IAF Congress. It was held in Washington, DC, USA, 28 August – 5 September, to celebrate the International Space Year.

The World Space Congress – I was mainly intended to gather a wide representation of the world space community in order to create a meeting with such a critical mass to enable significant statements to be made regarding the future preparation and planning of space research world wide. This Congress was very successful. It was estimated that more than 10 000 people participated in the various meetings and assemblies.

During the Congress, a number of awards were made among which, as relevant to crystallography, were the COSPAR International Cooperation Medal (1992) to Professor Hubert Curien and the Zel'dovich Award for Commission G (Materials Science in Space) to Stefan van Vaerenbergh.

The next World Space Congress – II is scheduled for the year 2000, very probably at the same location in Washington.

ICSU Committee on the Teaching of Science

No meeting was held in 1992.

Finances

The audited accounts of the year 1992 are given at the end of this Report. For comparison, the figures for 1991 are provided in italics. The accounts are presented in Swiss Francs.

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 Swiss Francs at 31 December 1992 have been translated into Swiss Francs in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into Swiss Francs by applying the rates of exchange appro-

priate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, an apparent loss has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 361310. This loss has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1992. It should be noted that this loss in Swiss Francs is not a real loss of money, but rather a loss on paper resulting from the accounts being expressed in Swiss Francs.

Investments are noted in the balance sheet at their market value at 31 December 1992. The difference between revalued cost and market value has been shown as an adjustment in order that the investments can be stated at cost. This prevents the fluctuations in value from influencing the General Fund. The revalued cost is obtained by converting the cost of investments in the currencies of purchase into Swiss Francs using the exchange rates operative on the balance sheet date.

The total of SwFr 493769 with the banks at the end of the year was represented by Dfl 3054 and US \$614 with the Amsterdam-Rotterdam Bank, US \$44967 with Merrill Lynch, £178637 with the National Westminster Bank and SwFr 23384 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, excluding stocks of unsold publications but including the loss of SwFr 361310 resulting from fluctuations in rates of exchange, have decreased during the year, from SwFr 5455503 to SwFr 5325909.

Transfers of SwFr 150000 and SwFr 50000 were made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund and the *Journal of Applied Crystallography* Fund, respectively. A transfer of SwFr 150000 was made to the Research and Education Fund from the General Fund and a transfer of SwFr 20000 was made to the Ewald Fund from the General Fund. A transfer of SwFr 25000 was made to the President's Fund from the General Fund to provide additional funds for cases of special need.

Beneath the detailed figures of the expenditure and income for each fund account, the balance at 1 January, 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.

The General Fund account shows a deficit of SwFr 8989, before the transfers totalling SwFr 195000 to the Research and Education Fund, the President's Fund and the Ewald Fund, as compared with a surplus of SwFr 217338 in 1991, before transfers totalling SwFr 110000 to the Research and Education Fund and the President's Fund. The administrative expenses were SwFr 304323 in 1992 as compared with SwFr 264408 in 1991. Of this amount, SwFr 91297 was charged to the publications of the Union.

SwFr 19343 was given for general support of scientific meetings, in addition to SwFr 90850 for financial support to young scientists attending meetings, which appears in the expenses of the Research and Education Fund, and SwFr 13818 in special grants from the President's Fund. SwFr 2849 was spent in assisting the work of the non-publishing Commissions. The expenses of the Union representatives on other bodies were SwFr 7314. The cost of

the two Finance Committee meetings held in 1992 was SwFr 15701, whilst the Executive Committee meeting cost SwFr 37528. The Union received SwFr 16632 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 131720. Interest on bank accounts and investments credited to the General Fund was SwFr 266268.

The President's Fund, the Publications and Journals Development Fund, the Research and Education Fund and the Ewald Fund received interest, at a nominal rate of 8% per annum, on the balances in the funds.

The President's Fund account therefore received interest of SwFr 1005, in addition to the already mentioned transfer of SwFr 25000 from the General Fund. Grants totalling SwFr 13818 were paid from the fund.

The *Acta Crystallographica* account for 1992 shows a surplus of SwFr 275139 before the transfer of SwFr 150000 to other fund accounts, as compared with a surplus of SwFr 219564 in 1991 before transfers of SwFr 50000.

The subscription rates were increased for 1992. The number of paid subscriptions to all sections of *Acta*, including 95 personal subscriptions in 1991 and 92 in 1992, decreased from 1050 in 1991 to 1005. For the number of paid subscriptions to the separate sections of the journal, those to Section A increased from 268 in 1991 to 276, those to Section B increased from 195 to 208 and those to Section C increased from 135 to 144. As usual, the cost of the technical editing office has been divided between the *Acta Crystallographica* and the *Journal of Applied Crystallography* accounts in percentages based on the number of text pages published during the year, namely 83 and 17%, respectively, for 1992. For 1991, the percentages were 81 and 19%. The technical editing costs for *Acta Crystallographica* were SwFr 593862 as compared with SwFr 462936 in 1991. The journal's accounts have also been charged with administration expenses as in previous years and as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a surplus of SwFr 52221 before the transfer of SwFr 50000 to the Publications and Journals Development Fund, as compared with a deficit of SwFr 5527 in 1991. The number of subscriptions, including 113 personal subscriptions in 1991 and 108 in 1992, decreased from 1022 in 1991 to 1006 in 1992.

The *Structure Reports* account shows a deficit of SwFr 9357 in 1992 as compared with a surplus of SwFr 17198 in 1991. One A Series volume and one B Series volume were published in 1992 (only one A Series volume in 1991). Editorial expenses were SwFr 90188 as compared with SwFr 13670 in 1991, but the level of these expenses does fluctuate from year to year. The net income from sales was SwFr 143172 in 1992 as compared with SwFr 43097 in 1991.

The *International Tables* account shows a surplus of SwFr 46637 as compared with a deficit of SwFr 5263 in 1991. Volume C was published in early 1992 and Volume B will be published in 1993. The net sales income of SwFr 171721 derived mostly from the sales of Volumes A and C.

The Book Fund is credited with the sales of the remaining publications of the Union including those of *Molecular Structures and Dimensions*, for which until 1991

there had been a separate fund account. The main sales income was from the *Historical Atlas of Crystallography*, edited by J. Lima de Faria.

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 SwFr 122 640 for computer expenses, including the purchase of computing equipment and software for the Chester office, all relate to the technical editing of the journals. SwFr 90 850 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union, was charged to the Research and Education Fund account.

President's Fund Account for the year ended 31 December 1992

	1992	1991	
Grants	13,818	23,395	Swiss Francs
<i>Excess of income over expenditure carried to balance sheet</i>	12,187	—	Interest (Note 6)
	<u>26,005</u>	<u>23,395</u>	Transfers from other Funds:
			General Fund
Balance at 1 January	26,377	36,042	<i>Excess of expenditure over income carried to the balance sheet</i>
Difference between income and expenditure	12,187	- 11,448	
Fluctuations in rates of exchange	- 2,450	1,783	
Balance at 31 December	<u>36,114</u>	<u>26,377</u>	
			1992
			1,005
			25,000
			<u>26,005</u>
			1991
			1,947
			10,000
			<u>11,448</u>
			<u>23,395</u>

International Tables Account for the year ended 31 December 1992

	Swiss Francs		Swiss Francs	
	1992	1991	1992	1991
Publication expenses:				
Reprinting Volume A	40,471	-	87,410	65,044
Typesetting Volume B	-	9,515	5,939	3,111
Printing and Typesetting Volume C	48,364	1,216	17,032	30,309
			121,674	-
			232,055	98,464
Editorial expenses:				
Editorial honoraria	8,465	8,085		
Secretarial assistance, postage and office equipment	12,354	23,444		
Technical Editing	15,430	35,867	60,334	25,600
			171,721	72,864
<i>Excess of income over expenditure carried to balance sheet</i>				
	46,637	-	-	5,263
	171,721	78,127	171,721	78,127
Balance at 1 January	129,062	125,600		
Difference between income and expenditure	46,637	-5,263		
Fluctuations in rates of exchange	-11,149	8,725		
Balance at 31 December	164,550	129,062		

Book Fund Account for the year ended 31 December 1992

	Swiss Francs			Swiss Francs	
	1992	1991		1992	1991
Publication expenses:			Transfer from <i>Molecular Structures and Dimensions</i> Fund	-	5,315
· Book series expenses	735	57	Sale of copies, net of		
· <i>Atlas of Crystallography</i>	1,183	16,136	· Publisher's commission on sales	4,550	6,776
· <i>World Directory of Crystallographers</i> ,			· <i>Atlas of Crystallography</i>	179	256
8th Edition	242	48,937	· <i>Crystallographic Databases</i>	389	-52
· Sundry publications	6	11	· <i>Escher Drawings</i>	99	30
			· <i>Early Papers</i>	124	39
			· <i>Fifty Years of Electron Diffraction</i>	22	66
			· <i>World Directory of Crystallographers</i> ,	382	1,381
			8th Edition		
			· <i>Molecular Structures and Dimensions</i>		
			Royalties		
			· <i>Escher Drawings</i>	400	400
			· Book series - IUCr Crystallographic		
			· Symposia	3,777	1,040
				4,177	1,440
<i>Excess of income over expenditure</i>	8,716	-			5,232
<i>carried to balance sheet</i>	10,882	65,141		10,882	65,141
Balance at 1 January	3,495	8,491			
Difference between income and expenditure	8,716	-5,232			
Fluctuations in rates of exchange	-776	236			
Balance at 31 December	11,435	3,495			

Research and Education Fund Account for the year ended 31 December 1992

	Swiss Francs			Swiss Francs	
	1992	1991		1992	1991
Expenses:			Transfers from other Funds:		
Young Scientists' Support	90,850	53,804	General Fund	150,000	100,000
1989 ECM Fund creditor	2,697	13,007	Interest (Note 6)	44,336	40,484
Visiting Professorship Programme	9,665	145			
IUCr publications	—	202			
		<u>67,158</u>			
<i>Excess of income over expenditure</i>					
<i>carried to balance sheet</i>	91,124	73,326			
	<u>194,336</u>	<u>140,484</u>		<u>194,336</u>	<u>140,484</u>
Balance at 1 January	657,412	539,640			
Difference between income and expenditure	91,124	73,326			
Fluctuations in rates of exchange	-47,547	44,446			
Balance at 31 December	<u>700,989</u>	<u>657,412</u>			

Ewald Fund Account for the year ended 31 December 1992

	Swiss Francs			Swiss Francs	
	1992	1991		1992	1991
Selection Committee and expenses	1,629	253	Transfers from other Funds:		
			Acta Crystallographica	20,000	15,000
			General Fund	19,173	15,567
			Interest (Note 6)		
<i>Excess of income over expenditure</i>					
<i>carried to balance sheet</i>	37,544	30,314			
	<u>39,173</u>	<u>30,567</u>		<u>39,173</u>	<u>30,567</u>
Balance at 1 January	241,294	194,720			
Difference between income and expenditure	37,544	30,314			
Fluctuations in rates of exchange	-17,712	16,260			
Balance at 31 December	<u>261,126</u>	<u>241,294</u>			

Cash Flow Statement for the year ended 31 December 1992

	1992	Swiss Francs 1991
Net cash outflow from operating activities	- 388,986	- 125,773
Returns on investments		
Interest received	62,520	89,851
Investment income	312,396	348,647
	374,916	438,508
Net cash inflow from returns on investments		
Investing activities		
Purchase of office equipment	- 5,680	- 3,917
Purchase of investments	- 1,568,914	- 1,197,533
Disposal of investments	1,717,825	633,090
	143,231	- 568,360
Net cash inflow/(outflow) from investing activities		
Increase/(decrease) in cash and cash equivalents before and after financing	129,161	- 255,625

Notes to the Financial Statements

1. Accounting Policies

(a) Accounting convention

The financial statements are prepared under the historical cost convention 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.

The revalued cost of fixed assets and investments referred to in the balance sheet and Note 4 to the accounts arises by applying this method.

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 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.

(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 of unsold copies of Union publications

Stocks of unsold copies of publications are not valued for accounting purposes.

(e) Expenditure on premises

Expenditure on renovation and refurbishing 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 fully depreciated in the year of purchase.

(g) Investment income

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

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. It therefore follows that the effect of fluctuations in exchange rates will normally only arise at the year end when the figures are reported in Swiss Francs.

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

	1992	1991
Netherlands Guilders	1.2500	1.2588
Danish Crowns	4.2918	4.3365
Pounds Sterling	0.4583	0.3951
US Dollars	0.6944	0.6993

The net assets of the Union at 1 January 1992 (SwFr 5,455,503) would have had the value of US \$3,815,033 or £2,155,469 if expressed in those currencies.

At 31 December 1992, these assets (SwFr 5,325,909) would have had the value of US \$3,698,311 or £2,440,864 respectively, being a decrease of US \$116,722 or an increase of £285,395 from the previous year.

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.

4. Investments

	Holding at revalued cost 1 January 1992	Additions during the year	Swiss Francs Disposals/ Redemptions during the year	Fluctuations in rates of exchange	Holding at revalued cost 31 December 1992
Held by Merrill Lynch					
(Corporate Government Securities)					
US \$20,692 GNM P146535-2016	28,803	-	- 5,240	52	23,615
US \$58,544 GNM P169332-2016	81,041	-	- 11,015	252	70,278
US \$150,000 US Treasury November 2004 (Mutual Funds/Unit Investment Trusts)	64,383	-	- 61,682	- 2,701	-
2,231 Units ML Capital Fund/CLB (US \$)	90,889	59,614	-	- 20,823	129,680
US \$4,750 Temple Worldwide Fund G	71,661	-	-	501	72,162
US \$4,750 Temple Worldwide Fund I	71,661	-	-	501	72,162
US \$785 Haussman Holdings	364,710	64,874	-	8,448	438,032
US \$5,139 Global Equity Portfolio (Certificates of deposit)	72,287	-	- 75,320	3,033	-
US \$50,000 FHLMC 8.5% Sep. 15 20RG	70,266	-	- 27,249	- 570	42,447
US \$50,000 CITI CDT Cards 8.25% Nov. 15 193	71,613	-	-	500	72,113
US \$75,000 British Gas France	110,275	-	-	771	111,046
US \$75,000 GEC	108,233	-	-	757	108,990
US \$8,000 MLST World income portfolio	114,772	-	-	802	115,574
Held by Foreign & Colonial					
34,298 Units Reserve Asset Fund Class D (US \$)	897,650	31,578	- 437,288	- 15,305	476,635
11,964 Units Reserve Asset Fund Class L (£)	291,849	208,014	- 8,439	- 68,569	422,855
43,064 Units Reserve Asset Fund Class O (US \$)	784,239	-	- 796,612	12,373	-
11,026 Units Reserve Asset Fund Class X (£)	278,377	450,047	- 200,521	- 58,382	469,521
17,617 Units Reserve Asset Fund Class H (ECU)	353,322	31,407	- 12,043	- 25,354	347,332
20,929 Units Reserve Asset Fund Class C (US \$)	-	445,458	-	22,761	468,219
11,080 Units Reserve Asset Fund Class M (US \$)	-	277,922	-	- 7,758	270,164
Held by National Westminster Bank					
£400,000 (1991 £458,933) cash on one year deposit	1,161,560	-	- 149,042	- 139,718	872,800
	<u>5,087,591</u>	<u>1,568,914</u>	<u>- 1,784,451</u>	<u>- 288,429</u>	<u>4,583,625</u>

Investments are noted in the balance sheet at their market value at 31 December 1992. The difference between revalued cost and market value has been shown as an adjustment in order that the investments can be stated at revalued cost. This prevents the fluctuations in market value from influencing the General Fund.

The revalued cost is obtained by converting the cost of investments in the currencies of purchase into Swiss Francs using the exchange rates operative on the balance sheet date.

Included in investments above is SwFr 872,800, which is invested in a one year bank deposit account at National Westminster Bank, Jersey which is due to mature on 31 August 1993. It is the intention of the officers of the Union to reinvest this money on maturity. This money is not considered to be part of the general deposit and savings accounts available as day to day working capital of the Union and has therefore not been included within the current assets of the Union.

5. Bank Interest

	Swiss Francs	
	1992	1991
National Westminster Bank PLC		
Manchester SMMO Account	10,545	47,935
Manchester Business Reserve Account	7,600	6,678
Manchester Capital Reserve Account	10,111	-
Amsterdam-Rotterdam Bank NV		
Current Guilder Account	4	14
Guilder Savings Account	35	84
US \$ Account	6	14
Union Bank of Switzerland		
Current Swiss Francs Account	28	-
Merrill Lynch		
CMA Account	3,558	8,308
Foreign & Colonial		
Cash balances	149	211
Interest from Munksgaard	30,484	26,607
	<u>62,520</u>	<u>89,851</u>

6. Investment Income

	Swiss Francs			Swiss Francs	
	1992	1991		1992	1991
GEC	8,121	1,766	Allocated to President's Fund	1,005	1,947
British Gas	9,220	777	Allocated to Ewald Fund	19,173	15,567
ML Capital Fund	8,437	4,082	Allocated to Publication and Journals		
P146535-2016	2,429	2,677	Development Fund	44,134	49,011
P169332-2016	6,994	7,850	Allocated to Research and Education Fund	44,336	40,484
Temple Worldwide Fund G	5,942	6,177	Balance left in General Fund	203,748	241,648
Temple Worldwide Fund I	4,583	8,130			
Foreign and Colonial Fund M	7,872	-			
Foreign and Colonial Fund H	31,407	25,037			
Foreign and Colonial Fund X	54,004	37,128			
Foreign and Colonial Fund D	31,578	67,329			
Foreign and Colonial Fund L	16,985	8,780			
Foreign and Colonial Fund O	-	19,705			
FHLMC	5,738	6,059			
MLST World income portfolio	7,080	7,535			
CITI CDT Cards	5,827	5,881			
National Westminster Bank deposit account	106,179	139,744			
	<u>312,396</u>	<u>348,657</u>		<u>312,396</u>	<u>348,657</u>