### International Union of Crystallography

### **Report of the Executive Committee for 1989**

### **Extraordinary General Assembly**

An Extraordinary General Assembly was held in London on 19 December. It had been called by the Executive Committee, at its meeting in July 1989, to consider its recommendation that the US Adhering Body be asked to organize the 1993 IUCr General Assembly and Congress, and that the General Assembly and Congress scheduled to be held in Beijing in 1993 be postponed to 1996.

Twelve Adhering Bodies sent delegates. Postal responses had been received from 16 Adhering Bodies, who did not send delegates. The remaining seven Adhering Bodies did not reply or send delegates. The delegates present were given a summary of the postal responses, of which nearly all supported the Executive Committee recommendation. The President explained the background to the Executive Committee decision made in July 1989. He told delegates that, prior to the Extraordinary General Assembly, assurances had been sought from the China Association for Science and Technology (CAST) on the arrangements for the Congress and, particularly, on the free circulation of scientists including young Chinese scientists at present in other countries but who might wish to return to China for the Congress. Copies of that letter, and the reply from CAST giving such assurances, were distributed to delegates. The Vice-President of the IUCr, Y.-q. Tang, also answered questions concerning the possibility of holding a Congress successfully in China.

After an extensive and detailed debate it was decided that the 1993 General Assembly and Congress would be held in Beijing. This decison will be presented to the Bordeaux General Assembly in July 1990 for final approval.

### Meetings

The IUCr sponsored the following meetings held during 1989:

1. International Conference on the Use of X-ray Crystallography in the Design of Anti-viral Agents, Kona, Hawaii, USA, 6-8 February 1989.

2. Symposium on Crystallographic and Modelling Methods in Molecular Design, Gulf Shores, Alabama, USA, 30 April-3 May 1989.

3. Meeting on Crystallography of Biological Macromolecules: Methods and Results, Como, Italy, 16-19 May 1989.

4. Third International Meeting on Quasicrystals. Incommensurate Structures in Condensed Matter, Vista Hermosa, Mexico, 29 May-2 June 1989.

5. International Workshop on the Rietveld Method, Petten, The Netherlands, 13-15 June 1989.

6. Gordon Conference on Electron Distributions and Chemical Bonding, Plymouth, New Hampshire, USA, 3-7 July 1989. 7. International Workshop on Accurate Crystal Structure Determination at High Pressure, Münich, Federal Republic of Germany, 24-25 July 1989.

8. Symposium on Symmetry of Structure, Budapest, Hungary, 13-19 August 1989.

9. Third International Conference on Crystallization of Biological Macromolecules, Washington, DC, USA, 13-19 August 1989.

10. Symposium on Organic Crystal Chemistry, Poznań-Rydzyna, Poland, 14-17 August 1989.

11. Twelfth European Crystallographic Meeting, Moscow, USSR, 20-29 August 1989.

12. Ninth International Hydrogen Bond Conference, Zeist (Utrecht), The Netherlands, 10-15 September 1989.

The Executive Committee met in Rowton, near Chester, England, in July. It also held a special meeting in London on 19 December, prior to the Extraordinary General Assembly on that day. The Finance Committee met twice, in Trömso in March/April and in Rowton immediately prior to 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 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) appointment of new staff in the IUCr office in Chester;

(3) upgrading of office technology in the IUCr office in Chester and expansion of this office;

(4) future of *Structure Reports* and their co-operation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre;

(5) consideration of the report of the Working Party on Crystallographic Information, and the development of electronically assisted publication;

(6) progress with Volumes B and C of International Tables;

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

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

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

(10) investment policy;

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

(12) consolidation of the Ewald Fund and appointment of the Selection Committee for the second Ewald Prize;

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

(14) free circulation of scientists;

(15) discussion of the arrangements of the Bordeaux General Assembly and Congress with the Programme Committee;

### INTERNATIONAL UNION OF CRYSTALLOGRAPHY

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

				Full A	rticles	Short Form	nat Papers	Short Com	nunications	Fast Comm	unications
Vol.	Year	Number of Pages*	Number of Papers	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length
A40 B40 C40	1984	$\begin{array}{c} 728\\ 616\\ 2126 \end{array} 3470$	$123 \\ 99 \\ 811 $ 1033	$\begin{pmatrix} 109 \\ 99 \\ 789 \end{pmatrix}$ 208	$ \begin{array}{c} 6 \cdot 2 \\ 6 \cdot 2 \\ 2 \cdot 7 \end{array} \right\} 6 \cdot 2 $			$\frac{14}{22} \right\} 36$	$\frac{1\cdot 1}{0\cdot 8} \bigg\} 0\cdot 9$		
A41 B41 C41	1985	$\begin{array}{c} 624\\ 456\\ 1836\end{array}$ 2916	$114 \\ 67 \\ 703 \\ 884 \\ 703 \\ 884$	$\left. \begin{smallmatrix} 108 \\ 66 \\ 686 \end{smallmatrix} \right\}$ 174	$\begin{array}{c} 5\cdot4\\ 6\cdot4\\ 2\cdot6\end{array}$	— 8		$\begin{pmatrix} 6\\1\\9 \end{pmatrix}$ 16	$\left.\begin{array}{c}0\cdot8\\0\cdot6\\0\cdot7\end{array}\right\}0\cdot7$		
A42 B42 C42	1986	588 640 1892	$98 \\ 90 \\ 732 $ 920	$\begin{pmatrix} 85\\ 89\\ 648 \end{pmatrix}$ 174	$ \begin{array}{c} 6\cdot 3 \\ 7\cdot 0 \\ 2\cdot 7 \end{array} 6\cdot 7 $	— 	  1·6	$ \begin{array}{c} 13\\1\\9 \end{array} \right\} 23$	$\left.\begin{array}{c}1\cdot1\\2\cdot2\\0\cdot9\end{array}\right\}1\cdot1$		
A43 B43 C43	1987	840 584 2472	$128 \\ 100 \\ 995 $ 1223	$(114) \\ 91 \\ 817 $ 205	$ \begin{array}{c} 6 \cdot 5 \\ 6 \cdot 3 \\ 2 \cdot 7 \end{array} 6 \cdot 4 $	 174	$\frac{-}{1\cdot7}$	$ \begin{array}{c} 14\\ 9\\ 4 \end{array} $ 27	$ \left.\begin{array}{c} 1\cdot3\\ 0\cdot9\\ 0\cdot9\\ 0\cdot9 \end{array}\right\}1\cdot1 $		
A44 B44 C44	1988	$ \begin{array}{c} 1104\\ 680\\ 2240 \end{array} 4024 $	$159 \\ 104 \\ 897 \end{pmatrix} 1160$	$150 \\ 100 \\ 712 $ 250	$\begin{pmatrix} 6 \cdot 3 \\ 6 \cdot 4 \\ 2 \cdot 5 \end{pmatrix} 6 \cdot 4$	 174	 1.5	$ \begin{array}{c} 9\\ 4\\ 11 \end{array} $ 24	$ \begin{array}{c} 1 \cdot 1 \\ 0 \cdot 3 \\ 0 \cdot 3 \end{array} $ 0 \cdot 6		
A45 B45 C45	1989	$\begin{array}{c} 920\\ 600\\ 2030 \end{array} \} 3550$	$     \begin{array}{c}       143 \\       94 \\       806     \end{array}     1043 $	$122 \\ 90 \\ 550 \\ 212$	6·6 6·6} 2·8	 239	— — 1·9	$     \begin{bmatrix}       14 \\       4 \\       17     \end{bmatrix}     35   $	$ \begin{array}{c} 0.9\\0.5\\0.8 \end{array} \right\} 0.8$	7	3.4

### Acta Crystallographica

### Journal of Applied Crystallography

				Full A	rticles	Sh Commu	ort nications	Crysta	l Data	Comj Prog		Short	Items§
Vol.	Year	Number of Pages*	Number of Papers	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length
17	1984	488	104	66	6.2	11	1.5	7	0.5	7	2-4	14	0.9
18	1985	546	108	80	5.5	9	1.8	5	0.4	7	3.3	7	0.8
19	1986	492	104	71	6.1	12	1.6	10	0.4	7	1.9	8	0.8
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	6	0.7

\* Excluding indexes.

† Volume A40 includes, in addition, 542 pages of abstracts communicated to the Hamburg Congress.

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

(16) review of the activities of the Commissions;

(17) establishment of an *ad interim* Commission on Synchrotron Radiation;

(18) review of IUCr representation on the Scientific and Regional Associates and on other bodies;

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

### Publications

Volume 45 of Acta Crystallographica and Volume 22 of the Journal of Applied Crystallography were published, as were Volumes 49A, 49B and 54A of Structure Reports, and reprints of Volumes II and IV of International Tables for X-ray Crystallography, and Volume A and the Brief Teaching Edition of Volume A of International Tables for Crystallography.

### **Adhering Bodies**

A list of Adhering Bodies of the IUCr was published in the Report of the Executive Committee for 1988 [*Acta Cryst.* (1989), A**45**, 740-741]. An updated list will be published in *Acta Crystallographica* Section A in due course, in the Report of the Bordeaux General Assembly.

### Work of the Commissions

### Commission on Journals

Volume 45 of Acta Crystallographica (Acta) was published in 1989, and included a total of 1043 papers (a 10% decrease from 1988) received from 51 countries, and an overall total of 3550 pages (an 11% decrease from last year).

The average length of full articles in Acta increased to 5.3 pages in 1989 from 5.1 pages in 1988 (see Table 1). Median publication times for these full articles, the average

elapsed time between the published acceptance and nominal publication dates, were 4.8 months for Acta A, 4.7 months for Acta B, and 6.1 months for Acta C. Corresponding publication times in 1988 were 5.0, 5.3, and 4.0 months, respectively. Median publication times in 1989 for Short Communications were 5.1 months for Acta A, 3.2 months for Acta B, and 4.0 months for Acta C. The median publication time for Fast Communications papers in Acta A was 1.4 months and for Short Format papers in Acta C 5.3 months.

A total of 36 inorganic, 8 organometallic and 45 organic papers appeared in Section B in 1989 compared with 37, 15 and 42, respectively, in 1988. By contrast, the distribution of papers in Section C was 95 inorganic, 228 organometallic and 483 organic in 1989, compared with 110 inorganic, 266 organometallic and 520 organic articles in 1988.

Volume 22 of the Journal of Applied Crystallography (JAC) was published in 1989. A total of 125 papers was published (a 26% decrease from 1988), received from 29 countries. Overall, the number of pages decreased to 642 in 1989 from 996 in 1988. While the number of papers published in JAC this year was smaller than in 1988, the 'Small Angle Scattering' issue produced in 1988 resulted in a larger-than-usual increase of an additional 69 papers. With that taken into consideration, the papers published in JAC during 1989 actually reflect an increase over previous years.

The average length of full articles in JAC was 6.7 pages in 1989, compared to 5.7 pages in 1988. The median publication time for full articles was 5.4 months for JAC, down from 5.9 months in 1988. The median publication time for Short Communications and Computer Programs was 2.6 months in 1989, up slightly from 2.2 months in 1988.

Section A of Acta Crystallographica converted to a monthly publication beginning in January 1989, in order to accommodate the new Fast Communications section that was approved by the Commission on Journals in 1988. It was anticipated that the average publication time for Fast Communications would be about three months, but the 7 papers that were accepted were published in an average time of 1.4 months. Co-editors will encourage authors to consider more frequent use of Fast Communications.

There is an increasing backlog of *Acta* Section C structural papers, both with Co-editors and with the Technical Editor in Chester, resulting in the increased publication time for these papers. However, with new computer equipment and checking procedures instituted in Chester, and plans by the Commission on Journals at its 1990 meeting in Bordeaux to address proposed changes in the procedures for handling structural papers, it is hoped that this backlog will decrease during the coming year.

Peter Lindley, Wolfram Saenger, Marjorie Harding and John Spence were appointed as new Co-editors of *Acta* during 1989. Roberto Colella retired after nine years as an *Acta* Co-editor, and the Commission extends its warm thanks to him for the commitment in time and energy he made in performing his duties so well.

### Commission on Structure Reports

Volumes 49A (396 pp.) and 54A (328 pp.) (Metals and Inorganic Compounds for 1982 and 1987, respectively) were published in 1989. Volume 55A (Metals and Inorganic Compounds for 1988) is with the publisher and will appear in 1990.

Volume 49B (1861 pp. Organic Compounds for 1982) was published in 1989. Co-editorial work is nearing completion on Volumes 50B and 51B (Organic Compounds for 1983 and 1984, respectively) and continues for Volume 52B (Organic Compounds for 1985). Material is being gathered for the 10-year Organic Index (Volume 47B).

### Commission on International Tables

The Executive Committee of the IUCr considered the series *International Tables for Crystallography* at its meetings in July 1989, and interviewed the Editors of Volumes B and C on 18 July. Though certain gaps in the original plans for these volumes still remained, it was felt that the contributions already received plus those that could be confidently expected within a few months would make acceptable publications. The Editors of Volumes B and C were therefore instructed to send to the Technical Editor the remaining sections for publication, with an absolute deadline of 31 December 1989, and to hold over to a second edition any contributions still outstanding at that date.

Professors V. Kopsky and D. B. Litvin have prepared a detailed plan for a volume on *Subperiodic Symmetry Groups*. Their plan will be considered by the Commission and the Executive Committee at meetings in Bordeaux in July 1990.

Much time has been spent by the Chairman of the Commission and others within the IUCr in studying the practicability of preparing a volume on multidimensional crystallography. The quantity of material makes it difficult to plan even a volume on four-dimensional crystallography, and it is not entirely clear whether the theory is complete for higher dimensions. The subject is very important in connection with modulated structures and quasicrystals, and the Commission hopes to be able to make definite proposals at Bordeaux.

Discussion continued on two other proposals (*Crystallographic Computing*; *Mathematics for Modern Crystallography*). During the meeting of the Executive Committee the Editor of Volume B put forward outline proposals for these volumes. Such volumes are likely to be of great value to the crystallographic community, but the appropriate format needs further consideration. The formats so far considered were (i) Volumes of *International Tables* and (ii) Monographs, such as in the IUCr/Oxford University Press Series. This question will be further discussed during the Bordeaux meetings of the Commission.

Detailed reports on Volumes A-D are given in the following paragraphs.

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

The second edition of Volume A was reprinted in May 1989; it contains corrections of a few errors as well as new diagrams for the hexagonal space groups and the tetragonal space groups of geometric crystal class 4/mmm.

Preparations for the third edition have continued. Two main changes are intended:

(i) New diagrams for the remaining tetragonal space groups (classes 4 to  $\overline{42m}$ ) were completed in December 1989. Extensive revisions of the cubic space-group diagrams are under way. All these diagrams are prepared by Mr R. A. Becker (Aachen).

(ii) Work on the more detailed characterization of the subgroups of the plane and space groups has continued; see the 1988 Commission Report.

The second edition of the *Brief Teaching Edition* of Volume A was reprinted with corrections in September 1989.

### Volume B (Reciprocal Space; Editor U. Shmueli)

The period to which this report pertains was devoted to the organization and reviewing of outstanding contributions, to the completion of Chapter B.1.1 Reciprocal Space in Crystallography (by the Editor) and to activities related to the discussions with the Executive Committee, held in July 1989. It appears that Volume B will consist of nineteen chapters, comprising a selection of mathematical and statistical methods of crystallography, methods of crystal structure determination from X-ray and electron diffraction data, computational and graphical treatments of crystal and molecular geometry, topics in crystal physics related to diffuse scattering and scattering from paracrystalline phases, and dynamical theories of X-ray and electron diffraction. Two contributions are still in the final stages of revision, and four invited contributions have been postponed to a later edition of the volume.

The possibility of transferring via electronic mail almost arbitrarily complicated texts manifested itself to the Editor during the period of this report. It should be pointed out that most scientific word processors are equipped with relevant translating routines, and transmission of scientific material between author and editor, via this route, is a convenient and rather inexpensive proposition.

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

Much of the year has been devoted to chasing delayed contributions and providing linking paragraphs and cross references. A few gaps in the original plan remained at the expiry of the deadline set by the Executive Committee; some are being filled by condensation and updating of material from Volumes II-IV. The original concept of Volume C, it may be remembered, evolved at meetings of the Executive Committee in Montreal in 1981 as a 'quick and dirty' editorial condensation of the non-obsolete parts of Volumes II-IV. It soon became obvious that such a volume would be unworthy of the IUCr, and new expert contributions were sought. To a great extent the search for new contributions was successful.

### Volume D (Physical Properties of Crystals; Editor B. T. M. Willis)

Work on Volume D officially began in September 1988, though preparations had begun considerably earlier. The Table of Contents was approved by the Executive Committee and is published in *Acta Cryst.* (1989), A**45**, 743. It consists of six parts.

The first part, 'Mathematical Introduction', is substantially complete. It is concerned with the use of tensors to represent the physical properties of crystals, at a level of presentation similar to that of the book *Physical Properties* of Crystals by J. F. Nye (1985). The last chapter in this part deals with the reduction in the number of independent components of a tensor by the symmetry operations of the crystallographic point group. The remaining parts describe the macroscopic properties of crystals, intrinsic or extrinsic. The *intrinsic* properties depend on the inherent nature of the crystal (structure, chemical composition, ...), whereas *extrinsic* properties are associated with faults (point defects, dislocations, ...). Most of the properties to be dealt with in Volume D are extrinsic. The second part, 'Mechanical Properties', is in first draft.

### Commission on Biological Macromolecules

The structural analysis of biological macromolecules continues to be a successful activity and a number of structures of great importance for understanding biochemical and biological principles have been elucidated in the last year. The interdisciplinary character of this crystallography is emphasized by the increasing reliance on synchrotron radiation and advances in computational power. This has been reflected in an increasing number of small workshops, held at national and international levels, specifically designed to bring the application of new techniques to the whole community.

The policy on deposition of crystallographic data has been accepted throughout the crystallographic and associated communities and it is hoped that this will lead to a better practice on making coordinates available.

The Commission has begun to consider establishing criteria through which the correctness and quality of refined protein crystal structures can be assessed. This is now seen to be particularly important with the expansion of the subject and the growth of many new laboratories. The Commission feels it is imperative that the tradition of excellence and reliability associated with X-ray structural research into macromolecules should be continued. It considers that this will be ensured by the recognition, within the community, that certain crystallographic and structural criteria have to be met before such structures can be safely published. It is expected that discussions on this matter will take place within the Commission and throughout the community. There will be a discussion session on crystallographic accuracy and criteria at the XV IUCr Congress in Bordeaux.

### Commission on Charge, Spin and Momentum Densities

The activities of the Commission were summarized in its Newsletters Nos. 1 and 2, which were published in *Acta Cryst.* [(1989), A**45**, FC15-FC17; (1990), A**46**, FC1-FC4], and were sent to everyone on the updated mailing list compiled at Sagamore.

The highlight of the year was the Gordon Research Conference on Electron Distribution and Chemical Bonding, which provided excellent opportunities for discussions of recent results and new trends.

A Symposium on Chemical Bonding and Lattice Dynamics by Diffraction Methods was held in Moscow in connection with the XII European Crystallographic Meeting in August 1989.

Those Commission members present at the Gordon Conference, and other interested participants, discussed suggestions for the programme of the XV IUCr Congress and proposals for new Commission projects. At this Congress there will be an Open Commission Meeting and two Microsymposia on the subjects suggested by our Commission: Open Commission Meeting on Accuracy of Experimental Electron Densities; Microsymposia on The Application of Charge Densities to Computer Simulation and Molecular Design and on Extinction.

Two new Commission projects have been suggested, which will be discussed in more detail at Bordeaux: Evaluation and/or Measurement of the Electron Density in Perovskite Structures and Quantum Mechanical Description of Electronic Structure from Experimental Charge and Momentum Densities.

The next Sagamore Conference will be held in Konstanz, Federal Republic of Germany, 1-7 September 1991.

### Commission on Crystal Growth and Characterization of Materials

During 1989 the Commission continued its organizational work on the following events sponsored by the IUCr.

(a) First International Conference on Epitaxial Crystal Growth, to be held in Budapest, Hungary, 1-7 April 1990. The Commission is acting as part of the Programme Committee.

(b) International School on Crystal Growth and Crystallographic Assessment of Industrial Materials, to be held at Sitges, Spain, 13-25 May 1990. The Commission is helping to organize the school, formally acting as the Steering and Programme Committees. The school is mainly intended to provide information and expertize for young scientists from developing countries in geographical areas such as North Africa, the Middle East and Latin America.

In addition, the Commission is organizing a Microsymposium on Crystal Growth in Microgravity at the XV IUCr Congress in Bordeaux. This Microsymposium will concentrate on how crystallographic methods are expected to play a role in the structural definition of space materials, rather than on reports of new trends and developments as regards crystal growth in space.

### Commission on Crystallographic Apparatus

During 1989 the Commission continued to work actively on several projects.

(i) The X-ray Attenuation Project (D. C. Creagh): This was inaugurated more than a decade ago and, although on a number of occasions it seemed to reach a conclusion, interest by crystallographers in the project and its findings has caused the project to be regenerated. Laboratories throughout the world are still making measurements on the standard specimens and reporting their results. Two papers have been published [Creagh & Hubbell (1987). Acta Cryst. A43, 102-112; Creagh & Hubbell (1990). Acta Cryst. A46, 402-408]. Other papers will ensue. It is worth noting that there has been an upsurge of interest by crystallographers in the accuracy of crystallographic data tables, of which the attenuation data tables are one.

(ii) The Single-Crystal Lattice-Parameter Project (G. DeTitta): Progress on this project has been slow: necessarily so because it is essential to characterize the specimens to be used in international collaborative projects very carefully. Considerable interest exists in this project as evidenced by the incorporation of sessions on accuracy in lattice-parameter measurements at meetings of both the American Crystallographic Association and Society of Crystallographers in Australia in the past two years.

(iii) The Accuracy in XAFS Project (R. Frahm, H. Oyanagi, J. Wong and D. C. Creagh): The aim of this

project is the creation of standard procedures for the collection, analysis and interpretation of XAFS spectra. To do this one must first acquire, and characterize, standard materials for use by other laboratories. A start has been made in that specimen materials have been acquired and characterized and preliminary measurements were made by Oyanagi and Creagh in 1989. Some of the material tested proved to be unsuitable for use in a round-robin experiment of the kind we envisage. Further discussion of this project will take place at the XAFS VI conference in York, England, in August 1990. It is anticipated that further testing will take place in Japan in November 1990.

(iv) International Tables for Crystallography, Volume C: The Commission has been involved extensively in the time-consuming task of providing data for these tables and has produced sections on X-ray spectroscopy, X-ray absorption, anomalous dispersion and radiation safety. It also sought to initiate a project on the re-measurement of a number of X-ray wavelengths which are thought to be in error but failed to attract sufficient funding for this project even though a demonstrable need exists for better more accurate data.

(v) Open Commission Meeting, Bordeaux (H. Hashizume and D. C. Creagh): Enthusiastic activity by Professor Hashizume has ensured that the meeting on Area Detectors in X-ray Diffraction will be very successful with nearly two hundred abstracts being submitted.

The Commission has been host to two special committees, the High Pressure Group and the Inter-Commission Committee on Synchrotron Radiation, the latter being organized jointly with the Commission Neutron Diffraction.

(i) The High Pressure Group (Chairman: H. Schulz) has organized a highly successful workshop sponsored by the IUCr following the AIRAPT meeting in Paderborn, Federal Republic of Germany. 82 participants from 13 countries attended the Workshop on Crystal Structure Determination at High Pressure – Future Developments. The participation included 15 young scientists, which augurs well for the future of this research activity.

(ii) The Inter-Commission Committee on Synchrotron Radiation was set up to establish the need, or otherwise, for a separate IUCr Commission on Synchrotron Radiation, but it never really started to function. This led the IUCr Executive Committee to set up such a Commission on an *ad interim* basis until the Bordeaux General Assembly. The Inter-Commission Committee has therefore been disbanded.

### Commission on Crystallographic Computing

No report has been received from the Chairman of the Commission.

### Commission on Crystallographic Data

The main area of Commission activity in 1989 centred around development of the free-format Crystallographic Information File (CIF). This work is being carried out in conjunction with the IUCr Working Party on Crystallographic Information and the Commission on Journals. The CIF is based on the self-defining text archive and retrieval file structure of S. R. Hall. It is being designed as a vehicle for machine-readable submissions to *Acta Cryst.* Considerable progress has been made on the selection of descriptor field names and on their precise definition. The file structure itself has also undergone some modifications as a result of this process. The requirements of different chemical structure types, *i.e.* metals/alloys, inorganics, molecular compounds and proteins, are being taken into account. A test manuscript, submitted as a CIF via electronic mail to Chester, has been successfully processed to camera-ready copy by desktop publishing software. Some tidying of these proposals is required in early 1990. The CIF project, and possibilities for machine-readable submissions to Acta Cryst. will be the subject of a Microsymposium at the XV IUCr Congress in July 1990.

Sales of the Commission monograph *Crystallographic* Databases have now covered its production costs. Some 350 copies have been sold since publication in August 1987. The Commission report on Standardization of Unit Cell Data was revised during 1989 and will be presented for acceptance at Bordeaux.

Several members of the Commission met informally at the meeting of the American Crystallographic Association in Seattle in July 1989. Discussions centred on the CIF project noted above.

### Commission on Crystallographic Nomenclature

Three major reports, prepared by the Commission's Subcommittee on Statistical Descriptors in Crystallography (Chairman: D. Schwarzenbach), its *ad hoc* Committee on the Nomenclature of Symmetry (Chairman: P. M. de Wolff) and its Subcommittee on the Nomenclature of Inorganic Structure Types (Chairman: J. Lima-de-Faria), were completed and brought to publication during the year.

The first report, 'Statistical Descriptors in Crystallography', was published in Acta Cryst. (1989), A45, 63-75. In addition to providing a definition of the major statistical terms used in papers on crystallography, the report discusses the statistical basis upon which crystal structure refinement procedures depend, considers the influence of defects in the model used for refinement and the choice and significance of the weighting schemes employed, and makes a series of recommendations designed to improve the use of statistical methodologies in crystallography.

The second report, 'Definition of Symmetry Elements in Space Groups and Point Groups', published in Acta Cryst. (1989), A45, 494-499, redefines symmetry elements in terms of their fundamental and carefully defined geometric elements. The work of the *ad hoc* Committee was extended during the year to a consideration of the printed and graphical symbols of symmetry elements.

The third report, 'Nomenclature of Inorganic Structure Types', published in Acta Cryst. (1990), A46, 1-11, develops a self-consistent nomenclature of crystal-chemical formulas that offers much greater structural insight for inorganic materials than is possible with traditional chemical formulas.

The year was also marked by an upsurge in the use of electronic mail for communication within the Commission. With only one member not network connected, discussions and interactions came closer to the level expected at meetings in person. In consequence, a new major nomenclature problem has been identified and methods for dealing effectively with it are in the process of being worked out.

### Commission on Crystallographic Teaching

The main activities of the Teaching Commission in 1989 have been the organization of a Winter School in Bangkok, Thailand, 7-15 February 1990, and of a session on The Teaching of Crystallography: How to Engage Science Students of the 1990s and Beyond to be held at the XV IUCr Congress in Bordeaux.

At present our efforts are concentrated on the Pamphlet Series and the Visiting Professorship Programme. Experiences from Teaching Schools have highlighted the need for individually specialized teaching topics and methods for students in different locations throughout the world. The aim is to have these two programmes adequately address the perceived needs of groups requesting teaching assistance and to ensure their successful implementation.

### Commission on Electron Diffraction

Work continued on the proposed multi-author book *Electron Diffraction Techniques*, which is sponsored by the Commission and will be published in the IUCr/Oxford University Press Series *IUCr Monographs on Crystallography*. However, the deadline for completion of the chapters, December 1989, passed with only about half the chapters in near-final form and by March 1990 two key chapters were still outstanding. Nevertheless, a publication date in 1990 may still be possible.

A proposal for a survey on the computer programs being used for the calculation of the intensities of high-resolution electron micrographs and electron diffraction patterns of crystals was discussed at a meeting held in Las Vegas, Nevada, USA, in March 1989. The coordinator of the project, Dr D. Van Dyck, has now formulated the proposal which will be circulated in 1990. Publication of the results of the survey is anticipated.

Proposals by the Commission to the Programme Committee of the XV IUCr Congress were received favourably and there will be an Open Commission Meeting on Convergent Beam Electron Diffraction and a Microsymposium on Surface Structure by Electron Diffraction and Other Methods.

An unusual situation has arisen in relation to the Commission membership, in that more than half the members are leaving because their terms have expired or because they do not wish to continue on the Commission. Procedures have been initiated to find new Commission members, providing a well balanced and active Commission whilst conforming with the recommendation of the Executive Committee for a reduction in the number of members from 10 to 8.

### Commission on Neutron Diffraction

At the Perth General Assembly, the IUCr Executive Committee requested the Commissions on Neutron Diffraction and on Crystallographic Apparatus to appoint a Sub-committee of four, two from each Commission, to coordinate activities of their Commissions with the synchrotron community whenever possible, and to make recommendations to the Executive Committee on the desirability of establishing a Commission on Synchrotron Radiation. The two members appointed from the Commission on Neutron Diffraction were D. E. Cox and G. Lander. Although the Sub-committee chairman failed to report to the Executive Committee, the above-mentioned two members, after discussions with members of the Commission and other members of the neutron and synchrotron community, recommended that a separate Commission on Synchrotron Radiation be established. This was done by the Executive Committee, on an *ad interim* basis until the Bordeaux General Assembly.

After much deliberation, the members of the Commission unanimously recommended to the IUCr Executive Committee that Gordon and Breach be permitted to use the Commission's mailing list in their publication of a newsletter *Neutron News*, to be mailed to a very large audience, about 6000 people compared with mailings to about 800 for the previous newsletter. Registered users will receive copies free of charge, similar to the arrangement whereby synchrotron users receive Synchrotron Radiation News free. The first issue of Neutron News was mailed in early March 1990 and the second issue went to press later that month.

The Commission supported and helped organize a Microsymposium at the XV IUCr Congress on Dynamical Aspects of Neutron Scattering. Another Microsymposium, on Neutron Diffraction in Materials Science Research, was organized by other members of the neutron community. The Commission also gave its support to two satellite meetings of the Congress; one in Paris beforehand, on Short Range Order in Ill-Ordered Materials, and one in L'Alpe d'Huez afterwards, on Complementary Applications of Diffraction by Neutrons and by X-ray Synchrotron Radiation.

### Commission on Powder Diffraction

The major event during 1989 involving the Commission was the International Workshop on the Rietveld Method, held at the Stichting Energieonderzoek Centrum Nederland (ECN) in Petten, The Netherlands, 13-15 June. There were about 150 participants, a number very much at the upper edge of the range the planners thought acceptable. The scientific programme consisted of 18 invited lectures and 45 contributed posters. The programme sought to emphasize the current status, problems and further development of the method itself, rather than the many important applications to current scientific problems. The Workshop was fortunate to have Dr Rietveld present both as a lecturer and as an active member of the Organizing Committee. It was at the beginning of his still-continuing career at the ECN that Dr Rietveld wrote the program and papers in 1967 and 1969 which have given the method his name. The ECN was the host organization and took care of all financial matters except the IUCr grants to young scientists. Fifteen such grants totalling \$5 055 were approved and 13 grantees actually attended and received their grants. By all accounts, the workshop was very successful.

A book, tentatively entitled *The Rietveld Method* and based on the 18 invited papers, is in the scientific editing process and will be published in the IUCr/Oxford University Press Series *IUCr Monographs on Crystallography*.

Newsletters 2 and 3 were issued in 1989 under the editorships of Z. Bojarski and T. Yamanaka, respectively.

D. K. Smith (Pennsylvania State University) started a Program Information Exchange Bank (of computer programs for analyses of powder diffraction data) and accepted appointment as a Consultant to further develop and operate the Bank.

Plans are well developed for the Congress Satellite Meeting on Powder Diffraction in Toulouse, 16-19 July 1990. Substantial outside support has been obtained (CNRS; JCPDS). The meeting promises to be well attended and scientifically significant for powder diffraction.

The Rietveld Refinement Round-Robin project, led by R. J. Hill, has now been fully launched. About 25 intending participants have signed up. Both X-ray and neutron powder diffractionists are involved. The sample materials, one simple and one complex, plus sets of both neutron and X-ray data on a third material (lead sulfate) for local Rietveld refinement of the structure, have been distributed. A preliminary report is planned for the Satellite Meeting in Toulouse.

A Rietveld Summer School for Beginners to be held in Cieszyn, Poland, 9-11 August 1990, received IUCr sponsorship and financial support in the form of IUCr grants for young scientists and some travel funds for the four lecturers/instructors. Three of these lecturers met and developed the detailed curriculum for the School. Hands-on experience, running Rietveld refinements on a personal computer, is to be an important ingredient.

The Commission was fortunately able to use the opportunity of the presence of most of the members at the Rietveld Workshop to hold a three-part meeting of the entire membership. This face-to-face meeting was very productive in reviewing, critiquing and further planning the various Commission projects.

The Commission requests the assistance of the crystallographic and diffraction community to help it become more aware of the various meetings, activities and needs related to powder diffraction in all parts of the world. The Commission would also appreciate suggestions for other or expanded activities that would be of benefit to the powder diffraction community.

### Commission on Small Molecules

During 1989 the Commission helped organize a symposium in Poland, proposed topics and speakers for the scientific programme for the XV IUCr Congress in Bordeaux, and continued its programme on International Cooperation in Intensity Data Collection.

The Symposium on Organic Crystal Chemistry, Poznań-Rydzyna, Poland, 14-17 August 1989, featured 30 invited lectures and oral contributions on polymorphism, molecular interaction in crystals and analysis of inter- and intramolecular forces and presentations describing frontier research in low-temperature and neutron diffraction analysis of structures. The 56 contributed posters covered a wide range of topics, including biologically active small molecules, organic compounds of chemical interest, crystal growth, powder diffraction and protein studies. A dozen countries were represented, including many crystallographers from the USSR.

The Commission submitted proposals for the programme of the XV IUCr Congress in Bordeaux. Suggestions for 25 lectures were grouped under four major topics, with alternative speakers suggested for many of the lectures.

The Commission encouraged the organization of the Third International Symposium on Computational Chemistry: Molecular Modelling - Theory and Experiment, to be held at Schloss Elmau, Federal Republic of Germany, 22-26 October 1990. The purpose of these symposia is to bring together experimentalists and theoreticians interested in a broad range of structural studies, to foster exchange of ideas and to encourage collaboration. Seven new international collaborations were initiated in the project International Cooperation in Intensity Data Collection, and a number of new data sets were collected through collaboration previously initiated as part of this project.

The Commission is encouraging the organization of a satellite meeting on molecular dynamics at ECM-13, to be held in 1991 in Ljubljana, Yugoslavia. This would encourage participation of spectroscopists who will be holding an adjoining meeting in Yugoslavia.

### Ad interim Commission on Modulated Structures, Polytypes and Quasi-crystals

No report has been received from the Chairman of the Commission.

### Ad interim Commission on Synchrotron Radiation

At its meeting in July 1989, the Executive Committee of the IUCr decided to set up this Commission, *ad interim* until the XV General Assembly in Bordeaux. It invited J. R. Helliwell to serve as Chairman, who accepted readily. A draft set of the terms of reference was drawn up and approved by the Executive Committee, after wide consultation between the Chairman and members of the relevant scientific community. The agreed draft terms are being published in a variety of crystallographic newsletters. The goals of the Commission are, briefly, to provide a focus of organization and information for aspects of diffraction experiments at synchrotron-radiation sources worldwide, and so facilitate access to appropriate instruments, to maintain and improve standards and to organize meetings.

Proposals for the membership of the Commission were made and accepted. Most of the proposed members agreed to serve on the *ad interim* Commission.

### 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 1989 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1989 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1990, but approved in 1989, are listed below:

1. Winter School on Crystallography of Natural Materials for Science and Industry, Bangkok, Thailand, 7-15 February 1990.

2. First International Conference on Epitaxial Crystal Growth, Budapest, Hungary, 1-7 April 1990.

3. International School on Crystal Growth and Crystallographic Assessment of Industrial Materials, Sitges, Barcelona, Spain, 13-25 May 1990.

4. Symposium on Short Range Order in Ill-Ordered Materials, Orsay, near Paris, France, 16-18 July 1990 (satellite meeting of Bordeaux Congress).

5. Symposium on Powder Diffraction, Toulouse, France, 16-19 July 1990 (satellite meeting of Bordeaux Congress).

6. Symposium on Symmetry in Physical Space and in Superspaces. Physical Applications: Quasicrystals, Incommensurate Phases, Châtenay-Malabry, near Paris, France, 29-31 July 1990 (satellite meeting of Bordeaux Congress). 7. Symposium on Complementary Applications of Diffraction by Neutrons and by X-ray Synchrotron Radiation, near Grenoble, France, 29-31 July 1990 (satellite meeting of Bordeaux Congress).

8. International School on Crystallographic Computing, Bischenberg, near Strasbourg, France, 29 July-5 August 1990 (satellite meeting of Bordeaux Congress).

9. Summer School for Beginners with the Rietveld Method, Cieszyn, Poland, 9-11 August 1990.

10. Iberoamerican School on Crystallography and XI Iberoamerican Congress on Crystallography, Mérida-Mérida, Venezuela, 30 September-13 October 1990.

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. 43 papers presented at the International Conference on Applications and Techniques of Small-Angle Scattering, held at Argonne, 26-29 October 1987, were published in the December 1988 issue of the Journal of Applied Crystallography, Vol. 21, pp. 582-885. 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 six months in advance of the date of the meeting, writing to the Chairman of the Sub-committee. The present Chairman is E. N. Maslen. A new Chairman will be appointed at Bordeaux. 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**

### Asian Crystallographic Association (AsCA)

The primary present objective of AsCA is to provide Asian crystallographers with information and news about crystallographic activities in the region, and in other parts of the world. In 1989 two AsCA newsletters were distributed widely within the 16 countries in the Asian region, as well as to the Executive Committees of other international associations.

The AsCA represents countries which differ enormously in their resources and relative expenditure on crystallographic research. Its aim is to provide, through communication and cooperation, a sharing of the expertize and equipment of the scientifically advanced members with less developed member countries. Until now this role has been assumed mainly by the IUCr Commissions, by way of activities such as the Commission on Crystallographic Teaching Schools in Tianjin, People's Republic of China, in 1988 and Bangkok, Thailand, in 1990. It is intended that, in the future, the AsCA will play a more prominent role in the organization and sponsorship of these events, and ultimately will be in a position to organize conferences of its own. Initially this will probably be done in conjunction with one of the regular national meetings in the region.

### European Crystallographic Committee

The Twelfth European Crystallographic Meeting (ECM-12) was held in Moscow, 20-29 August 1989. The Opening Lecture by L. M. Blinov was on Structure and Properties of Liquid Crystals, and was followed by a concert and reception. The scientific programme continued with four General Lectures, several Microsymposia and about 1000 poster sessions, followed by post-ECM Symposia.

The annual meeting of the European Crystallographic Committee was held on 22 August, during ECM-12. It received reports on ECM-12 and heard plans for ECM-13, to be held in Ljubljana, Yugoslavia, 25-30 August 1991, as well as for meetings in 1992 and 1994. The President of the IUCr spoke to the meeting about the Extraordinary General Assembly to be held on 19 December in London.

### International Organization for Crystal Growth (IOCG)

The main activity of the IOCG during 1989 was the organization of the Ninth International Conference on Crystal Growth (ICCG-9) and the Seventh International Summer School on Crystal Growth (ISSCG-7). Both events were hosted in Japan by the Japanese Association for Crystal Growth (JACC).

ICCG-9 was held in Sendai, 20–25 August 1989. There were well over 1000 participants and the conference consisted of 5 plenary papers, 79 invited papers and 740 contributed papers. This was an increase of 30% compared with the total number of papers presented at the previous ICCG's, which reflects the trend of crystal growth to expand its interests and activities. The proceedings of ICCG-9 will be published in 1990 as a single issue of J. Cryst. Growth.

ISSCG-7, held in Zao, 26-31 August, had about 120 participants. The school provided a high-level programme of lectures that covered a wide range of topics.

During the IOCG General Assembly, which took place during ICCG-9, the membership of the IOCG Executive Council was renewed for the triennium 1989-92. The officers are: B. Cockayne (UK), President; A. A. Chernov (USSR), Vice-president; R. F. Sekerka (USA), Vicepresident; M. Schieber (Israel), Secretary; E. Kaldis (Switzerland), Treasurer; R. Kern (France), Past president.

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

The general structure and modes of operation of the JCPDS have been detailed in previous annual reports and remain similar. It is, however, an organic organization, so some change is a constant of its existence. There is a constant drive toward development of better data acquisition, review and distribution methods. One of the new editorial procedures involves appointment of standing consultants for particular areas covered by the Powder Diffraction File (PDF), e.g. minerals. All powder data sets on minerals are, then, to be processed through this (4 person) group. Improved throughput is expected. The organization is growing physically, also, and more space is needed at the headquarters site. The number of members was 114 as of March 1989. All are volunteers. A large fraction of them seem to be actively, busily involved in the various task groups.

There is a continuing trend toward inclusion of more data of other kinds along with the diffraction data. In part, this trend is augmented by the success of the CD ROM as a medium for the database; it has plenty of space for other data, also. In fact, at the March meeting it was said that the JCPDS was going to approach the IUCr to assess possible interest in 'publishing' the International Tables for *Crystallography* on CD ROM (separately, not with the PDF). No such approach has, in fact, been made.

The JCPDS has voted to change its Articles of Incorporation to include in its purposes 'activity relating to materials characterization and other charitable, educational or scientific activity generally, as defined under the Internal Revenue Code of 1986'. The Grants-in-Aid programme remains a very important one for the JCPDS. An interesting example of work in identifying subsets of the PDF that would be particularly useful is that of zeolites. It was reported at the March meeting that a search through the PDF had found nearly 400 zeolites which were 'hiding' in the file: that is, they were not identified or classified as zeolites. By the fall meeting, they were all collected in a book edited by P. Bayliss. By scanning lots of journals, the Minerals Project found about 4100 sets of powder diffraction data of minerals which had not previously been published and about 100 new minerals.

Future editions of the PDF will move toward using the JCAMP format. For a description of the format, see, for example, R. S. McDonald and P. A. Wilks, 'JCAMP-DX: a Standard Form for the Exchange of Infrared Data in Computer Readable Form', *Applied Spectroscopy* (1988), **42**, 151-162. The electron diffraction PDF has been put on CD ROM. Tests show about 85-90% success in phase identification with this database.

As a result of initiatives taken by the IUCr representative, the JCPS is co-sponsoring and giving \$14 000 support to the IUCr Congress Satellite Meeting on Powder Diffraction, Toulouse, 16–19 July 1990, and will hold a JCPDS workshop there. The JCPDS will also co-sponsor the First European Powder Diffraction Conference, Munich, March 1991, and will hold another workshop there.

The JCPDS Board chose to subsidize the journal *Powder* Diffraction, rather than let the subscription rate go up to cover costs, in order to encourage more subscriptions. Inquiries of the editors of *Powder Diffraction* revealed no discontent with the relationship between it and J. Appl. Cryst. The relevant Editors and Co-editors communicate with each other and, on occasion, exchange manuscripts.

### **Representatives on Other Bodies**

### International Council for Scientific and Technical Information (ICSTI)

The International Council for Scientific and Technical Information (ICSTI) held its 1989 General Assembly and associated technical meetings in Orléans, France, 20-26 May.

Numeric Data Group. The main activity of the Group continues to be the compilation of a Directory of Numeric Databases. The IUCr representative is engaged in editing the replies of the crystallographic databases to the Group's questionnaire.

Group on Education and User Needs. A study is in progress to determine the nature, size, scope, content and results of ongoing programs for (i) training scientists and engineers in the use of computerized information and data services and products; and (ii) developing simplified userfriendly search software specially designed for scientists and engineers. At his own request, A. J. C. Wilson, the IUCr representative on ICSTI, was relieved of his responsibility as Chairman of this Group.

Other Committees and Groups. Because of the overlapping of sessions, it was possible for the IUCr representative to attend only the Finance Committee, the Chemistry Working Group, and the Technical Activities Coordinating Committee (TACC). The Chemistry Working Group considered a draft paper by Dr G. Poetzscher of FIZ Chemie on User Needs in Chemical Information. It was felt to be useful but in need of much revision and rewriting; suggestions were received from several ICSTI members. A. J. C. Wilson agreed to undertake the rewriting, and the revised paper has been submitted to the Journal of Chemical Information and Computer Science. A shortened version will be presented at the International Symposium on the Future of Scientific, Technological and Industrial Information Services to be held in Leningrad 28-31 May 1990. The TACC is being reorganized. Again at his request, A. J. C. Wilson was relieved of the chairmanship of the Committee on Statutes and By-Laws. To maintain continuity he remains Vicechairman for the time being.

Technical session. There was a technical session on Bibliometric Techniques and New Added-Value Products. Bibliometric techniques provide a method for comparing the 'productivity' of individuals, laboratories or countries, and there was a lively interest in the six talks. Most of such work is based on the Science Citation Index, and thus publications in journals not covered by the SCI are not represented. There was a lively criticism of the papers, of which at most two showed a full appreciation of the weaknesses as well as of the strengths of the methods.

General Assembly. The General Assembly met twice. The formalities for the admission of the International Union of Pure and Applied Physics (IUPAP) as a 'new' Member in Class A were completed, and the Institut National de la Santé et de la Recherche Medicale (INSERM) was admitted as a new Member. [IUPAP had been a member of the ICSU Abstracting Board, but had not agreed to automatic transfer to membership of ICSTI.] J. R. (Ron) Smith, for twenty years the Chairman of the TACC and its predecessors, was elected as an Honorary Member.

The decision made in 1988 was confirmed: the bookkeeping will be simplified by using French francs for the main accounts, and converting only the balance sheet and summaries into dollars. The General Assembly fixed the scale of dues in French francs; the conversion involves no general increase or decrease, though some Members lose and others gain from the variations of the dollar/own currency/franc exchange rates. For the IUCr and other Unions the annual dues become FFr 3000. As this was a regular triennial General Assembly, a new Executive Committee was elected. The Officers are Edward Kennedy (BIOSIS), President; Barrie Stern (Elsevier), Vice-president; Daniel Confland (DIST), General Secretary; and Kent Smith (US NLM), Treasurer.

The second session of the General Assembly was a 'celebration of the fortieth anniversary', with four short talks: Introduction (Jacques Michel, outgoing President); Forty Years of ICSU AB/ICSTI (A. J. C. Wilson); Main Technical Achievements of ICSU AB/ICSTI (Mel Day); and The Future of ICSTI (Edward Kennedy, incoming President). The text of A. J. C. Wilson's talk has been deposited at the IUCr office.

The next meeting is scheduled to take place in Gatlinburg, Tennessee, USA, 13-16 May 1990.

.

### Committee on Data for Science and Technology (CODATA) of the International Council of Scientific Unions

CODATA did not meet during 1989, but several publications were issued. A list of titles can be obtained from the IUCr representative.

CODATA has its own task groups, working groups, commissions and committees with various objectives, and the IUCr could participate in some of them. These are CODATA Referral Database, Artificial Intelligence and Computer Graphics, Network Steering Committee, Fundamental Physical Constants, Materials Database Management, Hybridoma Data Bank, Biological Macromolecules, Microbial Strain Data Network, Biological Databases, Terminology and Nomenclature Used in Biology, Critically Evaluated Phase Equilibrium Data, Chemical Thermodynamic Tables, Geothermodynamic Data, Environmental Databases, Industrial Data, Multisatellite Thematic Mapping, Data Sources in Far-Eastern Countries, and Systematic Identification of Foods in Numerical Data Banks. More task groups may be formed in respect of the IUCr's activities; the IUCr representative recommends nomination of members for the groups on CODATA Referral Database, on Artificial Intelligence and Computer Graphics and on Biological Macromolecules.

### Committee on Space Research (COSPAR) of the International Council of Scientific Unions

No report has been received from the IUCr representative.

### Committee on the Teaching of Science (CTS) of the International Council of Scientific Unions

CTS met in 1989 in Paris. Most of its activities are directed to the teaching of science in developing countries, where teaching is difficult or impossible because of a lack of instruments, and therefore the important task is the development and maintenance of low-cost equipment. The training of technicians is also an important activity of CTS. One of the future goals of CTS is to popularize the teaching of science in general. This is considered to be most important, and essential if science is to survive.

Committee on Science and Technology in Developing Countries (COSTED) of the International Council of Scientific Unions

The IUCr representative received no communications from COSTED during 1989.

### Interdivisional Committee on Nomenclature and Standards (IDCNS) of the International Union of Pure and Applied Chemistry

IDCNS reviews all relevant recommendations originating in IUPAC Commissions and Divisions for publication in *Pure & Applied Chemistry*. About 50 such documents are reviewed annually and a copy of each is received by the IUCr representative. A document of interest to many crystallographers will be the new two-part edition of *Inorganic Nomenclature* (the Red Book), scheduled to appear in 1990. The IDCNS meets on alternate years in association with IUPAC General Assemblies, and in the UK the other years. The representative attended the meeting held in 1989 immediately prior to the 35th IUPAC General Assembly, in Lund, Sweden. This provided a useful introduction to the complex interactions between major international bodies charged with standardizing the names and values of important quantities. Neither IDCNS nor the IUCr is at present represented on the Comité Consultatif des Unités du Conférence Générales des Poids et Mesures. Efforts are now being made to achieve IDCNS representation.

### Commission on the Structure and Dynamics of Condensed Matter of the International Union of Pure and Applied Physics

The main activity of this Commission is to give preliminary examination to applications for sponsorship by IUPAP of conferences within its field of interest and to make appropriate recommendations to IUPAP. The work is done by correspondence. There are no remarkable actions to be reported during 1989.

### Action Committee on Conferences and the Condensed Matter Divison of the European Physical Society

In March 1989, the Committee on Conferences discussed the refereeing system in connection with the handling of conference proposals. The main questions were (1) should referees also look into the selection of invited speakers and their geographical distribution, and (2) could it be tolerated that, in certain conferences, the same people rotate in the International Programme Committee? About 70 EPS meetings received approval or sponsorship.

At a special meeting in November 1989, the EPS President summarized recent decisions of the Council. The former Advisory Committees had been renamed Action Committees. The newly named Action Committee on Conferences would aim to co-ordinate the works of other committees, divisions and national societies via a 'task force' of four or five people. The Committee also considered how to organize study conferences in physics and in other domains, similar to the Gordon Conferences in the USA, perhaps under the appealing name of Fermi Conferences.

By special arrangement, the IUCr representative on the EPS Action Committee on Conferences has been invited regularly to the meetings of the board of the Condensed Matter Division, when he repeatedly drew the members' attention to the activities of those IUCr Commissions of particular relevance to the Division, and requested all members to inform the IUCr Executive Secretary of meetings for announcement in the Forthcoming Meetings section of the *Journal of Applied Crystallography*. During the December 1989 meeting, the IUCr representative suggested co-operation between the *ad interim* Commission on Synchrotron Radiation of the IUCr and the corresponding, recently created, Interdivisional Group of the EPS. The CMD organizes annual conferences, which include topics close to crystallography.

### **International Council of Scientific Unions**

The IUCr representative attended the 1989 meeting of the ICSU General Committee and associated meetings of the Working Group of Physics, Chemistry, and Earth and Space Science Unions, 11-15 October, in Lisbon, Portugal.

The free circulation of scientists was, once again, one of the major topics for discussion. No progress was reported on the requirement by India and Japan for scientists from South Africa to sign a repudiation document if they wished to attend a meeting in either of these countries. On the other hand, the participants at the ICSU meeting were very pleased to learn from the IUCr representative that changes had been made to Danish law which permitted journals published in Denmark (including Acta Crystallographica and the Journal of Applied Crystallography) to be distributed to South Africa.

There were discussions on possible changes to the ICSU Statutes and Rules of Procedure, and to the frequency of ICSU General Committee meetings and General Assemblies. No decisions will be made before the next General Assembly, in 1990.

The major international programmes of ICSU are the International Geosphere-Biosphere Programme, the World Climate Research Programme, Scientific Aspects of National Disasters and the International Space Year. The IUCr is only involved directly with the last of these programmes, in materials science in space in co-operation with the ICSU Committee on Space Research (COSPAR).

### Finances

The audited accounts of the year 1989 are given at the end of this Report. For comparison, the figures for 1988 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 1989 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, a gain has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 202 627. This gain has been divided amongst the Fund Accounts in direct proportion to the balances on these accounts at 31 December 1989. 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 1989. 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 600 073 with the banks at the end of the year was represented by Dfl 86 311 and US \$275 with the Amsterdam-Rotterdam Bank, US \$70 592 with Merrill Lynch, £162 412 with the National Westminster Bank and SwFr 6383 with the Union Bank of Switzerland. The bank accounts with the National Westminster Bank USA were closed during 1989.

The balance sheet shows that the assets of the Union, excluding stocks of unsold publications but including the gain of SwFr 202 627 resulting from fluctuations in rates of exchange, have increased during the year, from SwFr 4 491 458 to SwFr 5 183 168.

No new fund accounts were established in 1989. A transfer of SwFr 40 000 was made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund and two transfers of SwFr 40 000 were made to the Research and Education Fund, one from the *Acta Crystallographica* Fund and the other from the General Fund.

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 263 985, before the transfer of SwFr 40 000 to the Research and Education Fund, as compared with a surplus of SwFr 123 784 in 1988. The administrative expenses were SwFr 199 340 in 1989 as compared with SwFr 214 911 in 1988. Of this amount, SwFr 60 331 was charged to the publications of the Union.

SwFr 14 056 was spent on supporting scientific meetings, SwFr 7438 was required for expenses of non-publishing Commissions and SwFr 11 114 for travel expenses of the Union representatives on other bodies. The cost of the two Finance Committee meetings held in 1989 was SwFr 15 313, whilst the Executive Committee meeting cost SwFr 30 360. The Union received SwFr 16 428 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 133 500. Interest on bank accounts and investments credited to the General Fund was SwFr 350 260.

The President's Fund account received no donations and no grants were paid from the fund.

The Acta Crystallographica account for 1989 shows a surplus of SwFr 229 909 before the transfer of SwFr 80 000 to other fund accounts, as compared with a surplus of SwFr 239 829 in 1988 before similar transfers of SwFr 120 000.

The subscription rates were maintained unchanged from 1988 and have now not been increased since 1983. Less pages were published in 1989 than in 1988, because of the implementation of new technologies and staff shortages in the technical editing office and at the typesetters, but the costs per page have increased significantly, when expressed in Swiss Francs, partly because of changes in the exchange rates of the Danish Krone, the Pound Sterling and the US Dollar as compared with the Swiss Franc.

The number of paid subscriptions to all sections of Acta, including 113 personal subscriptions in 1988 and 100 in 1989, decreased from 1113 in 1988 to 1097. However, the number of paid subscriptions to the separate sections of the journal increased from 244, 163 and 125 in 1988 to 262, 181 and 133 in 1989 for Sections A, B and C, respectively. 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 84 and 16% respectively for 1989. For 1988 the percentages were 80 and 20%. The technical editing costs for Acta Crystallographica were SwFr 334 754, excluding the costs of office refurbishment, as compared with SwFr 277 820 in 1988. 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 surplus of SwFr 42 707, as compared with a surplus of SwFr 11 637 in 1988 before the transfer of SwFr 15 000 to the Publications and Journals Development Fund. The number of pages published in 1989, 642 pages, was more than in recent years, except for 1988 when the proceedings of a meeting were published and the journal consisted of 996 pages. The number of subscriptions, including 107 personal subscriptions in 1988 and in 1989, decreased from 1026 in 1988 to 1022 in 1989.

The Structure Reports account shows a surplus of SwFr 60 765 in 1989 as compared with a deficit of SwFr 34 575 in 1988. Two A Series volumes and one B Series volume were published in 1989, so that the sales income was considerably higher than in 1988 when only two A Series volumes were published. Editorial expenses were much less than those of 1988 but the level of these expenses does fluctuate from year to year. Publishing and editorial expenses in 1989 were SwFr 60 043 and SwFr 37 181 respectively, as compared with SwFr 23 261 and SwFr 61 619 in 1988. The net income from sales was SwFr 157 989 in 1989 as compared with SwFr 50 305 in 1988. The large increase resulted from the publication of the B Series volume in 1989.

The International Tables account shows a deficit of SwFr 46 867, as compared with a surplus of SwFr 33 706 in 1988, because of much higher publication and editorial expenses. The increase in publication expenses arose because Volume A, Volume II and Volume IV were reprinted, in addition to the costs of reprinting the Teaching Edition of Volume A and typesetting Volumes B and C which occurred in both years. There was also a significant increase in technical editing expenses, being mainly work on Volumes B and C. The net income from sales of SwFr 88 526 derived mostly from the sale of 370 copies of Volume A, but 360 copies of the Teaching Edition of Volume A were also sold.

The Book Fund includes the sales of the remaining publications of the Union. SwFr 881 was received from the sales of Escher Kaleidozyklen, the remaindered stock of which was purchased by the Union in 1988. SwFr 6671 was received from the sales of Crystallographic Databases, compiled by the Commission on Crystallographic Data and published in 1987. This publication has proved to be extremely popular. SwFr 324 was received from the sales of Fifty Years of X-ray Diffraction. SwFr 472 was received from the sales of Symmetry Aspects of M. C. Escher's Periodic Drawings, as well as SwFr 250 royalties for the Japanese edition of this book. SwFr 542 was received from the sales of Early Papers on Diffraction of X-rays by Crystals, SwFr 348 from the sales of Fifty Years of Electron Diffraction and SwFr 419 from the sales of the Seventh Edition of the World Directory of Crystallographers, which was published in 1986. Sales of sundry publications yielded SwFr 405.

As usual, the *Molecular Structures and Dimensions* account shows no surplus, because this account was charged with a contribution (SwFr 3629) towards the publication costs of Volume 15, the last volume to be published. Because no volume has been published since 1984, the sales income is small.

For the first time, the income for the Publications and Journals Development Fund account and for the Research and Education Fund account includes interest as well as transfers from other fund accounts. The interest has been calculated at a nominal rate of 8% on the balance in the fund during the year, this being the formula used for crediting the Ewald Fund with interest since 1986. The expenses of SwFr 50 481 in the former account for computer expenses, including the purchase of computing equipment for the Chester office, all relate to the technical editing of the journals. For the latter account the main expense was SwFr 78 996 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union.

The only expense for the Ewald Fund in 1989 was the expenses of the Selection Committee's work in examining the nominations for the second Ewald Prize and making its recommendation to the Executive Committee. The balance in the fund at 31 December 1989 was SwFr 218 494.

+				IP	4 I E	ZR	192	11		NA	L	UNI		Or	CKIS	IA	LLU	UKAPH
	90		£C1,£K£,1	8,660	121.310		6,025	1 570 148	01.06/77/60		10,262	1,296,538		3.177.224	17,696		4,491,458	
	rancs 1988	68,268	1,324,885										3,254,803 -77,579					
	Swiss Francs		600,073	11,123	342,577		8,900	067 673	106407		cov, 112	685,610		4.477.612	19,946		5,183,168	
	1989	44,190	688,000										4,748,245 -270,633					
Balance Sheet as at 31 December 1989		CURRENT ASSETS Cash at banks Current accounts	Deposit and savings accounts	Cash with Union officials	Debtors, accrued income and payments in advance	Subscriptions from Adhering	Bodies, due for 1989		Deduct Creditors, accrued	charges and income received	іп адуансе	NET CURRENT ASSETS INVESTMENTS (Note 4)	At market value Change in market value	At revalued cost	FIXED ASSETS Office equipment at revalued cost, less depreciation			
e Sheet as a	1988		900,605	16,034	1,828,802	382,661	68,246	216,729 11.053		5,881		493,518	341,705 196,224	4.491.458			4,491,458	
Balanc		Balance at 31 December 1989	1,170,342	16,686	2,090,453	442,674	134,260	116,773	10/100	6,120		543,020	372,377 218,494	5.183.168			5,183,168	
	Swiss Francs 89	Excess of income over expenditure for the year	223,985		149,909	42,707	60,765	-46,867 467		I		28,274	16,115 13,728	489.083				
	Sw 1989	Fluctuations in rates of exchange (Note 2)	45,752	652	81,722	17,306	5,249	6,911 460	Ì	239		21,228	14,557 8,542	202.627				
		As at 1 January 1989	900.605	16,034	1,858,802	382,661	68,246	216,729	rrn*11	5,881		493,518	341,705 196,224	4 491 458				
			FUND ACCOUNTS General Fund	President's Fund	Acta Crystallographica Journal of Applied	Crystallography	Structure Reports	International Tables	Molecular Structures	and Dimensions	Publications and Journals	Development Fund Research and	Education Fund Ewald Fund					

### Report of the Auditors to the International Union of Crystallography

We have audited the financial statements on pages 884-896 in accordance with Auditing Standards.

In our opinion, the financial statements give a true and fair view of the state of affairs of the Union at 31 December 1989 and of its excess of income over expenditure and source and application of funds for the year then ended. We have not been requested by the Union to consider the requirements of Swiss Company Law as regards these financial statements.

27 March 1990 Manchester, England

**Chartered** Accountants

Signed: TOUCHE ROSS & CO

884

International Union of Crystallography

### INTERNATIONAL UNION OF CRYSTALLOGRAPHY

	3,000 14,333	133,500 136,199 105,685	ļ			65,030														457,747
incs 1988				48,176	16,059	795														
Swiss Francs	16,428	133,500 262,998 87,262	39,422			60,331														599,941
1989				44,682	14,894	755														
	Grant received from ICSU COSTED Grant received from Unesco subvention to ICSU	Bodies Bodies Interest on investments (Note 6) Interest on bank accounts (Note 5)	Profit on disposal/redemption of investments	Amounts charged to the lollowing journals and publications: Acta Crystallographica	Journal of Applied Crystal- lography Melocular Semietrons and	Morecular structures and Dimensions														
	4,010				214,911			I	I	33,251	21,588	4,868	02371	7,531	36,500	7,034	2,740	I	123,784	457,747
ncs 1988		5,740 18,430	5,764 2,417 2,225	5,22 1,931	176,066 1,338															
Swiss Francs	4,835				199,340			23,306	25,321	30,360	15,313	11,114	4 873	7,438	14,056	ł	I	40,000	223,985	599,941
1989		6,680 21.383	2,645	526 422	166,356 1,328															
	Subscriptions to ICSU and ICSU bodies Administration expenses:	General Secretary and Treasurer: honorarium and secretarial assistance Audit and acconutancy charges	Legal and professional fees	Travelling expenses Bank charges Executive Secretary's office:	Salaries and expenses Depreciation of office equipment		Fifteenth General Assembly and	Programme Committee	Extraordinary General Assembly Meeting of the Executive	Committee	Finance Committee expenses Travel Exnenses of 111Cr	Representatives on other bodies	Working Party on Crystallographic Information	Commission expenses	Sponsorship of meetings	investments	Logo competition	Research and Education Fund	excess of income over expenditure carried to balance sheet	

General Fund Account for the year ended 31 December 1989

Figures showing how the balance at 31 December is obtained are given on the following page.

### INTERNATIONAL UNION OF CRYSTALLOGRAPHY

885

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

	1989	1988
Balance at 1 January	900,605	726,428
Difference between income and expenditure	223,985	123,784
Fluctuations in rates of exchange	45,752	50,393
Balance at 31 December	1,170,342	900,605

# President's Fund Account for the year ended 31 December 1989

	Swiss France	Francs		Swiss Francs	Francs
	1989	1988		1989	1988
Grants	I	I	Donations received	I	I
Excess of income over expenditure carried to balance sheet	1	Ι			
	I	I		I	1
Balance at 1 January	16,034	15,137			
Difference between income and expenditure Fluctuations in rates of exchange	<u></u> 652	<u></u> 897			
Balance at 31 December	16,686	16,034			

~			1.290.622	3,500	·				1,294,122	
rancs 1988	1,309,567 38,398	36, <i>998</i> 	1,384,963							
Swiss Francs 9			1.367.631	2,142					1,369,773	
1989	1,378,642 31,348	54,078 1,183 6,595 662	1,472,508 104.877							
Subscriptions to Volume 45	(1988 Volume 44) Sale of back numbers and single copies Aiffreicht charced to	subscribers subscribers Sale of microfiche back volumes Net profit on reprints Royalties and copyright fees	Less Publisher's commission on sales	Income from advertisements (net)						
~			641,531		364,586	48,176	120,000	119,829	1,294,122	1,634,964 119,829 104,009 1,858,802
rancs 1988	473,815 96,150 20.020	589,985 11,538 15,165	24,843	33,157 18,854 29,691	266,725 11,095 5,064		60,000 60,000			
Swiss Francs			667,925		427,257	44,682	80,000	149,909	1,369,773	1,858,802 149,909 81,722 2,090,433
1989	462,305 98,801 38 875	599,931	15,338 51,735 921	40,519 19,757 26,477	322,133 12,621 5,750		40,000 40,000			enditure
Publication expenses:	Printing and binding Volume 45 (1988 Volume 44) Distibution and postage	Net loss on reprints Printing Index to Volume 43	Printing Index to Volume 44 Five Year Index 1983-1987 Microfiching back volumes	Editorial expenses: Editorial honoraria Secretarial assistance Postage and sundries	l echnical Editing: Salaries and expenses Computer expenses Depreciation of office equipment	Administration expenses Transfers to other Funds:	Publications and Journals Development Fund Research and Education Fund	Excess of income over expenditure carried to balance sheet		Balance at 1 January Difference between income and expenditure Fluctuations in rates of exchange Balance at 31 December

Acta Crystallographica Account for the year ended 31 December 1989

887

Swiss Francs	255,501 12,989	5,526 	18,339 255,677	10,800				3,363	269,840		
Swiss	266,492 12,166 7 201	7,691 1,428 253 18,030	19,606 268,424	I				ł	268,424		
	to Volume 22 <i>me 21</i> ) 26 numbers and 1 ss rged to 1	mes 2	on sales	Contribution toward cost of printing Conference Proceedings			Erones of orranditures often income	extracts of experiments over income carried to balance sheet			
		155,201			83,580	16,059	15,000	1	269,840	364,612 -3,363 21,412	122 100
Francs	127,562 127,562 12,322 5,015	144,899 7,542 2,760	7,022	1,602 4,235	66,681 2,774 1,266						
Swiss	X	132,814			78,009	14,894	1	42,707	268,424	382,661 42,707 17,306	473 674
1020	100,723 14,503 8,028	123,254 3,690 5,870	6,571	2,967 3,613	61,359 2,404 1,095					enditure	
	Publication expenses: Printing and binding Volume 22 (1988 Volume 21) Distribution and postage Airfreight costs	Twenty Year Index 1968-87 Net loss on reprints Microfiching back volumes	Editorial expenses: Editorial honoraria	Secretarial assistance Postage and sundries	Computer expenses Computer expenses Depreciation of office equipment	Administration expenses Transfers to other Funds: Publications and Journals	Development Fund Evers of income oner expenditure	carried to balance sheet		Balance at 1 January Difference between income and expenditure Fluctuations in rates of exchange	Ralance at 31 December

Journal of Applied Crystallography Account for the year ended 31 December 1989

### INTERNATIONAL UNION OF CRYSTALLOGRAPHY

		daw am			the second of the same and any top support of the second s				
	1989	Swiss Francs	1088 1988			1989	Swiss Francs	ncs 1988	
Publication expenses: Printing and binding Volumes 400, 400 and 540					Sale of copies Volumes 49A, 49B and 54A (1988 Volumes 50A and 53A)	181 714		57 387	
_	46,450 13.593	60.043	14,761 8.500	23.261	Earlier volumes and indexes	31,785	I	12,123	
ļ		,			Less Publisher's commission	213,499		69,510	
ia y expenses	36,209 972	37,181	61,318 301	61,619	on sales	55,510	157,989	19,205	50,305
		I			Excess of expenditure over income				
carried to balance sheet		60,765		I	carried to balance sheet		I		34,575
	, u	157,989	ı n	84,880			157,989		84,880
Balance at 1 January		68,246		99,002					
Difference between income and expenditure Fluctuations in rates of exchange	ture	60,765 5,249		-34,575 3,819					
Balance at 31 December		134,260	•	68,246					

## Structure Reports Account for the year ended 31 December 1989

	1989	Swiss Francs	s 1988			1989	Swiss Francs	uncs 1988	
	34,905				Sale of copies Volume A	77,731		82,636	
dition	7,580 9 550		7,523		I caching Edition of Volume A Volumes II, III and IV	6,771 35,097		9,797 31,243	
Typesetting Volume C 1. Reprinting Volumes II and IV 2.	14,339 26,362 9	92,745	16,643 	32,487	Less Publisher's commission	119,599	00 676	123,676	
	11,690	ł	9,012		011 34103	C/N'IC	070'00	CC0,2C	91,041
Secretarial assistance, postage and office equipment 11 Technical Editing 1	16,154 14,804 4	42,648	9,982 6,454	25,448					
Excess of income over expenditure carried to balance sheet		1		33,706	Excess of expenditure over income carried to balance sheet		46,867		1
	13	135,393		91,641			135,393		91,641
Balance at 1 January Difference between income and expenditure Fluctuations in rates of exchange	·	216,729 -46,867 6,911		170,896 33,706 12,127					
Balance at 31 December	17	176,773	! 1	216,729					

International Tables Account for the year ended 31 December 1989

•		3					
	Swis	Swiss Francs			Swiss Francs	ICS	
	1989	1988		1989		1988	
Publication Expenses:			Sale of copies, net of				
Escher Kaleidozyklen	50	9,173	Publisher's commission on sales				
Crystallographic Databases	110	1,236	Escher Kaleidozyklen		881		3,352
Ronk series expenses	١	86	Crystallographic Databases		6,671		4,986
Atlas of Crystallography	9.957	ļ	Fifty Years of X-ray Diffraction		324		110
World Directory of Crystallographers.			Escher Drawings		472		342
8th Edition	696	I	Early Papers		542		86
			Fifty Years of Electron Diffraction		348		187
			World Directory of Crystallographers,				
			7th Edition		419		910
			Sundry publications		405		133
			Rovalties				
			Escher Drawings	250		593	
			Book series - IUCr				
			Crystallographic Symposia	968	1,218	2,061	2,654
Excess of income over expenditure					1		
carried to balance sheet	467	2,265					
	11,280	12,760			11,280		12,760
				п			
	11 053	8.170					
Difference between income and expenditure	467	2,265					
Fluctuations in rates of exchange	469	618					
- - - -	11 000	11 053					
Balance at 31 December	11,707						

### Book Fund Account for the year ended 31 December 1989

Molecular Structures and Dimensions Account for the year ended 31 December 1989	305Sale of copies1989Swiss Francs305Less Publisher's commission5,9241,487795on sales1,5404,3843871,100	1,100     4,384     1,100       5,552     5,552       329	5,881	Publications and Journals Development Fund Account for the year ended 31 December 1989	Transfers from other funds:       1989       Swiss Francs       1989         Acta Crystallographica       40,000       60,000         Journal of Applied Crystallography       38,755       -         Interest       38,755       -
tres and Dime	Swiss Francs 1988 3,629 	4,384 5,881 239	6,120	rnals Developr	200155 FTAILCS 1988 88,126 80,126
Molecular Structu	Publication expenses: Publication expenses: Salarites Administration expenses <i>Excess of income over expenditure</i> <i>for the year</i> : University of Cambridge TUCr carried to balance sheet	4 Balance at 1 January Difference between income and expenditure Fluctuations in rates of exchange		Publications and Jour	Expenses: Expenses: Computer expenses: Purchase of computer equipment and software Programming and Acordament 32 761 500

		SWISS FIRICS	EICS .				SWISS FT
	1989		1988			1989	
Expenses: Computer expenses: Purchase of computer	002 21		264 00		Transfers from other funds: Acta Crystallographica Journal of Applied Crystallography	40,000 	
equipment and soltware Programming and development	32,761	50,481	00,120 10,141	98,267	Interest	cc/,85	
- Excess of income over expenditure carried to balance sheet		28,274		1	Excess of expenditure over income carried to balance sheet	I	
		78,755		98,267		78,755	
Balance at 1 January		493,518		489,170			
Difference between income and expenditure Fluctuations in rates of exchange	iditure	28,274 21,228		-23,267 27,615			
Balance at 31 December		543,020		493,518			

23,267 98,267

### INTERNATIONAL UNION OF CRYSTALLOGRAPHY

892

	I		ONION OF CRISTALLC	JORATHI	675
	Swiss Francs 1988 60,000 	14,282 74,282		Swiss Francs 1988 13,900 13,550 27,450	
1989	1989 40,000 24,825	104,825		5. 1989 15,680 15,680	
Research and Education Fund Account for the year ended 31 December 1989	Transfers from other Funds: Acta Crystallographica General Fund Interest	Excess of expenditure over income carried to balance sheet	372,377 341,705 Ewald Fund Account for the year ended 31 December 1989	Bequest and donation Interest	
ttion Fund Account	ncs 1988 74,189 — 14,282	74,282 336,867 - 14,282 19,120	341,705 d Account for the	Swiss Francs 1988 2,912  24,538  27,450	160,706 24,538 10,980 196,224
and Educe	Swiss Francs 1989 Swiss Francs 10 96 50 50 88,710	16,115 104,825 341,705 16,115 14,557	372,377 Ewald Fun	1989 	196,224 13,728 8,542 218,494
Research	198 Expenses: 198 History of the Union 210 Young Scientists' Support 78,996 ACA Video Grant 8,050 Report on Teaching 606 Crystallography 606 IUCr Publications 848	Excess of income over expenditure carried to balance sheet Balance at 1 January Difference between income and expenditure Fluctuations in rates of exchange	Balance at 31 December	Prize Cost of medals Selection Committee and expenses Excess of income over expenditure carried to balance sheet	Balance at 1 January Difference between income and expenditure Fluctuations in rates of exchange Balance at 31 December

### Statement of Source and Application of Funds Year ended 31 December 1989

	Swiss Francs		
	1989	1988	
Source of funds			
Excess of income over expenditure for the year	489,083	228,635	
Fluctuations in rates of exchange	202,627	251,319	
	691,710	479,954	
Adjustment for items not involving the movement of funds:			
Depreciation	8,173	7,669	
Fluctuations in rates of exchange on office equipment and investments	-173,632	-131,667	
Profit/loss on sale/redemption of investments	-39,422	7,034	
Total generated from operations	486,829	362,990	
Increase in creditors, accrued charges and income received in advance	44,453	109,381	
Proceeds of sale/redemption of investments	1,199,992	2,214,935	
	1,731,274	2,687,306	
Application of funds	. ,		
Increase in debtors and accrued income (including subscriptions)	-224,142	-950	
Purchase of office equipment	-11,332	-5,555	
Purchase of investments	-2,286,417	-2,814,523	
Movement in net liquid funds	-790,617	-133,722	
<b>1</b>			

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.

### 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:

	1989	1988
Netherland Guilders	1.2547	1.3541
Danish Crowns	4.3234	4.6111
Pounds Sterling	0-3975	0-3771
US Dollars	0-6211	0.6944
European Currency Unit (ECU)	N/A	0.5990

The total assets of the Union at 1 January 1989 (SwFr 4,491,458) would have had the value of US 3,118,868 or £1,693,729 if expressed in those currencies.

At 31 December 1989 these assets (SwFr 5,183,168) would have had the value of US 3,219,266 or £2,060,309 respectively, being an increase of US 100,398 or £366,580 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

		S	wiss Francs		
	Holding at revalued cost 1 January 1989	Additions during the year	Disposals/ Redemptions during the year	Fluctuations in rates of exchange	Holding at revalued cost 31 December 1989
Held by Rothschild Asset Management Limited					
£300,000	795,545	<u> </u>	_	-40,889	754,656
(Old Court International Reserves Limited)	·				
Held by Merrill Lynch					
(Corporate Government Securities)					
US \$120,000 TIGR.SER15-89RG	146,229	_	169,585	23,356	_
US \$22,434 GNM P146535-2016	33,342		1,233	5,356	37,465
US \$65,395 GNM P169332-2016	97,533		3,805	15,481	109,209
US \$36,000 US Treasury May 1991		44,695		4,736	49,431
US \$36,000 US Treasury May 1996		83,202	90,925	7,723	
US \$84,000 US Treasury May 2001		44,973		4,765	49,738
US \$84,000 US Treasury August 2001		114,916	125,988	11,072	
US \$150,000 US Treasury November 2004	_	78,790		-3,602	75,188
US \$150,000 US Treasury May 2005	_	234,093	225,682	-8,411	
(Mutual Funds/Unit Investment Trusts)			,	-,	
US \$50,000 USA Income portfolio	71,644	_	87,068	15,424	_
US \$45,246 GSIF 1B GNMASRS	57,652		66,784	9,132	
2,231 Units ML Capital Fund/CLB (US\$)	36,032	37,786		6,756	80,574
4,306 Units ML Basic Fund/CLB (US\$)	72,042	45,331		11,506	128,879
US \$4,750 Temple Worldwide Fund G		83,688	_		83,688
US \$4,750 Temple Worldwide Fund I	_	83,688	_	_	83,688
US \$365 Haussman Holdings	_	167,133		6,377	173,510
US \$5,000 Global Equity Portfolio		76,446	_	5,918	82,364
(Certificates of deposit)		,		-,	,
US \$50,000 CD Calif Fedl S&L	72,000		75,500	3,500	_
US \$100,000 Coast Fedl		151,000	159,000	8,000	_
US \$100,000 CD Richmond	_	151,000	155,000	4,000	_
US \$50,000 FHLMC 8.5% Sep. 15 20RG	_	79,110		2,948	82,058
US \$50,000 CITI CDT Cards 8.25% Nov. 15 193	_	80,627	_	3,005	83,632
Held by Foreign & Colonial		00,021		-,	
34,298 Units Reserve Asset Fund Class D (US\$)	822,938	53,410	_	92,879	969,227
9,126 Units Reserve Asset Fund Class L (£)	147,201	89,319	_	-13,750	222,770
33,482 Units Reserve Asset Fund Class 0 (US\$)	294,697	342,107	_	44,879	681,683
27,575 Units Reserve Asset Fund Class X $(\pounds)$	530,369	245,103	_	-45,620	729,852
	3,177,224	2,286,417	1,160,570	174,541	4,477,612
					<del></del>

Investments are noted in the balance sheet at their market value at 31 December 1989. 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.

6. Investment Interest

136,199

342,258

5. Bank Interest

	Swiss	s Francs		Swiss	Francs
	1989	1988		1989	1988
National Westminster Bank PLC			ML Basic value fund	5,552	2,800
Manchester Deposit Account	413	889	ML Capital fund	6,977	2,090
Manchester SMMO Account	39,777	73,635	P146535-2016	3,386	1,886
Manchester Business Reserve Account	6,900	8,790	P169332-2016	9,901	5,569
Amsterdam-Rotterdam Bank NV	.,	-,	CD Lomas	, <u> </u>	764
Current Guilder Account	59	69	4.5% Swiss Federal 1983-1995	_	611
Guilder Savings Account	524	878	4.75% Swiss Confederation 1984-1994	_	6,409
Guilder 1 month deposits	2,530	6.829	5.625% International Bank for		
ECU 1 month deposit		3,049	Reconstruction and Development	_	9,552
US\$ Accounts	13	21	9.5% New Zealand 1985-1992	_	16,689
Union Bank of Switzerland			CD Goldome	3,953	´ —
Current Account	36	63	GSIF 1B GNMASRS	· _	5,185
Merrill Lynch			10.5% Treasury Stock 1989	_	37,560
CMA Account	15,743	8,431	13.75% Treasury Stock 1993	_	8.869
Foreign & Colonial	,	,	14.5% Treasury Stock 1994	_	6,611
Cash balances	12	_	15.25% Treasury Stock 1996		9,847
Interest from Munksgaard	21,170	16,527	15.5% Treasury Stock 1998	_	7,043
Interest on officers' petty cash accounts	85	54	US Federal		7,598
			USA Income	3,402	4,274
	87,262	119,235	CD Valley		2,046
			Foreign and Colonial Fund X	98,790	
Allocated to Ewald Fund		13,550	Foreign and Colonial Fund D	52,302	
Balance left in General Fund	87,262	105,685	Foreign and Colonial Fund L	79,772	_
			Foreign and Colonial Fund O	73,894	
	87,262	119,235	CD Coast	1,219	_
			CD Richmond	1,150	
			CD Calif Fed S&L 89	1,100	—
			CITI CDT Cards	553	_
			Withholding tax recovered	4,872	5,053
				346,823	140,456
			Less: Rothschild management fees	4,565	4,257
				342,258	136,199
			Allocated to Ewald Fund	15,680	
			Allocated to Publication and Journals	-	
			Development Fund	38,755	—
			Allocated to Research and Education	24.925	
			Fund Balance left in General Fund	24,825	136,199
			Datance left in General Fund	262,998	130,199

### 896