

International Union of Crystallography

Report of the Executive Committee for 1991

Meetings

The IUCr sponsored the following meetings held during 1991:

1. First European Powder Diffraction Conference, Munich, Germany, 14-16 March 1991.
2. Intensive Course in X-ray Structure Analysis, Aston, England, 18-24 March 1991.
3. International Workshop on Methods of Structure Analysis of Modulated Structures and Quasicrystals, Bilbao-Lekeitio, Spain, 29 April-4 May 1991.
4. Third European Conference on Crystal Growth, Budapest, Hungary, 5-11 May 1991.
5. Second European Workshop on Crystallography of Biological Macromolecules, Como, Italy, 13-16 May 1991.
6. International Workshop on Magnetism, Magnetic Materials and Their Applications, La Habana, Cuba, 21-29 May 1991.
7. 18th Course 'Static, Kinematic and Dynamic Aspects of Crystal and Molecular Structure', Erice, Italy, 30 May-9 June 1991.
8. International Conference on Polytypes, Modulated Structures and Quasicrystals, Balatonszékplak, Hungary, 20-24 August 1991.
9. Thirteenth European Crystallographic Meeting, Trieste, Italy, 25-30 August 1991.
10. Conference on Charge, Spin and Momentum Densities, Konstanz, Germany, 1-7 September 1991.
11. Summer School on Neutron Scattering, Oxford, England, 17-27 September 1991.
12. International School on Materials for Electronics: Growth, Properties and Applications, Trieste, Italy, 18 November-6 December 1991.

The Executive Committee met in Chester, England, in August. The Finance Committee met twice, also in Chester, in March and then in August 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 and other matters concerning the IUCr journals;
- (2) publication of a new Section (Section D) of *Acta Crystallographica* on Biological Crystallography;
- (3) appointment of new staff in the IUCr office in Chester;
- (4) upgrading of office technology in the IUCr office in Chester and expansion of this office;
- (5) future of *Structure Reports* and its cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre;
- (6) developments of the STAR file, the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* papers and other uses of CIF;
- (7) progress with Volumes B and C of *International Tables*;

- (8) establishment of an international crystallographic newsletter;
- (9) approval of the audited accounts for the previous year;
- (10) the General Fund estimates and the level of the unit contribution;
- (11) investment policy;
- (12) funding and uses of the Publications and Journals Development Fund and the Research and Education Fund;
- (13) appointment of the Selection Committee for the third Ewald Prize;
- (14) sponsorship and financial support for meetings, including young scientists' support;
- (15) discussion of the arrangements for the Beijing General Assembly and Congress;
- (16) review of the activities of the Commissions.

Publications

Volume 47 of *Acta Crystallographica* and Volume 24 of the *Journal of Applied Crystallography* were published, as were Volume 56A of *Structure Reports* and the Eighth Edition of the *World Directory of Crystallographers*.

Adhering Bodies

A recent 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].

Work of the Commissions

Commission on Journals

Volume 47 of *Acta Crystallographica* (*Acta*) was published in 1991, and included a total of 1336 papers (a 7% increase from 1990) received from 50 countries, with an overall total of 4630 pages. Manuscripts received by Co-editors continued to increase, with 1465 papers received in 1991.

The average lengths of full articles in *Acta A* and *Acta B* in 1991 increased to 7.2 and 7.4 pages, respectively, while *Acta C*'s full articles and Short Format papers showed little change at 2.7 and 1.8 pages. Median publication times for these full articles, the average elapsed time between the published acceptance and nominal publication dates, were 5.2 months for *Acta A*, 5.8 months for *Acta B* and 7.0 months for *Acta C*. The median publication times for *Acta A* increased as a result of its appearing bimonthly in 1991. *Acta B* continued to increase in size, with a corresponding slight increase in publication time. The clearing of a backlog of *Acta C* papers contributed to a decrease in its publication time. Median publication times in 1991 for Short Communications were 4.8 months for *Acta A*, 6.1 months for *Acta B* and 6.1 months for *Acta C*. The median publication times

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

<i>Acta Crystallographica</i>											
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
A43†	1987	840	128	114	6.5	—	—	14	1.3	27	1.1
B43		584	100	91	6.3	—	—	9	0.9		
C43		2472	995	817	2.7	174	1.7	4	0.9		
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	1.7	391	1.8	7	0.6		

Journal of Applied Crystallography

Vol.	Year	Number of Pages*	Number of Papers	Full Articles		Short Communications		Fast Communications (from 1990) Crystal Data (1986–1989)		Computer Programs		Short Items§	
				Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length
20	1987	538	105	70	5.7	12	2.0	4	0.5	15	3.1	4	0.6
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

* Excluding indexes

† Volume A43 includes, in addition, 360 pages of abstracts communicated to the Perth Congress.

‡ 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 on Small-Angle Scattering, Leuven, Belgium, 1990.

for Fast Communications papers in *Acta A* and *Acta B* were 1.8 and 1.3 months, respectively, and for Short Format papers in *Acta C* 6.1 months.

A total of 53 inorganic, 13 organometallic and 62 organic papers appeared in Section B in 1991, compared with 47, 13 and 63, respectively, in 1990. The distribution of papers in Section C was 115 inorganic, 358 organometallic and 603 organic in 1991, compared with 128 inorganic, 294 organometallic and 557 organic articles in 1990.

The number of papers published for Volume 24 of the *Journal of Applied Crystallography (JAC)* in 1991 was 176, compared with 105 for 1990, reflecting the appearance of the Small-Angle Neutron Scattering special issue. The number of pages was 1102 (560 in 1990) and the median publication time for full articles was 7.0 months (5.6 months if the SANS issue is excluded).

The average length of full articles in *JAC* was 5.7 pages in 1991, compared with 5.6 pages in 1990. The average length for Short Communications and Computer Programs

was 2.3 pages in 1991, compared with 2.0 pages in 1990. Papers were received from 30 countries.

The Executive Committee approved the establishment of the new Section D of *Acta Crystallographica*, entitled *Biological Crystallography*. The initial publication date is January 1993. Dr Jenny P. Glusker of The Fox Chase Cancer Center in Philadelphia will serve as Editor of *Acta D*.

Angelo Gavezzotti and Hans Burzlaff retired as *Acta* Co-editors at the end of 1991, after handling a total of over 900 manuscripts during their terms. Mario Nardelli joined as Co-editor of *Acta*, following his retirement as President of the IUCr.

Commission on Structure Reports

Volume 56A (Metals and Inorganic Compounds for 1989; 293 pp.) was published in 1991. Volumes 57A (Metals and Inorganic Compounds for 1990; 339 pp.) and 51B (Organic Compounds for 1984; 2094 pp.) were sent to the printer in 1991. Work is nearing completion on Volume 50B (Organic

Compounds for 1983) and is well in hand for Volume 52B (Organic Compounds for 1985). The final stages of the preparation of the 10-year Index, Volume 47B, are in progress.

Commission on International Tables

No meeting of the Commission was held during 1991. Detailed reports on the individual volumes are given below.

Volume A (Space-Group Symmetry; Editor Th. Hahn)

Work on the subgroups of space groups continued throughout the year; new ways of presenting and extending the subgroup data in Volume A received particular attention.

New thoroughly re-designed diagrams for the cubic space groups were completed in December 1991. They contain, among other improvements, new symbols for the 'inclined' two- and threefold axes; explicit graphical indication of the horizontal $\bar{4}$ axes (instead of their twofold 'subaxes'); complete sets of 'heights' (as fractions) for the horizontal fourfold axes and the $\bar{4}$ inversion points in the cubic systems, as well as for the symmetries $4_2/m$ and $6_3/m$ in the tetragonal, hexagonal and cubic space groups.

The third edition of Volume A, with many revisions, went to press in January 1992.

Volume B (Reciprocal Space; Editor U. Shmueli)

Some progress was achieved during 1991 in the preparation and processing of the proofs of the various Chapters and Sections of Volume B.

The transmission of corrected galley proofs to the Technical Editor was completed during the spring of 1991. The page proofs of all the Chapters and Sections of Parts 1 and 2 of Volume B were prepared, received and distributed among the authors by the Technical Editor and his staff. All the authors but one submitted to the Editor corrected page proofs, usually accompanied by suggested indexing terms.

The main editorial activity during the year was related to checking the various proofs and to related correspondence.

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

The making up of the galley proofs into page proofs was completed early in the year and Volume C went to press in December 1991.

The nature of the volume, consisting of many sections on very diverse subjects, has required more detailed indexing than has been usual in earlier volumes, and it has been necessary to adopt a smaller type size and a more condensed format. For the first time there is a name index (11 pages in four columns), and the subject index occupies 17 pages in three columns.

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

At the invitation of the Editor, a working party of nine persons met in Paris in June 1991. This group defined the outline of the volume, which will consist of three parts (Part 1: Tensorial Aspects of Physical Properties; Part 2: Symmetry Aspects of Excitations; Part 3: Symmetry Aspects of Structural Phase Transitions. Twinning and Domain Structures). This outline and a preliminary list of potential

authors were accepted by the Executive Committee at its August 1991 meeting. It is planned that the first drafts of papers should be ready by the end of 1992 and that their harmonization should be completed by the end of 1993, so that the volume could be sent to the Technical Editor in 1994.

It is planned that detailed tables giving the irreducible representations of the point groups and the magnetic groups, the independent components of tensors up to the sixth rank in the same groups, as well as the relationships between tensor components in equivalent twin domains, will be accessible *via* software on a diskette which will accompany the volume.

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

Volume E consists of three parts: Part 1: Subperiodic Group Tables: Frieze Groups, Rod Groups, and Layer Groups; Part 2: Subperiodic Groups and their Relationship to Space Groups; Part 3: Symmetry of Planes in Crystals.

Part 1 is complete, except that the diagrams have not as yet been professionally drawn. It is anticipated that this part will soon be sent to Professor Hahn, who has agreed to read the manuscript of Volume E for consistency with Volume A in nomenclature, style and presentation.

Part 2 is nearing completion and Part 3 is partially done. Computer-system incompatibilities arose on the move of one of the Editors to Fiji and have caused some delays; these difficulties have now been rectified.

Commission on Biological Macromolecules

The determination of protein and macromolecular structures continues to be carried out successfully in an increasing number of laboratories throughout the world. The most spectacular among many achievements are the structure determinations of the SV40 polyoma virus and the complex between the growth hormone and its receptor.

The success in protein crystallography and the general acceptance of data deposition created a bottleneck at the Brookhaven Protein Databank and necessitated a review of the data deposition procedures. This flood of structures led to the appearance of an annual volume *Macromolecular Structures*, in which all published structures are reviewed briefly and their crystallographic details listed. This is proving to be a popular and desirable development. There is also increasing publication in *Acta Crystallographica* and the decision to begin a new section of that journal on Biological Crystallography will meet some of the demands for journals for macromolecular crystallography.

The concerns that published macromolecular structures should be crystallographically sound has been widely recognized. There is growing use of various criteria which are being included in papers submitted for publication. As yet there is no simple universal formula for correctness, and the range in data quality and resolution will always make this difficult.

Commission on Charge, Spin and Momentum Densities

The Commission has continued to encourage all activities devoted to the accurate determination of density distributions in position and momentum space, where this promotion is not restricted to the crystallographic community but includes physicists and chemists who are interested in

fundamental problems of the ground-state properties of condensed matter. This widespread activity is in accordance with the main aim of the Commission, namely to bring together crystallographers whose principal interest is to investigate chemical bonding with scientists of those fields of physics and chemistry which are contributing to the fundamental understanding of bonding both from the quantum-theoretical point of view and from the different experimental methods providing access to this problem.

The most important activity of the Commission in 1991 was the organization of the Xth Sagamore Conference, held 1-7 September in Konstanz, Germany, with the Commission acting as the Programme Committee.

The topics of the Conference covered the main more classical fields of the Commission's activity, such as electron and spin densities in position and momentum space in relation to solid-state properties both theoretically and experimentally. Experimental developments were emphasized, such as magnetic photon scattering by utilizing the unique properties of synchrotron-radiation sources, the application of positron annihilation to momentum density and Fermi-surface topology of high- T_c superconductors. Special attention was paid to the problem of the dynamics of ground-state properties (dynamic structure factor), with respect to both electrons and ions in crystalline solids and the problem of reconstructing quantum-mechanical quantities, e.g. density matrices, from experimental data.

The Commission held two business meetings during the Sagamore Conference. The main topics of these meetings were organizing further activities (Gordon Conference 1992, Beijing IUCr Congress 1993 and XIth Sagamore Conference 1995) and collecting information about the progress of current Commission projects.

There was widespread interest in the Commission project on quantum-mechanical description of electronic structure from experimental charge and momentum densities, documented by a long list of persons who offered to take part in the project, which has led the promotor of the project, W. Weyrich, to agree to organize annual meetings at Konstanz dedicated to this topic.

Commission on Crystal Growth and Characterization of Materials

Work has continued on previously planned projects and organizational work for future initiatives has also been undertaken.

During the European Crystallographic Meeting (ECM-13), the Commission organized a Microsymposium on Crystal Growth, to present and discuss various aspects of crystal growth and characterization of materials and promote closer relationships between the crystallographic and crystal-growth communities. Emphasis was placed on organic crystals, materials which are of increasing interest for their applications in many fields.

The most important activity of the Commission during the year concerned the organization of a School in Trieste for young scientists of developing countries. The International School on Materials for Electronics: Growth, Properties and Applications was held 18 November-6 December and was attended by 67 participants from 28 countries, selected from more than 400 applicants.

The Commission has also helped organize the Third European Conference on Crystal Growth (ECCG-3),

Budapest, 5-11 May, with the sponsorship of the Union and the approval of the IOGG. The proceedings of the International School on Crystal Growth and Crystallographic Assessment of Industrial Materials (organized by the Commission in Sitges, Spain, in 1990) were published under the title *Crystalline Materials: Growth and Characterization* (1991), edited by R. Rodriguez-Clemente & C. Paorici, Zurich: Trans Tech Publications.

Commission on Crystallographic Apparatus

During 1991, a number of existing projects have continued and planning has progressed on other projects.

1. *The X-ray Attenuation Project (D. C. Creagh)*. The publication of Volume C of *International Tables for Crystallography*, which contains the tables of absorption coefficients and dispersion corrections, brings to an end work on this project. The tables are a theoretical compilation rather than a compilation of experimental results, because the experimental results are fragmentary and inaccurate. Sooner or later an effort has to be made to obtain good experimental data.

2. *Single-Crystal Lattice-Parameter Project (G. De Titta)*. This project is going forward but it is not progressing as rapidly as was hoped. It is, however, a difficult project to organize and results may only be forthcoming in the next triennium.

3. *The Accuracy in XAFS Project (H. Hashizume, R. Fourme and D. C. Creagh)*. The aim of this project was to set up standard procedures for use in XAFS experiments. Two reports on standard procedures of XAFS have now been produced by the XAFS community [the latest publication being *Physica (Utrecht)* (1989), B158, and *X-ray Absorption Fine Structure* (1991), edited by S. S. Hasnain, New York: Horwood] and some additional comments have been incorporated in Section 4.2.3. X-ray Spectroscopy in *International Tables for Crystallography*, Vol. C (1992). Crystallographers should note that negotiations with the National Nuclear Data Centre at NSLS, Brookhaven, have resulted in the setting up of an XAFS data centre. Enquiries as to how to use this data set should be made through the Director of the NNDC, Dr S. Pearlman. In 1992, at the XAFS VII Conference (Kobe, Japan), decisions will be taken as to the future of the XAFS organization. The major decision to be made is whether the XAFS body wishes to remain as a separate entity, in much the same form as it is at present, or whether it should apply to become a Commission of the IUCr.

4. *Evaluation of Two-Dimensional Detectors*. Investigations are still under way to determine whether it would be possible to create a system for setting up criteria for satisfying and evaluating the data performance of area detectors of all kinds. Considerable input to this project has been given by Russian groups, whose contributions have been coordinated by L. Malakhova.

5. *X-ray Diffraction at High Pressures (R. Nelmes)*. This group within the Commission has been extremely active and very effective in undertaking its tasks. It ran a very successful workshop at SERC Daresbury in conjunction with the Synchrotron Radiation Instrumentation Conference, Chester, England, in July 1991. It is also planning to hold a workshop in the USA in May 1992, to be organized by Dr L. Finger in collaboration with the Commission on Powder Diffraction. The group is also actively involved in

the organization of Microsymposia and Plenary Lectures at the Beijing IUCr Congress.

6. *Absolute Light-Atom Structure Determination (L. Malakhova)*. Professor Malakhova is in the early stages of organizing a collaborative venture involving a number of laboratories within Russia and Europe, at this stage to determine light-atom structures using anomalous-dispersion and three-beam techniques. It is hoped that this project will commence in the next triennium and that the results might be available at the end of that triennium.

Commission on Crystallographic Computing

The following list gives the main activities of the Commission during 1991.

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

(2) Detailed planning of the Veszprém School on Crystallographic Computing to be held in Balatonfüred, Hungary, 1-7 June 1992 was carried out. The local organizing committee of this school is chaired by Dr K. Simon. The Commission acts as the core of the international Programme Committee. The Commission Chairman visited the proposed site and the members of the Organizing Committee. The School site has been changed from Veszprém to Balatonfüred for organizational reasons.

(3) Planning of a School on Crystallographic Computing initially to be held in Shanghai, China, as a satellite meeting to the XVI IUCr Congress with local Organizing Committee headed by Professor Zheng Pei-ju were continued. In June 1991, the Commission Chairman learnt of the resignation of Professor Zheng Pei-ju. A replacement site (Hefei) and a new Organizing Committee Chairman (Professor Fan Cheng-gao) have been contacted. The Commission will act as the core of the international Programme Committee and as a source of organizational advice and contacts. Owing to the change of site, the planning of this School is not as advanced as usual.

(4) Attempts to instigate a world-wide bulletin board for crystallographic news were continued.

Commission on Crystallographic Data

The activities of the Commission in 1991 have centred around the completion of the core version of the Crystallographic Information File (CIF) and its implementation for machine-readable submissions to *Acta Crystallographica*. Data-name definitions were finalized and a data-name dictionary was constructed. A manuscript describing the CIF was prepared and published in *Acta Cryst.* (1991), A47, 655-685. Further extensions of CIF to cover powder data and additional specific requirements of macromolecular crystallography are currently being examined by subject experts. Results will be published in due course. Integration of the CIF with the standard molecular data (SMD) format is in abeyance whilst the future of the SMD project is decided by the Chemical Structure Association.

As part of the finalization of the CIF core, a CIF generated by the XTAL system was used to test the in-house data checking and desktop publication systems at the IUCr Editorial Offices in Chester. As a result, the paper published in *Acta Cryst.* (1991), C47, 2276-2277 was generated automatically from CIF input.

The new procedures for CIF submissions to *Acta Cryst.* were summarized in an Editorial written in collaboration with the Commission on Journals and the Working Party

on Crystallographic Information. The Commission also assisted in the drafting of new *Notes for Authors* which embody CIF procedures.

The Commission is now keen to encourage developers of software packages for crystal structure determination to include CIF generators within new software releases. Indications are that a CIF generator will be included in future releases of *SHELX* and *SHELXTL*.

Commission on Crystallographic Nomenclature

Membership of the Commission increased sharply following the XV General Assembly. All members are *ex-officio* appointments as Editors of the Union's journals, each volume of *International Tables* and *Structure Reports*. In addition, the Chairmen of the IUCr/OUP Book Series Committee and the Commission on Crystallographic Teaching are now also members *ex officio*, to give a total strength of 11 members.

The primary work of the Commission in 1991 was conducted by its *ad hoc* Committee on the Nomenclature of Symmetry, its Subcommittee on the Nomenclature of *N*-Dimensional Crystallography, and by the Editors of Volume E of *International Tables*. The *ad hoc* Committee completed its report entitled *Symbols for Symmetry Elements and Symmetry Operations*. The report, which recommends use of several new or redefined printed symbols for symmetry elements, was accepted in December 1991 by the Commission and sent to the Executive Committee for final approval and publication in *Acta Cryst.*

The Subcommittee set up a Working Group with the limited task of comparing and evaluating the existing nomenclatures of crystal families, crystal systems and Bravais lattices in four dimensions followed by the presentation of a recommended nomenclature. The first task was completed late in 1990; however, an agreed choice between alternative nomenclature systems has not yet been reached.

The editors of Volume E of *International Tables*, V. Kopsky and D. B. Litvin, have proposed new recommendations for the Nomenclature, Symbols and Classification of the Subperiodic Groups for consideration by the Commission, since the IUCr was not previously concerned with subperiodic groups and their symbols and nomenclature. By the end of 1991, an advanced revision of these recommendations had been prepared. A final version for Commission approval is expected soon.

A proposal to study the variety of mathematical symbols used in the crystallographic literature to denote identical operations, followed by the preparation of a single recommended set of symbols, was received. In view of the extensive standards provided in *Mathematical Signs and Symbols for use in the Physical Sciences and Technology* (ISO/X1) and IUCr policy of following relevant nomenclature standards already adopted by other major international bodies, the proposal was not approved.

Commission on Crystallographic Teaching

The main activities of the Commission in 1991 were:

1. *The IUCr Visiting Professor Programme*. Information on this programme is being circulated widely to many countries through their National Committees for Crystallography. Different countries and organizations have their own specific requirements for input of crystallographic teaching. C. H. L. Kennard was a visiting Professor at the

University of Peradeniya, Sri Lanka. There were approximately 40 students involved in his course. A Visiting Professor was planned for the University of Hanoi but visa delays made this impossible. The idea will be reconsidered at a later date if the visa situation improves. Dr Ward Robinson will be a Visiting Professor at the Institute of Applied Chemistry and Jilin University, China, in May 1992.

2. *Teaching Schools*. Sponsorship for a Beginner's School on Powder Diffraction in 1993 is under consideration.

3. *Pamphlet Programme*. The Pamphlet series is being revived and several pamphlets are now being written. A list of instructions to pamphlet writers is being made. Copies of the first 19 pamphlets may be obtained from Polycrystal Book Service, Box 3439, Dayton, Ohio 45401, USA.

4. *ICSU Teaching Programme*. The Chairman, J. P. Glusker, attended a meeting of the ICSU Committee on the Teaching of Science in Paris in May 1991. It was very useful to find out how other Teaching Commissions disseminated information.

Commission on Electron Diffraction

The Commission project to produce a book, *Electron Diffraction Techniques*, has progressed slowly but is reaching a conclusion, with considerable modification imposed by the large amount of material submitted and delays by some authors. The work will now appear in two volumes. Volume 1 has been submitted to the publishers in camera-ready form and should appear before the end of 1992. A somewhat smaller Volume 2 should follow soon after, if the tardy authors finish their nearly complete chapters. These volumes will be published in the IUCr Monographs on Crystallography Series by Oxford University Press.

An on-going survey of computer programs used for the calculation of intensities of electron diffraction patterns and high-resolution images is being conducted by D. Van Dyck on behalf of the Commission.

Plans are well advanced for a Summer School to be held in Beijing in 1993, in the week prior to the IUCr Congress. The topic will be Electron Crystallography, but limited to the determination of the structures of crystals and gas molecules by use of high-energy (10 keV or more) electrons using diffraction modes. The topics of low-energy electron diffraction, other techniques for surface study and high-resolution electron microscopy have become too broad to include within the Summer School programme, but it is anticipated that they will be well represented within the programme of the IUCr Congress.

The Commission welcomes M. Van Hove from Berkeley, USA, as a new member of the Commission to represent low-energy electron diffraction and associated areas.

Commission on Neutron Diffraction

The Commission proposes to organize or sponsor a number of Microsymposia at the 1993 IUCr Congress, including some in common with other Commissions. Just prior to the Congress, there will be a satellite meeting on neutron scattering.

During 1991 some initiatives of the IUCr Executive Committee were discussed by the Commission and, with certain modifications, were strongly approved. One concerned a major database of all crystallographers which, as well as allowing more flexible updating of the *World Directory of Crystallographers*, could be used by conference organizers

and for informal contacts between scientists. Another was to produce an IUCr Newsletter which would include some of the Commission Newsletters.

A mailing list of neutron diffractionists maintained by the Commission was supplied to several conference organizers during the year. (Enquiries to mason@frill.bit-net). It was updated from the much larger list used for distribution of *Neutron News*, kindly made available by the publishers.

Neutron News, edited by G. Lander, continues as the outstanding means of communication with neutron scientists everywhere. Although its audience is much wider than our diffraction community, we have a special relationship with *Neutron News* and the Commission Chairman contributes regularly to it.

Present and former Commission members contributed to a teaching course known as Hercules and based at several European reactors and synchrotrons. In this programme about 50 graduate students and post-doctoral workers from many countries spent nearly two months in theory lectures and hands-on experiments with X-radiation and neutrons. A Workshop on Neutron and Synchrotron Radiation Studies of Materials at Brookhaven in May 1992 is also aimed at scientists wishing to use the wide range of techniques available at modern user facilities for materials characterization. The Commission wishes to encourage any such initiatives which emphasize the complementarity of neutrons and other radiations.

Commission on Powder Diffraction

During 1991, the Commission was actively involved in several projects and in planning and preparations for future meetings and workshops/schools.

Publications. The project of establishing a Program Information Exchange Bank on computer programs for powder diffraction data analysis has been conducted by D. K. Smith, Consultant to the Commission. The first phase of this project came to fruition with the publication of a categorized and annotated list of more than 280 programs with informative discussion of each category as *Powder Diffraction Program Information 1990 Program List* in *J. Appl. Cryst.* (1991), **24**, 369–402. Periodic updates are intended.

The first phase of the Rietveld Refinement Round-Robin Project (R. J. Hill) has been completed and published in *J. Appl. Cryst.* (1992), **25**, 589–610. 23 participants provided the results included in this publication, which were for 18 refinements with X-ray data and 20 with neutron data, using 11 different Rietveld analysis programs.

The manuscripts for a multi-author book, *The Rietveld Method*, were given to Oxford University Press at the end of 1991, for publication in the IUCr Monographs on Crystallography Series.

Two Commission Newsletters appeared in 1991; no. 6 in May and no. 7 in November.

Powder diffraction database format. The Commission recognizes that a single universally accepted format/system for archiving and exchanging powder diffraction data of all kinds is highly desirable. The CIF/STAR system is being used by the IUCr for other crystallographic data. It is highly acclaimed by those who have reviewed it for potential use with powder diffraction data. Therefore, the Commission is working with other groups to develop the dictionaries and other items needed for such use and to encourage adoption of the resulting powder diffraction subset of the

CIF/STAR system by all who produce, store and use powder diffraction data.

Future meetings and workshops or schools. The Commission did much preparatory work in 1991 for events to take place in 1992 and 1993. These are (1) a Meeting on Accuracy in Powder Diffraction, Gaithersburg, USA, 26–29 May 1992; (2) a Summer School on the Rietveld Method, Cieszyn, Poland, 13–15 August 1992; (3) possible similar schools on the Rietveld Method in Brazil and Argentina; (4) a Fourth International Workshop on Crystallography, Aswan, Egypt, 16–26 January 1993 and (5) a Satellite Meeting on Powder Diffraction, Hangzhou, China, 31 August–2 September 1993, in connection with the XVI IUCr Congress in Beijing. Plans for a workshop or school in South Africa in 1991 have had to be abandoned.

Commission on Small Molecules

During 1991, the Commission proceeded with plans for future symposia mentioned below. The Symposium on Biomolecular Structure and Dynamics, scheduled to be held in Yugoslavia in September 1991, was cancelled because of the hostilities. One issue of the Commission newsletter was distributed in 1991. Although the Commission continues to maintain its programme of the international cooperation in the Intensity Data Collection Project, few requests for assistance were received in 1991.

The VIII Symposium on Crystal Chemistry will be held in Rydzyna, Poland, 26–30 July 1992. A Symposium on Molecular Structure will be held in Fuzhou, China, 30 August to 1 September 1993, as a Satellite Meeting of the XVI IUCr Congress in Beijing.

A Symposium entitled Toward the Small Molecule Crystallography of the 21st Century will be held in conjunction with the 1994 meeting of the American Crystallographic Association in Atlanta, Georgia. F. H. Herbststein has developed an extensive outline for a symposium with published proceedings that would summarize the accomplishments and strengths of the field of small-molecule crystallography and identify future directions. Major topics of the symposium include molecular structure and properties, real crystals as revealed by detailed diffraction studies, and the crystal as a dynamic system and a physical framework.

Commission on Synchrotron Radiation

The Commission has had a very active year in organizing meetings, in its Global Instrumentation Survey and in actively participating in discussions on the possibility of starting a *Journal of Synchrotron Radiation*.

A satellite meeting was organized in Trieste as an adjunct to ECM-13 entitled Synchrotron Radiation in Crystallography. It included a visit to the site of the ELETTRA machine, under construction in Trieste. A detailed report on the meeting is being published in *Synchrotron Radiation News*. A Satellite Meeting to the XVI IUCr Congress will also be held in August 1993.

The Global Instrumentation Survey is now coming to fruition. The details of the survey for macromolecular crystallography are now in press in *Synchrotron Radiation News*. The surveys for materials-science crystallography, EXAFS and fibre diffraction are at an advanced stage. The information collected has already been provided to a number of representatives and funding bodies.

Ad Interim Commission on Aperiodic Crystals

In April 1991, the IUCr Executive Committee approved the establishment of the Commission on an *ad interim* basis with the membership of J. M. Perez-Mato (Chairman), G. Chapuis, M. Farkas-Jahnke, M. L. Senechal and W. Steurer. It replaces the earlier *ad interim* Commission on Modulated Structures, Polytypes and Quasicrystals. Its terms of reference are as follows:

In the following by 'crystal' we mean any solid having an essentially discrete diffraction diagram, and by 'aperiodic crystal' we mean any crystal in which three-dimensional lattice periodicity can be considered to be absent. As an extension, the latter term will also include those crystals in which three-dimensional periodicity is too weak to describe significant correlations in the atomic configuration, but which can be properly described by crystallographic methods developed for actual aperiodic crystals.

(1) To promote the development of common methods and nomenclature for the crystallographic investigation of aperiodic crystals, including modulated structures, polytypes, incommensurate misfit or composite crystals, and quasicrystals.

(2) To promote and coordinate scientific interchange among groups working in the field of incommensurate structures, quasicrystals, polytypes and periodic crystals in general. In particular, to promote the dissemination of the existing methods for structural analysis, and support the development of new ones.

(3) To promote the exchange of adequate samples and/or experimental data sets of these crystals, so that they can be made available to a larger number of groups.

(4) To cooperate with the Commission on Crystallographic Nomenclature and other interested groups in the development of a standard nomenclature for dealing with higher-dimensional descriptions of aperiodic crystals.

(5) To promote cooperation between crystallographers working on aperiodic crystals and mathematicians working in the field of high-dimensional symmetry groups and/or aperiodic systems, and to stimulate the development of mathematical crystallography.

(6) To promote knowledge among crystallographers of superspace or high-dimensional-space methods as tools which can also be used to advantage in investigation of certain periodic crystal structures.

(7) To cooperate with other Commissions of the IUCr in establishing adequate guidelines and standards for articles to be published in IUCr journals reporting structural investigations of aperiodic crystals and theoretical investigations of aperiodic patterns.

(8) To promote and coordinate scientific meetings dealing with aperiodic crystals; in particular to continue the triennial series of meetings begun by the preceding Commission.

(9) To advise the IUCr on organizing or sponsoring sessions on aperiodic crystals and/or high-dimensional crystallography at Congresses.

During the year the Commission actively supported and helped organize two meetings. In April–May 1991, in Lekeitio, Spain, there was an International Workshop on Methods of Structure Analysis of Modulated Structures and Quasicrystals, which focused on the methods of struc-

ture determination of both incommensurate structures and quasicrystals. In August 1991, also under the auspices and support of the Commission, MOSPOQ 91 (International Conference on Polytypes, Modulated Structures and Quasicrystals) was held in Balatonszék, Hungary, in which the whole field of aperiodic crystals was represented with a multidisciplinary viewpoint. Both meetings were attended by more than 100 participants. On both occasions a majority of the members of the Commission were present and met to discuss its activities.

Following its terms of reference, the Commission has initiated plans for an international meeting on Aperiodic Crystals in Lausanne, Switzerland, in 1994. This meeting will continue and substitute for, on a triennial basis, the previous MOSPOQ meetings.

At the moment, the elaboration of a set of guidelines about the contents to be included in structural reports of incommensurately modulated structures and incommensurate composite crystals is a priority task. The Commission is also preparing a mailing list of all people interested and working in the field of aperiodic crystals. Personal requests to the Commission for inclusion on this mailing list are welcomed.

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 1991 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1991 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1992, but approved in 1991, are listed below:

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. Fourth 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. 1992 Gordon Research Conference on Electron Distribution and Chemical Bonding, Plymouth, New Hampshire, USA, 20–24 July 1992.
7. Symposium on Organic Crystal Chemistry, Poznan, 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. 1992 ACA Meeting, Pittsburgh, Pennsylvania, USA, 9–14 August 1992.
11. Eighth International Summer School on Crystal Growth, Palm Springs, California, USA, 9–14 August 1992, and Tenth International Conference on Crystal Growth, San Diego, California, USA, 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. Inaugural Conference of the Asian Crystallographic Association, Singapore, 13–16 November 1992.

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, Department of Chemistry, State University of New York at Buffalo, Acheson Hall, Buffalo, NY 14214, USA.

Applications for sponsorship of satellite meetings must be submitted through the Chairman of the Organizing Committee of the main meeting.

Regional Associates and Scientific Associates

American Crystallographic Association (ACA)

The ACA held its annual meeting in Toledo, Ohio, 21–26 July. There were a record 450 presentations at this meeting which honored Dr J. D. Dunitz of ETH-Zentrum, Zurich, with the Martin Burger award and Dr J. D. Jorgensen of Argonne National Laboratory with the B. E. Warren Diffraction Award.

Partly to recognize their new status as a Regional Associate, the ACA is in the process of revising their bylaws to include specifically representation from member countries. As an interim measure, the ACA Council has included representation from the Canadian National Committee. The Council is developing an initiative to encourage student participation in the annual meetings and will be holding a student mixer prior to its Pittsburgh meeting in August 1992.

The officers for 1992 are Keith Watenpaugh, President; Richard Marsh, Vice-president; Judith Flippen-Anderson, Past-president; Vivian Cody, Secretary; S. N. Rao, Treasurer.

Asian Crystallographic Association (AsCA)

No report has been received from the IUCr representative.

European Crystallographic Committee (ECC)

The friendly help of Professor L. Randaccio and others in Trieste saved ECM-13. With only one day of delay, and with enormous effort by the Slovenian organizers directed by Professor L. Golic, the meeting was opened by the Chairman of the ECC (Dr K. Huml) and there was a Plenary Lecture by Nobel Laureate Professor R. Huber. Although the atmosphere was somewhat pressed by the political events in neighbouring Yugoslavia, which unquestionably reduced the number of active participants to 238, the scientific programme was of the traditional standard. Of course, a few expected talks were cancelled. Both microsymbiosia and poster sessions were well presented.

The ECC met on 28 August when Albania and Turkey obtained observer status. The Chairman's report dealt with the exchange of crystallographic transformation. The question how to hold satellite meetings along with the main conferences started a controversial debate. While the Chairman was in favour of local meetings of special interest, others emphasized the advantage of satellite meetings clustered around a main conference, saving substantial travel costs. The united Germany is now represented by one delegate from the united German National Committee. The meeting received reports on the next European Crystallographic Meetings: ECM-14, Enschede, The Netherlands, 2-7 August 1992 and ECM-15 to be held in Leipzig, Germany in 1994.

Concerning ECM-16, the Committee accepted unanimously the invitation from the University of Lund, Sweden.

The proposal of the Swedish National Committee to form a European Crystallographic Association brought a lively discussion. While some delegates were afraid of a bureaucratic organization, others thought that it would be an excellent idea. The lengthy debate upon this important question was finally adjourned until the next meeting, to let national delegates consider the situation with care and responsibility.

International Organization for Crystal Growth (IOCG)

The main activity of the IOCG has been devoted to the organization of its two most important events due next year in the USA. They are the Tenth International Conference on Crystal Growth in San Diego and the Eighth International Summer School on Crystal Growth in Palm Springs.

These conferences traditionally bring together, every three years, the largest, most diverse, international body of the crystal-growth community, covering fields of interest which include crystallization theory, massive and thin-film crystal growth, processing, and characterization in its widest meaning. They are thus intended to provide a general framework within which all aspects of crystal growth are presented and discussed in order to favour the largest interaction among different backgrounds and experiences, including important crystallographic contributions.

More specialized conferences on particular aspects of crystal growth have been organized during the year by the various National Associations of Crystal Growth presently affiliated to the IOCG.

During 1991 the IOCG supported the Seventh International Conference on Vapour Phase and Epitaxy, held in Nagoya, Japan, 14-17 July. The proceedings have been published as a single issue of *J. Crystal Growth* (1991), Vol. 115.

Joint Committee on Powder Diffraction Standards-International Centre for Diffraction Data (JCPDS-ICDD)

The IUCr representative attended both meetings of the ICDD held during 1991.

Reports at one meeting demonstrated that digitized patterns offer many advantages over the old style 'd's and I's' listings. One is improved phase analysis, both qualitative and quantitative, in multiphase specimens. Successful identification of up to ten phases in a single specimen was reported. Immediate graphical comparison of the complete pattern of the unknown with known patterns was reported to be very important in helping to make an educated guess of phase identity and then to verify it. Another advan-

tage of the full digitized patterns over the old d's and I's listing is much more useful representation of 'imperfect' materials, such as clays and polymers, for which such things as asymmetry of the diffraction profiles are important parts of their characterization. Another possibly important use is for *ab initio* structure determination.

CIF/STAR. The importance of a comprehensive universal standard format for the archiving and exchange of 'similar' data meets little argument. The CIF/STAR system gets high marks from all knowledgeable reviewers for its potential for being such a standard for crystallographic data, including powder diffraction data obtained from a great variety of facilities, e.g. fixed and variable wavelengths, fixed or changing beam intensities, a great variety of optics, X-rays or neutrons or electrons, data from home laboratory or national/international facilities each of which has its own in-house data reduction system etc. One important aspect of the CIF/STAR system is that it communicates the experiment as well as the data.

Efforts to encourage the ICDD to work with the IUCr to make the CIF/STAR format a universal standard for powder diffraction data, as well as other crystallographic and related data, have not yet been successful. In 1990 work began on adopting the CIF format as the long-term future format of choice for the ICDD, including developing the definitions needed to extend the CIF/STAR format to powder diffraction data. The Commission on Powder Diffraction was asked to represent the IUCr interests in that work, with J. I. Langford as the IUCr representative.

At the Spring 1991 ICDD meeting, however, some new concerns arose, even though several ICDD members expressed appreciation of the quality and utility of the CIF format. On the CIF/STAR licensing issue, several members of the ICDD Board did not like the idea of charging a licensing fee to their customers, especially the original equipment manufacturers (OEM's) who would supply their own software to their customers and would probably revise the format anyway.

Discussions are still continuing and it is hoped that a mutually acceptable solution can be obtained.

Representatives on Other Bodies

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

The Board of this body met on 8 April in Exeter, England, and on 11 November in Pisa, Italy. Both meetings were attended by the IUCr representative, who received progress reports on future meetings in Prague (1992), Regensburg (1993) and Madrid (1994).

Debates continued on the problems of Conference Proceedings and the publication policy concerning the Division's conferences, with a preference for using the (UK) Institute of Physics Conference Proceedings Series.

Reports were received on the activities of several sections of the EPS and the IUCr representative reported on the Union's activities as well as the 1991 European Crystallographic Meeting.

Interdivisional Committee on Nomenclature and Standards (IDCNS)

The annual meeting of IDCNS, held 6-7 August 1991 in Hamburg, Germany, was attended by the alternate to the

IUCr representative, in order to reduce travel costs for the Union. Documents of interest to the IUCr include a new *Nomenclature System for X-ray Spectroscopy*, published in *Pure Appl. Chem.* (1991), 63, 735-746, superseding the Siegbahn notation, and the Third Edition of ISO Handbook 2 (*Units of Measurement*) which should become available early in 1992. Many IDCNS documents are circulated to the IUCr representative for comment. Eleven such documents were published or in press, ten were approved for public distribution and one was withdrawn in the period under review. Consideration is being given to expediting IDCNS procedures leading to the approval of IUPAC nomenclature documents for publication.

International Council for Scientific and Technical Information (ICSTI)

Following the ICSTI Council meeting, 11-12 May 1991 in Nancy, France, the IUCr representative was invited to serve on a committee to examine matters concerning Class A members (which includes the IUCr). However, his suggestions regarding more effective methods of communicating scientific information have not struck a responsive chord so far.

Recently he was invited to participate in a survey of information related to biotechnology. The information received so far gives the impression that structural information is of minimal significance in biotechnology, which is rather puzzling. The IUCr representative has indicated the areas where he felt he could make an effective contribution, which overlap with, but do not coincide with, the area suggested by the Chairman.

The next meeting of the Council, to be held in Berlin in May 1992, should throw some light on what ICSTI is actually doing.

International Council of Scientific Unions (ICSU)

The IUCr representative attended the 1991 meeting of the ICSU General Committee and associated meetings of the working group of Earth, Space, Physical and Mathematical Sciences, 25-27 September, at the Norwegian Academy of Sciences and Letters, in Oslo, Norway.

Many problems concerning the organization of ICSU and the major programmes in which the Council is involved were discussed. It was noted that 1991 was the 60th anniversary of ICSU's founding and that the ICSU activity in serving the scientific community around the world was going on, so, *inter alia*, it was pointed out that ICSU was more and more often being sought to give advice to governments and other outside bodies on scientific matters. The importance of ICSU's close cooperation with the scientific communities in central and eastern Europe was stressed.

Concerning the governance of ICSU, it was unanimously agreed that the principle of an approximate balance between the voting powers of the National and of the Union Members should be maintained.

Among common concerns and services, the problem of the enhancement of the availability of scientific literature to developing countries and that of the intellectual property aspects of the new generation of machine-readable text were considered.

On free circulation of scientists it was noted that the number of cases concerning visa difficulties was decreasing while other types of human rights issues involving the freedom of the pursuit of science were increasing.

Eleven short presentations were made by Union representatives highlighting exciting new developments in their scientific fields. The IUCr representative gave a broad presentation of the development of modern crystallography, citing particularly the achievements in the field of molecular reactivity, macromolecular biology, solid-state physics and materials science, and pointing out the importance of the crystallographic databases in connection with problems of drug design, biological activity and physical properties.

It was decided that the next meeting of the General Committee will be held in Jerusalem, 27-29 October 1992.

ICSU Committee on Data for Science and Technology (CODATA)

CODATA is an interdisciplinary Scientific Committee of ICSU which seeks to improve the quality, reliability, management and accessibility of data of importance to all fields of science and technology. Its membership consists of 21 National Members, 16 Scientific Unions, 5 Co-opted Members, 1 Affiliated Member and 27 Supporting Organizations.

CODATA sponsored four meetings in 1991. In conjunction with ICSTI, it completed a study to determine the concerns involved in access to data which was presented at the ICSU Executive Board. This study suggested several areas where CODATA and ICSTI might expand on the types of activities relevant to information access which they have traditionally performed. Examples are:

1. Education and training in the use of electronic information systems, including efforts in developing countries.
2. Education on the principles of copyright and intellectual properties.
3. Standardization of terminology, formats, classification systems and user interfaces.
4. Preparation of directories to information sources.
5. Documentation of the value of reliable data to technological progress.
6. Interchange of information on pricing strategies, promotion of information products and other issues.

CODATA, ICSTI and ICSU should be alert to problems of information access, especially at the political level, which may arise in the future.

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

This Committee was set up by ICSU in 1966 to promote Science and Technology in developing countries.

The IUCr representative informed COSTED about the activities of the IUCr Teaching Commission on the Visiting Professorship and Seminar programs, and about the IUCr policy of helping young scientists, particularly from developing countries, to attend meetings and schools sponsored by the IUCr.

The IUCr representative has received minimal communication about COSTED activities.

ICSU Committee on Space Research (COSPAR)

During 1991, the most important activity of COSPAR, an interdisciplinary scientific body concerned with the progress on an international scale of all kinds of scientific investigations carried out in space, was in the organization of the COSPAR Plenary Meeting and Associated Activities, to be held as part of the World Space Congress, 28 August-5 September 1992, in Washington, DC, USA. This Congress,

which will be organized in the framework of the International Space Year (an initiative formally endorsed by the UN General Assembly in 1989), is expected to have a great impact on the preparation and planning of global space research.

The list of the COSPAR symposia and scientific meetings planned during the Congress are reported in the COSPAR Information Bulletin No. 122, Dec. 1991. They include topics of relevance for the crystallographic research area, especially as regards the proposals of the COSPAR Commission on Materials Science in Space. The most relevant is a Symposium on Microgravity Research: Materials and Fluid Sciences, to be held 3 August–4 September 1992. This symposium will focus on scientific progress in gravity-dependent phenomena in fluids and materials accomplished in space flights. The most relevant themes which will be highlighted are: crystal growth from the melt, solution and vapour; diagnostics of microgravity parameters; glass transitions and amorphous materials; macromolecular crystals; multiphase phenomena in solids; solidification processes.

ICSU Committee on the Teaching of Science

No report has been received from the IUCr representative.

Finances

The audited accounts of the year 1991 are given at the end of this Report. For comparison, the figures for 1990 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 1991 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 appropriate to the individual dates of these transactions. As a consequence of the fluctuations in exchange rates, an apparent gain has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 368 982. This gain has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1991. It should be noted that this gain in Swiss Francs is not a real gain of money, but rather a gain 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 1991. 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 427 652 with the banks at the end of the year was represented by Dfl 3004 and US \$611 with the Amsterdam–Rotterdam Bank, US \$171 456 with Merrill

Lynch, £64 262 with the National Westminster Bank and SwFr 14 380 with the Union Bank of Switzerland.

The balance sheet shows that the asset of the Union, excluding stocks of unsold publications but including the gain of SwFr 368 982 resulting from fluctuations in rates of exchange, have increased during the year, from SwFr 4 773 398 to SwFr 5 455 503.

A transfer of SwFr 35 000 was made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund and a transfer of SwFr 100 000 was made to the Research and Education Fund from the General Fund. A transfer of SwFr 15 000 was made to the Ewald fund from the *Acta Crystallographica* Fund and a transfer of SwFr 10 000 was made to the President's Fund from the General Fund, to provide additional funds for cases of special need. The *Molecular Structures and Dimensions* Fund was wound up and its balance incorporated into the Book Fund, which was also credited with sales of *Molecular Structures and Dimensions* during 1991.

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 surplus of SwFr 217 338, before the transfers totalling SwFr 110 000 to the Research and Education Fund and the President's Fund, as compared with a surplus of SwFr 357 524 in 1990, before transfers totalling SwFr 225 000 to the same fund accounts. The administrative expenses were SwFr 264 408 in 1991 as compared with SwFr 239 644 in 1990. Of this amount, SwFr 79 322 was charged to the publications of the Union.

SwFr 1500 was given for general support of scientific meetings, in addition to SwFr 53 804 for financial support to young scientists attending meetings, which appears in the expenses of the Research and Education Fund, and SwFr 23 395 in special grants from the President's Fund. SwFr 12 367 was spent in assisting the work of the non-publishing Commissions. The expenses of the Union representatives on other bodies were SwFr 6161. The cost of the two Finance Committee meetings held in 1991 was SwFr 21 938, whilst the Executive Committee meeting cost SwFr 31 070. The Union received SwFr 16 740 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 132 610. Interest on bank accounts and investments credited to the General Fund was SwFr 331 499.

The President's Fund, the Publications and Journals Development Fund, the Research and Education Fund and the Ewald Fund receive 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 1947, in addition to the already-mentioned transfer of SwFr 10 000 from the General Fund. Grants totalling SwFr 23 395 were paid from the fund.

The *Acta Crystallographica* account for 1991 shows a surplus of SwFr 219 564 before the transfer of SwFr 50 000 to other fund accounts, as compared with a surplus of SwFr 224 290 in 1990 before transfers of SwFr 600 000.

The subscription rates were increased for 1991 and more pages were published in 1991 than in 1990. The number of paid subscriptions to all sections of *Acta*, including 100

personal subscriptions in 1990 and 95 in 1991, decreased from 1082 in 1990 to 1050. For the number of paid subscriptions to the separate sections of the journal, those to Section A remained unchanged from 1990 at 268, those to Section B increased from 187 to 195 and those to Section C decreased from 141 to 135. 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 81 and 19% respectively for 1991. For 1990 the percentages were 88 and 12%. The technical editing costs for *Acta Crystallographica* were SwFr 462 936, as compared with SwFr 370 551 in 1990. The journal's accounts have also been charged with administrative expenses as in previous years and as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a deficit of SwFr 5527, as compared with a surplus of SwFr 75 633 in 1990, before the transfer of SwFr 15 000 to the Ewald Fund. However, the number of pages published in 1991, 1102, was double the normal annual figure because of the publication of the proceedings of the International Conference on Small-Angle Scattering, Leuven, Belgium, 6–9 August 1990. 560 pages were published in 1990. The number of subscriptions, including 107 personal subscriptions in 1990 and 1991, decreased from 1032 in 1990 to 1022 in 1991.

The *Structure Reports* account shows a surplus of SwFr 17 198 in 1991 as compared with a surplus of SwFr 9670 in 1990. Only one A Series volume was published in each of these years. Editorial expenses were only SwFr 13 670 as compared with SwFr 28 612 in 1990, but the level of these expenses does fluctuate from year to year. The net income from sales was SwFr 43 097 in 1991 as compared with SwFr 53 148 in 1990.

The *International Tables* account shows a deficit of SwFr 5263, as compared with a deficit of SwFr 32 161 in 1990. These deficits will continue to occur until Volumes B and C are published and substantial sales income is received for both volumes. Volume C was published in early 1992 and Volume B should be published later in 1992. Virtually all the expenses incurred in 1990 and 1991 relate to these volumes. The net sales income of SwFr 72 864 derived mostly from the sale of 340 copies of Volume A, but 172 copies of the Teaching Edition of Volume A were also sold.

The Book Fund is credited with the sales of the remaining publications of the Union including, for the first time, those of *Molecular Structures and Dimensions*, for which until 1991 there had been a separate fund account. The main sales income was from the Eighth Edition of the *World Directory of Crystallographers*, which was published in December 1990. By the end of 1991 all but SwFr 5413 of the expenses for producing this *Directory* had been recovered from sales. 328 copies of the *Historical Atlas of Crystallography*, edited by J. Lima de Faria, were sold and it was reprinted in late 1991.

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 135 843 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 53 804 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.

Calculation of the balance of the General Fund Account at 31 December

	Swiss Francs	
	1991	1990
Balance at 1 January	1,131,584	1,170,342
Difference between income and expenditure	107,338	133,524
Fluctuations in rates of exchange	89,872	-171,282
Balance at 31 December	<u>1,328,794</u>	<u>1,131,584</u>

President's Fund Account for the year ended 31 December 1991

	Swiss Francs		
	1991	1990	1990
Grants	23,395	1,524	50
			1,286
<i>Excess of income over expenditure carried to balance sheet</i>	—	24,812	25,000
	<u>23,395</u>	<u>26,336</u>	—
Balance at 1 January	36,042	16,686	
Difference between income and expenditure	-11,448	24,812	
Fluctuations in rates of exchange	1,783	-5,456	
Balance at 31 December	<u>26,377</u>	<u>36,042</u>	
	1991	1990	1990
	1,947	—	50
Donations received			1,286
Interest (Note 6)	10,000		25,000
Transfers from other Funds:			
General Fund	11,448		
<i>Excess of expenditure over income carried to balance sheet</i>			
	<u>23,395</u>	<u>23,395</u>	<u>26,336</u>

Acta Crystallographica Account for the year ended 31 December 1991

	Swiss Francs		Swiss Francs	
	1991	1990	1991	1990
Publication expenses:				
Printing and binding Volume 47 (1990 Volume 46)	592,323	586,118	1,697,994	1,582,371
Distribution and postage	125,894	127,753	18,556	19,102
Airfreight costs	48,078	41,604	52,180	51,278
	<u>766,295</u>	<u>755,475</u>	<u>(4,589)</u>	<u>10,944</u>
Printing Acta Supplement to Volume A46	—	28,594	—	1,386
Biological crystallography journal	4,006	3,767	1,764,141	1,665,081
Index to Volume 46 (1990 Volume 45)	19,074	14,886	120,158	112,080
Documenter	16,118	17,758	<u>1,643,983</u>	<u>1,553,001</u>
		<u>820,480</u>	<u>1,960</u>	<u>1,170</u>
Editorial expenses:				
Editorial honoraria	43,846	33,746		
Secretarial assistance	21,684	19,981		
Postage and sundries	32,928	31,241		
Technical Editing:				
Salaries and expenses	437,470	342,151		
Computer expenses	18,677	19,966		
Depreciation of office equipment	6,789	8,434		455,519
				<u>53,882</u>
Administration expenses	59,492			
Transfers to other Funds:				
Publication and Journals Development Fund	35,000	500,000		
Research and Education Fund	—	100,000		
Ewald Fund	15,000	—		600,000
				<u>—</u>
<i>Excess of income over expenditure carried to balance sheet</i>	169,564	—	—	375,710
	<u>1,645,943</u>	<u>1,929,881</u>	<u>1,645,943</u>	<u>1,929,881</u>
Balance at 1 January	1,489,296	2,090,433		
Difference between income and expenditure	169,564	-375,710		
Fluctuations in rates of exchange	120,335	-225,427		
Balance at 31 December	<u>1,779,195</u>	<u>1,489,296</u>		

Book Fund Account for the year ended 31 December 1991

	Swiss Francs			Swiss Francs	
	1991	1990		1991	1990
Publication Expenses:			Transfer from <i>Molecular Structures and Dimensions</i> Fund		
<i>Escher Kaleidozyklen</i>	—	36	Sale of copies, net of	5,315	—
Book series expenses	57	187	Publisher's commission on sales		
<i>Atlas of Crystallography</i>	16,136	12,019	<i>Atlas of Crystallography</i>	6,776	7,922
<i>World Directory of Crystallographers</i> ,			<i>Escher Kaleidozyklen</i>	—	170
8th Edition	48,937	1,270	<i>Crystallographic Databases</i>	256	813
Sundry Publications	11	259	<i>Fifty Years of X-ray Diffraction</i>	—	133
			<i>Escher Drawings</i>	-52	787
			<i>Early Papers</i>	30	103
			<i>Fifty Years of Electron Diffraction</i>	39	56
			<i>World Directory of Crystallographers</i> ,		
			7th Edition	—	151
			<i>World Directory of Crystallographers</i> ,		
			8th Edition	44,658	136
			Sundry Publications	66	245
			<i>Molecular Structures and Dimensions</i>	1,381	—
			Royalties		
			<i>Escher Drawings</i>	400	300
			Book series-IUCr Crystallographic		
			Symposia	1,040	742
			Excess of expenditure over income		
			carried to balance sheet	5,232	2,213
				<u>65,141</u>	<u>13,771</u>
Balance at 1 January	8,491	11,989			
Difference between income and expenditure	-5,232	-2,213			
Fluctuations in rates of exchange	236	-1,285			
Balance at 31 December	<u>3,495</u>	<u>8,491</u>			

Research and Education Fund Account for the year ended 31 December 1991

	Swiss Francs		Swiss Francs	
	1991	1990	1991	1990
Expenses				
History of the Union	—	1,976	—	100,000
Young Scientists' Support	53,804	76,145	100,000	200,000
1989 ECM Fund creditor	13,007	—	—	300,000
Visiting Professorship Programme	145	—	40,484	—
IUCr publications	202	606	—	27,673
	<u>67,158</u>	<u>78,727</u>	<u>140,484</u>	<u>327,673</u>
<i>Excess of income over expenditure carried to balance sheet</i>	73,326	248,946	—	—
	<u>140,484</u>	<u>327,673</u>	<u>140,484</u>	<u>327,673</u>
Balance at 1 January	539,640	372,377	—	—
Difference between income and expenditure	73,326	248,946	—	—
Fluctuations in rates of exchange	44,446	-81,683	—	—
Balance at 31 December	<u>657,412</u>	<u>539,640</u>	<u>140,484</u>	<u>327,673</u>

Transfers from other Funds:
Acta Crystallographica
 General Fund

Interest (Note 6)

Ewald Fund Account for the year ended 31 December 1991

	Swiss Francs		Swiss Francs	
	1991	1990	1991	1990
Prize	—	26,582	15,000	—
Selection Committee and expenses	253	—	—	15,000
<i>Excess of income over expenditure carried to balance sheet</i>	30,314	5,700	15,567	17,282
	<u>30,567</u>	<u>32,282</u>	<u>30,567</u>	<u>32,282</u>
Balance at 1 January	194,720	218,494	—	—
Difference between income and expenditure	30,314	5,700	—	—
Fluctuations in rates of exchange	16,260	-29,474	—	—
Balance at 31 December	<u>241,294</u>	<u>194,720</u>	<u>30,567</u>	<u>32,282</u>

Transfers from other Funds:
Acta Crystallographica
Journal of Applied Crystallography
 Interest (Note 6)

Statement of Source and Application of Funds
Year ended 31 December 1991

	Swiss Francs	
	1991	1990
Source of funds		
Excess of income over expenditure for the year	313,123	312,758
Adjustment for items not involving the movement of funds:		
Fluctuations in rates of exchange	368,982	-722,528
Depreciation	12,488	13,210
Fluctuations in rates of exchange on office equipment and investments	-326,460	623,902
Profit on sale/redemption of investments	-19,121	-193,007
	349,012	34,335
Total generated from operations		
Increase in creditors, accrued charges and income received in advance	—	76,818
Proceeds of sale/redemption of investments	633,090	1,056,222
Decrease in debtors and accrued income (including subscriptions)	39,571	99,451
	1,021,673	1,266,826
Application of funds		
Decrease in creditors, accrued charges and income received in advance	-46,899	—
Purchase of office equipment	-3,917	-26,424
Purchase of investments	-1,197,533	-1,187,357
	-226,676	53,045
Movement in net liquid funds		
	-226,676	53,045

Net liquid funds include cash at banks and with Union officials.

Notes to the Financial Statements

1. Accounting Policies

(a) Accounting convention

The financial statements are prepared under the historical cost convention.

(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 within the General Fund Account when declared and added to the accumulated cost of investments. Other dividends are recognized within the General Fund 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:

	1991	1990
Netherland Guilders	1.2588	1.3464
Danish Crowns	4.3365	4.5512
Pounds Sterling	0.3951	0.4000
US Dollars	0.6993	0.7874

The total assets of the Union at 1 January 1991 (SwFr 4,773,398) would have had the value of US \$3,758,573 or £1,909,359 if expressed in those currencies.

At 31 December 1991 these assets (SwFr 5,457,687) would have had the value of US \$3,816,560 or £2,156,332

respectively, being an increase of US \$57,987 or £246,973 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 1991	Additions during the year	Disposals/ Redemptions during the year	Fluctuations in rates of exchange	Holding at revalued cost 31 December 1991
Swiss Francs					
Held by Merrill Lynch					
<i>(Corporate Government Securities)</i>					
US \$20,692 GNM P146535-2016	25,847	—	-301	3,257	28,803
US \$58,544 GNM P169332-2016	78,775	—	-7,840	10,106	81,041
US \$36,000 US Treasury May 1991	37,591	—	-42,919	5,328	—
US \$84,000 US Treasury May 2001	37,825	—	-37,825	—	—
US \$150,000 US Treasury November 2004	57,179	—	—	7,204	64,383
<i>(Mutual Funds/Unit Investment Trusts)</i>					
2,231 Units ML Capital Fund/CLB (US \$)	63,559	—	—	27,330	90,889
US \$ 4,750 Temple Worldwide Fund G	63,643	—	—	8,018	71,661
US \$ 4,750 Temple Worldwide Fund I	63,643	—	—	8,018	71,661
US \$ 785 Haussman holdings	227,686	110,612	—	26,412	364,710
US \$ 5,129 Global Equity Portfolio	64,199	—	—	8,088	72,287
<i>(Certificates of deposit)</i>					
US \$ 50,000 FHLMC 8.5% Sept 15 20RG	62,403	—	—	7,863	70,266
US \$ 50,000 CITI CDT Cards 8.25% Nov 15 193	63,600	—	—	8,013	71,613
US \$ 75,000 British Gas France	—	119,529	—	-9,254	110,275
US \$ 75,000 GEC	—	117,316	—	-9,083	108,233
US \$ 8,000 MLST World income portfolio	—	105,141	—	9,631	114,772
US \$ 60,000 Reynold RJOV	—	70,320	-80,840	10,520	—
Held by Foreign & Colonial					
34,298 Units Reserve Asset Fund Class D (US \$)	764,545	36,784	—	96,321	897,650
11,964 Units Reserve Asset Fund Class L (£)	288,274	—	—	3,575	291,849
43,064 Units Reserve Asset Fund Class O (US \$)	553,883	151,704	—	78,652	784,239
11,026 Units Reserve Asset Fund Class X (£)	725,326	—	-444,244	-2,705	278,377
17,617 Units Reserve Asset Fund Class H (ECU)	—	335,069	—	18,253	353,322
Held by National Westminster Bank (1990 Coutts)					
£458,933 cash on one year deposit	1,000,000	151,058	—	10,502	1,161,560
	<u>4,177,978</u>	<u>1,197,533</u>	<u>-613,969</u>	<u>326,049</u>	<u>5,087,591</u>

Investments are noted in the balance sheet at their market value at 31 December 1991. 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 1,161,560 which is invested in a one year bank deposit account at National Westminster Bank, Jersey which is due to mature on 28 August 1992. 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	
	1991	1990
National Westminster Bank PLC		
Manchester SMMO Account	47,935	63,730
Manchester Business Reserve Account	6,678	19,620
Amsterdam-Rotterdam Bank NV		
Current Guilder Account	14	22
Guilder Savings Account	84	71
Guilder 1 month deposit	—	3,718
US \$ Account	14	21
Merrill Lynch		
CMA Account	8,308	10,611
Foreign & Colonial		
Cash balances	211	243
Interest from Munksgaard	26,607	20,640
Interest on officers' petty cash accounts	—	84
	<u>89,851</u>	<u>118,760</u>

6. Investment Income

	Swiss Francs	
	1991	1990
GEC	1,766	—
British Gas	777	—
ML Basic Value Fund	—	2,699
ML Capital Fund	4,082	3,851
P146535-2016	2,677	2,772
P169332-2016	7,850	8,312
FHLMC 8.5% Sept 15 20RG	—	5,993
Temple Worldwide Fund G	6,177	4,788
Temple Worldwide Fund I	8,130	6,553
Global Equity Portfolio	—	1,599
Foreign and Colonial Fund H	25,037	—
Foreign and Colonial Fund X	37,128	101,986
Foreign and Colonial Fund D	67,329	58,004
Foreign and Colonial Fund L	8,780	48,450
Foreign and Colonial Fund O	19,705	6,999
FHLMC	6,059	—
MLST World income portfolio	7,535	—
CITI CDT Cards	5,881	5,816
National Westminster Bank/Coutts deposit account	139,744	48,333
	<u>348,657</u>	<u>306,155</u>
Less: Rothschild management fees	—	2,319
	<u>348,657</u>	<u>303,836</u>
Allocated to President's Fund	1,947	1,286
Allocated to Ewald Fund	15,567	17,282
Allocated to Publication and Journals Development Fund	49,011	36,027
Allocated to Research and Education Fund	40,484	27,673
Balance left in General Fund	241,648	221,568
	<u>348,657</u>	<u>303,836</u>