

## International Union of Crystallography

### Report of the Executive Committee for 1979

#### Personal Notes

Professor W. H. Zachariasen died on 19 December 1979. He was a member of the Union's Executive Committee between 1966 and 1972. An obituary has been published [*Acta Cryst.* (1980), A36, 739–740]. Professor L. O. Brockway died on 17 November 1979. He was Chairman of the Union's Commission on Electron Diffraction between 1957 and 1963. An obituary has been published [*J. Appl. Cryst.* (1980), 13, 106].

#### Meetings

The Union sponsored or co-sponsored the following meetings held in 1979: Inter-Congress Meeting on Modulated Structures, Kailua-Kono, Hawaii, USA, 22–25 March; Inter-Congress Symposium on Accuracy in Powder Diffraction, Washington DC, USA, 11–15 June; Fifth European Crystallographic Meeting, Copenhagen, Denmark, 13–17 August; Sagamore VI Conference on Charge, Spin and Momentum Densities, Mont Tremblant, Quebec, Canada, 19–25 August.

Four Commissions of the Union were able to hold business meetings during the year, mostly at relevant scientific meetings, and two Commissions organized scientific sessions at the Fifth European Crystallographic Meeting.

The Executive Committee met at Copenhagen, 10–13 August. The most important items of business dealt with were (1) sponsorship of meetings; (2) arrangements for the Twelfth General Assembly and Congress, including the membership of the Congress Programme Committee; (3) approval of the audited accounts for 1978; (4) possible change in the currency of the subscriptions paid by Adhering Bodies; (5) subscription rates and other matters concerning the Union's journals, including the establishment of in-house composition facilities; (6) appointment of a new publisher for *Structure Reports* and other publications of the Union; (7) the new volume on direct space of *International Tables for Crystallography*; (8) preparation of a book *Fifty Years of Electron Diffraction*; (9) preparation of a Sixth Edition of the *World Directory of Crystallographers*.

#### Appointments

The Executive Committee confirmed the appointment of Dr M. Hospital and Dr V. I. Simonov as Co-editors of *Acta Crystallographica* and Professor G. Kostorz as a Co-editor of the *Journal of Applied Crystallography*.

#### Publications

Volume 35 of *Acta Crystallographica* and Volume 12 of the *Journal of Applied Crystallography* were published in 1979,

as were Volumes 42B (1975) and 43A (1976) of *Structure Reports* and Volumes 9 and 10 of *Molecular Structures and Dimensions*.

#### Adhering Bodies

The latest list of Adhering Bodies of the Union, and the names and addresses of the Secretaries of the National Committees, is given in Table 1. A full list of memberships of National Committees is given in Annex IV to the Report of the Eleventh General Assembly and Congress [*Acta Cryst.* (1979), A35, 1021–1067]. The following changes to the memberships of committees had been communicated to the Executive Secretary by 1 June 1980:

Canada: Add L. T. J. Delbaere.

China, People's Republic of: Revised spelling of names: Tang You-qi (Chairman), Fu Heng, Gu Xiaocheng, Huang Jin-ling, Liang Dong-cai, Liang Jing-kui, Lu Jia-xi, Lu Xue-shan, Peng Zhi-zhong, Zhang Yuan-long.

Denmark: New membership: J. Danielsen (Chairman), B. Buras, R. Hazell, B. Jensen, B. Jerslev Lund, B. Lebeck, A. Lindegaard-Andersen, H. Micheelsen, R. Norrestam, O. Simonsen, J. Villadsen.

Egypt, Arab Republic of: M. S. Ahmed (Chairman), Y. M. Abbas, S. Abdel-Hady, A. M. Abdel-Reheim, I. S. Ahmed, N. A. Ahmed, M. A. E. Eid, M. S. Farag, M. E. E. Helmy, S. A. Mohammed, S. A. Saleh, F. H. Youssef.

Germany, Federal Republic of: New membership: K. Fischer (Chairman), H. Burzlaff, W. Eysel, K.-J. Range, K. Sanger, H. Stiller, H. Wondratschek.

USA: Omit C. N. Caughlan, J. R. Clark, P. Coppens and R. E. Marsh and add B. W. Matthews, R. E. Newnham, C. T. Prewitt, R. A. Sparks and B. J. Wuensch.

#### Work of the Commissions

##### Commission on Journals

Volume 35 of *Acta Crystallographica* and Volume 12 of the *Journal of Applied Crystallography (JAC)* were produced in 1979. The number of papers and pages in *Acta A* has very slowly increased over the last four years, see Table 2, whereas the number of both in *Acta B* decreased sharply in 1979 after reaching a maximum in 1977 and 1978. The number of manuscripts accepted in 1978 and 1979 were nearly identical, but 1978 started with a backlog of 108 more manuscripts than 1979. The information density on a page of *Acta* has continued to increase, resulting in a slightly shorter average length of paper in *Acta B*, hence reducing the production cost proportionately. The trend toward publishing crystal structure determinations as short structural

Table 1. *Adhering Bodies*

<i>Country</i>	<i>Category*</i>	<i>Adhering Body</i>	<i>Secretary of National Committee</i>
Argentina	I	Consejo Nacional de Investigaciones Científicas Técnicas	M. A. R. DE BENYACAR, Division Física del Solido, Comision Nacional de Energia Atomica, Av. del Libertador 8250. 1429 Buenos Aires
Australia	III	Australian Academy of Science	The Executive Secretary, Australian Academy of Science, PO Box 783, Canberra City, ACT 2601
Austria	I	Österreichische Akademie der Wissenschaften	A. PREISINGER, Institut für Mineralogie, Kristallographie und Strukturchemie der Technischen Universität Wien, Getreidemarkt 9, A-1060 Vienna
Belgium	II	Académie Royale des Sciences, des Lettres et des Beaux-Arts de Belgique	G. S. D. KING, Laboratorium voor Kristallografie, Katholieke Universiteit Leuven, Redingenstraat 16 bis, B-3000 Leuven
Brazil	III	Conselho Nacional de Desenvolvimento Científico e Tecnológico	S. CATICHA ELLIS, DESCM, Instituto de Física, Universidade Estadual de Campinas, Campinas, São Paulo 13100
Canada	III	National Research Council	C. P. HUBER, Division of Biological Sciences, National Research Council of Canada, Ottawa, Ontario K1A 0R6
Chile	I	National Committee for Crystallography	I. GARACOCHEA WITTKE, Departamento de Física, Universidad de Chile, Casilla 5487, Santiago
China, People's Republic of	IV	Academia Sinica	GU XIAOCHENG, Department of Biology, Beijing University, Beijing
Czechoslovakia	I	Československá Akademie Věd	A. LÍNEK, Fyzikální ústav, Československá Akademie Věd, Libeň, Na Slovance 2, 1980 40 Praha 8
Denmark	I	Royal Danish Academy of Sciences and Letters	B. LEBECH, Physics Department, Risø National Laboratory, DK-4000 Roskilde
Egypt, Arab Republic of	I	Academy of Scientific Research and Technology	S. ABDEL-HADY, Faculty of Engineering & Technology, Cairo Higher Institute of Technology, Helwan, Cairo
Finland	I	Suomalainen Tiedeakatemia	L. TAHVONEN, Department of Physics, University of Helsinki, Siltavuorenpenger 20c, SF-00170 Helsinki 17
France	IV	Académie des Sciences (Institut de France)	J. F. PETROFF, Association Française de Cristallographie, Tour 26, 4 place Jussieu, 75230 Paris CEDEX 05
German Democratic Republic	II	Vereinigung für Kristallographie in der GGW der DDR	H. PEIBST, Zentralinstitut für Elektronenphysik, Akademie der Wissenschaften der DDR, Mohrenstrasse 40/41, DDR-108 Berlin
German, Federal Republic of	IV	Arbeitsgemeinschaft Kristallographie	K.-J. RANGE, Fachbereich Chemie & Pharmazie, Institut für Chemie, Universitätsstrasse 31, 8400 Regensburg
Hungary	I	Magyar Tudományos Akadémia	L. ZSOLDOS, Research Institute for Technical Physics, Hungarian Academy of Sciences, PO Box 76, H-1325 Budapest
India	I	Indian National Science Academy	P. KRISHNA, Department of Physics, Banaras Hindu University, Varanasi 221005. Acting Secretary until February 1981: K. VENKATESAN, Organic Chemistry Department, Indian Inst. of Science, Bangalore-560 012
Israel	I	Israel Academy of Sciences and Humanities	Z. SHAKKED, Department of Structural Chemistry, The Weizmann Institute of Science, Rehovot
Italy	III	Consiglio Nazionale delle Ricerche	G. FILIPPINI, Istituto di Chimica Fisica, Università di Milano, Via Golgi 19, Milano
Japan	IV	Science Council of Japan	Y. TAKÉUCHI, Mineralogical Institute, Faculty of Science, The University of Tokyo, 3-1 Hongo 7-chome, Bunkyo-ku, Tokyo 113
Netherlands	III	Stichting voor Fundamenteel Onderzoek der Materie met Röntgen-en Elektronenstralen	The Executive Secretary, FOMRE, Laan van Meerdervoort 53d, 2517 AE's-Gravenhage
New Zealand	I	The Royal Society of New Zealand	J. M. WATERS, Chemistry Department, University of Auckland, Private Bag, Auckland
Norway	I	Det Norske Videnskaps-Akademi	CHR. RØMMING, Department of Chemistry, University of Oslo, PO Box 1033, Blindern, Oslo 3
Poland	I	Polska Akademia Nauk	A. PIETRASZKO, Instytut Niskich Temperatur i Badań Strukturalnych, Polskiej Akademii Nauk, Plac Katedralny, 1, 50-950 Wrocław

\* Adherence to the Union is in one of five Categories I–V, with corresponding voting powers and contributions as set out in Statutes 3-6, 5-5 and 9-4.

Table I (cont.)

Country	Category*	Adhering Body	Secretary of National Committee
South Africa	I	South African Council for Scientific and Industrial Research	P. LE R. MALHERBE, International Relations Division, CSIR, PO Box 395, Pretoria 0001
Spain	III	Consejo Superior de Investigaciones Cientificas	S. MARTÍNEZ-CARRERA, Instituto de Química Física 'Rocasolano', Consejo Superior de Investigaciones Cientificas, Serrano 119, Madrid 6
Sweden	II	Kungliga Vetenskapsakademien	S. ABRAHAMSSON, Department of Structural Chemistry, University of Göteborg, Medicinaregaten 9, S400 33 Göteborg 33
Switzerland	II	Schweizerische Gesellschaft für Kristallographie	W. M. MEIER, Institut für Kristallographie und Petrographie, Sonneggstrasse 5, ETH-Zentrum, CH-8092 Zürich
UK	V	The Royal Society	The Executive Secretary, The Royal Society, 6 Carlton House Terrace, London SW1Y 5AG
USA	V	National Academy of Sciences—National Research Council	H. STEINFINK, Department of Chemical Engineering, The University of Texas at Austin, Austin, TX 78712
USSR	V	Akademija Nauk SSSR	V. I. SIMONOV, Institute of Crystallography, Leninsky prospekt 59, Moscow 117333
Yugoslavia	I	Jugoslavenska Akademija Znanosti i Umjetnosti	B. KAMENAR, Laboratory of General and Inorganic Chemistry, Faculty of Science, Ulica Soc. Revolucije 8, 41 000 Zagreb

\* See footnote on preceding page.

papers continues, with 11% more appearing in this format than as full articles in 1979. The number of papers and pages in *JAC* increased sharply in 1979, excluding the contributions from the Fourth International Conference on Small-Angle Scattering published in 1978.

The publication time, the average number of months between the published date of acceptance and the nominal date of issue, for full articles for the years 1978 and 1979 was 5.3 and 4.8 for *Acta A*, 5.5 and 4.1 for *Acta B* and 5.4 and 5.4 for *JAC*. For short communications it was 4.0 and 4.2 for *Acta A*, 3.6 and 3.4 for *Acta B* and 4.8 and 5.2 for *JAC*, with 4.4 and 3.8 for short structural papers in *Acta B*. The reduction in publication time for most categories of papers, which continues the trend started in 1978, is the result of several factors, not least of which are the excellent efforts of the technical staff in Chester and the active cooperation of the printers in Colchester. It is unlikely that further significant reduction in publication time can be achieved until in-house computer phototypesetting is installed and fully operational in Chester.

The informal grouping of papers as inorganic, organometallic or organic, which was introduced in *Acta B*34, has been continued in *Acta B*35. The number of papers in each grouping of full articles was 117, 91 and 204: that of short structural papers was 87, 120 and 250 respectively in 1979. The ratio of organometallic to organic papers is similar for both categories of article but proportionately many fewer inorganic papers appeared as short structural papers. The expanded format of the *Index to Acta A* and *B*, containing a subject, chemical name, inorganic formula, organic formula, and author index, was first brought out in 1978 and was again used in 1979 to facilitate the location of interesting information by readers of *Acta*.

The European members of the Commission met in London, 15–16 June 1979, and the North American members met in Boston, 14 August 1979. The computerized verification by Co-editors of chemical connectivity relationships in crystal structure manuscripts has revealed numerical

errors in as many as 35% of the manuscripts received. In an attempt to reduce the computational burden on Co-editors, authors of structural papers are now requested to supply their connected computer listings giving both input data and output bond lengths and angles with their manuscript [*Acta Cryst.* (1979), B35, 2284–2285]. Detection of duplicate structural determinations is now being systematically undertaken in Chester. The importance of strict adherence to SI units was reaffirmed. The principle of dividing *Acta B*, after in-house computer phototypesetting becomes available in Chester, was unanimously endorsed. The names proposed for the sections are: Section A, *Foundations of Physical Crystallography*; Section B, *Structural Science*; Section C, *Crystal Structure Communications*. The present *Crystal Structure Communications* will be absorbed in Section C, with the enthusiastic agreement of its Editors. *JAC* will remain unchanged. Improved offprints, with preceding and following articles blanked out, will be made available. Atomic coordinates of macromolecular structure determinations will be deposited in the same way as other materials and also with a data bank in machine-readable form.

V. I. Simonov and M. Hospital were appointed Co-editors of *Acta* and G. Kostorz Co-editor of *JAC*.

#### Commission on Structure Reports

Volume 42B (Organic Compounds for 1976, 1131 pages in two parts) and Volume 43A (Metals and Inorganic Compounds for 1977, 393 pages) were published in 1979.

The following volumes are with the printer and should appear in mid-1980: (1) Volume 43B (Organic Compounds for 1977, about 1600 pages in two parts); (2) Volume 44A (Metals and Inorganic Compounds for 1978, 387 pages). The increase in size of the B volume, relative to that of the previous year, results from a continued large increase in the number of reports, which has already nullified the reduction in size produced by last year's minor format changes. Co-

Table 2. Survey of the contents of the Union journals

<i>Acta Crystallographica</i>															
Vol.	Year	Number of pages*		Number of papers		Full Articles				Short Structural Papers		Short Communications			
						Number	Average length	Number	Average length	Number	Average length	Number	Average length		
A30\	1974	874\	3812	172\	805	135\	605	6.0\	5.6	—	—	37\	69	1.2\	1.2
B30/		2938/		633/		470/		5.4/		131		2.6		32/	
A311†	1975	880\	3824	171\	885	140\	586	6.1\	5.4	—	—	31\	69	1.4\	1.3
B31/		2944/		714/		446/		5.2/		230		2.4		38/	
A32\	1976	1038\	4398	188\	1011	152\	687	6.0\	5.2	—	—	36\	64	1.1\	1.1
B32/		3360/		823/		535/		5.0/		260		2.5		28/	
A33\	1977	1046\	5020	201\	1192	181\	729	5.6\	5.3	—	—	20\	54	1.5\	1.4
B33/		3974/		991/		548/		5.2/		409		2.6		34/	
A341†	1978	1048\	4896	189\	1229	158\	668	6.0\	5.2	—	—	31\	71	1.3\	1.1
B34/		3848/		1040/		510/		5.0/		490		2.5		40/	
A35\	1979	1090\	4220	187\	1085	162\	574	6.0\	5.0	—	—	25\	54	1.5\	1.5
B35/		3130/		898/		412/		4.7/		457		2.5		29/	

*Journal of Applied Crystallography*

Vol.	Year	Number of pages*‡		Full Articles§		Short Communications		Crystal Data		Computer Programs		Short Items¶	
				Number	Average length	Number	Average length	Number	Average length	Number	Average length	Number	Average length
7‡	1974	638	183	81	5.1	10	1.5	18	1.4	2	1.0	11	0.6
8‡	1975	698	201	80	5.6	17	1.7	25	1.5	4	2.0	6	0.6
9	1976	514	136	71	6.2	19	1.6	25	1.6	3	1.7	18	0.5
10	1977	510	134	76	5.5	14	1.8	22	1.3	6	1.6	15	0.9
11‡	1978	733	167	47	5.5	11	1.6	20	1.2	3	2.0	12	1.0
12	1979	642	168	87	6.8	13	1.5	42	1.6	11	1.8	14	0.6

\* Excluding indexes.

† Volume A31 includes, in addition, 338 pages of abstracts communicated to the Amsterdam Congress and Volume A34 includes, in addition, 431 pages of abstracts communicated to the Warsaw Congress.

‡ Volume 7 includes 144 pages of 21 papers and 37 abstracts presented at the Third International Conference on Small-Angle Scattering, Grenoble, 1973. Volume 8 includes 149 pages of 18 papers and 50 abstracts presented at the International Discussion Meeting on Studies of Lattice Distortion and Local Atomic Arrangements, Jülich, 1974. Volume 11 includes 363 pages of 4 review papers, 50 contributed papers, and 17 extended abstracts presented at the Fourth International Conference on Small-Angle Scattering, Gatlinburg, 1977. The columns giving the number of pages and the number of papers in each volume include all these papers and abstracts, but the columns giving the number and average length of Full Articles do not include the Conference papers.

§ Excluding Lead Articles and Conference papers.

¶ Laboratory Notes, Meeting Reports and Letters to the Editor.

editorial work is proceeding on Volumes 44B, 45A and 45B. Volume 36 (Ten-Year Index, 1961–1970) is still not complete.

*Commission on International Tables*

As mentioned in the report for 1978, D. S. Fokkema obtained the complete print-out of the 17 plane groups and the 230 space groups in December 1978. With this achievement his work for the new *International Tables for Crystallography* was terminated.

In January and February 1979 a page make-up for all groups was prepared at Aachen and copies were distributed to all members of the editorial committee. On 22–24 March some contributors met at Aachen to check and discuss the lay-out and to continue work on the Introduction. During the summer the print-outs were checked and the final corrections and additions were made to the space-group diagrams. In

September and October the complete corrected material was sent to the Union's Technical Editor, D. W. Penfold, for final lay-out. Work on the Introduction continued through 1979. Early in 1980 the first three completed sections were transmitted to the Technical Editor for printing. Several other sections are close to completion.

*Commission on Charge, Spin and Momentum Densities*

The principal activity of the Commission was the Sagamore VI Conference organized by V. H. Smith Jr and held at Mont Tremblant, Quebec, Canada. Over one hundred participants were in attendance and recent advances in all aspects of electron density work were thoroughly discussed. The Commission met during the conference and held an open session at which conference participants were able to discuss current projects and future plans.

The oxalic acid project, organized by E. N. Maslen, is now

well under way. Neutron studies at the Institut Laue-Langevin in Grenoble and Brookhaven National Laboratory have been completed, and ten participating groups are making X-ray measurements. Independent charge density calculations have been made by H. Johansen and E. D. Stevens. M. S. Lehmann reported on his feasibility study for the establishment of a data bank for charge-density studies. He was authorized, as a consultant of the Commission, to continue the search for a suitable depository for a file containing form factors and standard deviations. A further project which was formulated is a study of charge, spin and momentum densities in vanadium by all the relevant techniques. P. J. Brown will organize this comprehensive investigation. The Commission's annual newsletter is now circulated to some 400 scientists.

#### *Commission on Crystal Growth*

The Commission held two closed meetings and an open meeting at the Fifth European Crystallographic Meeting in Copenhagen in August 1979. The Commission decided to expand its scientific interests into the field of materials research related to crystal growth. The Commission considered that a modification of its name was necessary, in order to give a clear statement of its expanded field of activity and to help the Union when it sought financial support for the Commission's activities in materials research, including the organization of schools in developing countries. The new name proposed to the Executive Committee is the Commission on Crystal Growth and Characterization of Materials. This expansion of the interests of the Commission was clearly demonstrated in the programme of the Sixth Course of the International School of Crystallography on 'New Crystallographic Perspectives in Materials Science', organized jointly by the Commissions on Crystal Growth and Crystallographic Teaching and held in April 1980 at the Ettore Majorana Center for Scientific Culture in Erice, Italy.

The preparations continue for a school in India, probably to be held in March 1981, on 'Crystal Growth and Characterization of Materials for Energy Conversion and Storage'. The purpose of the school will be to fill the gap between university education and the demands of modern technology in this field. The subject is of great interest not only for developing countries but also for highly industrialized countries.

It is proposed to hold an open meeting at the Twelfth Congress in 1981, presenting some highlights of non-classical crystallography important for materials science, as well as some recent developments in fundamental and applied materials research.

#### *Commission on Crystallographic Apparatus*

All Commission matters were dealt with by correspondence. The proposed business meeting of the Commission during the Fifth European Crystallographic Meeting was cancelled because very few members and consultants would have been able to attend.

1. *Microdensitometer Project* (S. Abrahamsson, P. Kierkegaard, G. Lundgren). Phase 1 of the project has been completed and a detailed report is in the press [*J. Appl. Cryst.* (1980), **13**, 318–337]. It evaluates measurements of film intensities performed in different laboratories. In phase 2

a comparison will be made between data from the same crystal recorded on film and on a diffractometer. This work has been delayed by the lack of a suitable X-ray film. CEA-verken in Sweden has been persuaded to develop a special film for diffraction work. Preliminary tests indicate very good film characteristics, and a report has been submitted to *JAC* for publication.

2. *Survey of Film Characteristics* (M. Elder, O. S. Mills). Equipment for the project has been built and is now being tested. Measurements on the films will begin in 1980. It is intended to evaluate various film properties such as relative speed for Cu K radiation, granularity at different optical densities, fog density, film factor, amount of silver per cm<sup>2</sup> film, characteristic curve, thickness and weight of coating. The speed and fog density will be measured again after a six-month interval. Some 30 film types will be tested.

3. *X-ray Attenuation Project* (D. C. Creagh). An organizing committee has been formed and the planning of the project is well advanced. Sources of incident X-ray beams will range from synchrotron radiation sources to radio-isotope sources. A diverse range of detectors will also be used. Silicon will initially constitute the standard specimen. An announcement of the project will be published in *Acta* and *JAC* [*Acta Cryst.* (1980), **A36**, 499; *J. Appl. Cryst.* (1980), **13**, 199–200].

4. *Radiation Safety Bibliography* (S. Martinez-Carrera). The bibliography on publications dealing with safety devices, radiation techniques and medical aspects of radiation accidents has been completed. Its wider distribution is being considered.

5. *Polarization Ratio Survey* (L. D. Jennings). There have been a number of enquiries indicating interest in contributing to this survey, announced in *Acta Cryst.* (1978), **A34**, 159. Several people have informally mentioned having made measurements. However, no actual unpublished results have been reported to the organizer as a result of the survey. Thus, in spite of the lapse of time since the announcement, it is still premature to make a formal report on the results of the survey. The organizer would be very pleased to hear of any way that additional measurements of the polarization ratio of monochromators could be included.

6. *Meetings.* (a) The Commission supported the Inter-Congress Symposium on Accuracy in Powder Diffraction held at Washington DC, 11–15 June 1979. A report of the meeting has been published [*J. Appl. Cryst.* (1978), **12**, 638–639]. (b) A meeting on radiation safety (W. de Camp, S. Martinez-Carrera) was planned during the Sixth European Crystallographic Meeting in Barcelona. However, a survey made in the USA showed that only a few regulatory agencies might attend. As this may indicate that members of these agencies are unaware of radiation safety aspects of diffraction work, a further attempt will be made to bring them together with scientists and manufacturers, at an Open Commission Meeting on Radiation Safety at the Twelfth IUCr Congress in 1981.

#### *Commission on Crystallographic Computing*

1979 was a particularly busy year, being dominated by preparations for the Winter School in Crystallographic Computing held in Bangalore, India, 4–14 January 1980. This event provided for 144 students from 19 countries to attend lectures and practical work sessions given by over 20

lecturers from 9 countries. Following the example of the successful school at Twente, Netherlands in 1978 much emphasis was placed on the work sessions which occupied about half the timetable and provided a large measure of group and individual tuition. It is clear that this feature was particularly appreciated.

The school took place at the Indian Institute of Science at the invitation of the Director and the Indian National Science Academy. It was inaugurated by Sir John Kendrew who gave a colourful account of the early days of protein crystallography and the part played by computers over 20 years ago.

The collected lectures and worked examples are being prepared for publication for the IUCr by the Indian Academy of Sciences and should appear during 1980.

#### *Commission on Crystallographic Data*

The Commission met during the Fifth European Crystallographic Meeting in Copenhagen. The various activities with which the members have been concerned are summarized below:

1. *Bibliography of Mathematical Crystallography*. Work on this compilation has been completed and it is hoped to have it printed as a monograph and made available from the Chester office.

2. *Standard Crystallographic File Structure*. The specifications of this exchange format have undergone various revisions and the current versions which are being reviewed are the July 1979 main document together with a supplementary note issued in December 1979.

3. *Protein Data Bank*. The protein data bank operated at Brookhaven has made dramatic progress in recent years. The Commission was asked to lend support to a proposal for continued funding of the project and this was done.

4. *Data Errors in Acta Crystallographica, Section B*. An analysis was made of some 1500 data sets which had been published in *Acta Cryst.*, Section B during the period 1977–78. In particular, the effect of careful checking by the editors was examined. Whereas the 1200 structures which had not been checked showed at least one error in 16.4% of them, the 300 structures which had been checked showed an error rate of only 6.5%.

5. *Standards for Powder Publications*. Following on the discussions which took place at the Warsaw Congress, the American Crystallographic Association has prepared a final report setting out recommended standards for the publication of powder data.

6. *Crystal Chemical Formulae*. There was considerable discussion at Copenhagen on the question of the crystallographic description of structure types and the classification of inorganic structures. This was stimulated by a paper on the crystal chemical formulae of simple inorganic crystal structures by E. Parthé.

#### *Commission on Crystallographic Nomenclature*

The principal activities of the Commission this year were concerned with the establishment of two *ad hoc* committees, under ground rules outlined in *Acta Cryst.* (1979), A35, 1072. The *ad hoc* Committee on the Nomenclature of Disordered, Modulated and Polytype Structures has now

been constituted with A. Guinier as Chairman and G. B. Bokij, K. Boll-Dornberger, D. E. Cox, J. M. Cowley, S. Đurović, H. Jagodzinski, P. Krishna, K. Kuchitsu, P. M. de Wolff and B. B. Zvyagin as members and with the Chairman of the Commission as an *ex officio* member. This committee has already begun its deliberations. The second *ad hoc* committee, on the nomenclature of symmetry operations and symmetry elements in space groups, is being appointed.

#### *Commission on Crystallographic Studies at Controlled Pressures and Temperatures*

No official meeting of the Commission was held during 1979, but several members met at the VIIth International Conference on High Pressure Science and Technology held at LeCreusot, France, in July–August. The extension of the study of transformations at specific pressures to the higher pressure region was discussed and preparations were made for a study of the semiconductor–conductor transformation in GaAs, which occurs in the region 180–193 kbar according to previous investigations. The results will be reported at the Ottawa meeting in 1981.

#### *Commission on Crystallographic Teaching*

The Commission organized an open session at the Fifth European Crystallographic Meeting in Copenhagen, which met with great success. It also held a closed meeting which was attended by five members and consultants. The Commission will also organize an open session and a closed meeting at the Sixth European Crystallographic Meeting to be held in Barcelona in July/August 1980.

The programme for the Spring School on 'New Crystallographic Perspectives in Material Sciences', to be held in Erice, Italy, 8–22 April 1980, has been finalized. Discussions are under way for the next Summer School on The Teaching of Crystallography to be organized by the Commission. A formal invitation has been received from Malaysia and has been accepted by the Commission, but the dates have not yet been determined.

The Pamphlet Project is continuing very actively under the editorship of C. A. Taylor. A first set of ten pamphlets will be published in 1980 with the support of a Unesco Contract and a second set is under preparation. Finally, a very interesting historical map of crystallography has been proposed by J. Lima-de-Faria.

#### *Commission on Electron Diffraction*

The current projects of the Commission include the following items:

1. *Preparation of a Book entitled 'Fifty Years of Electron Diffraction'*. The book will be in three sections, covering the starting period (de Broglie, Davisson and Germer, G. P. Thomson, and Kikuchi), the middle period (personal reminiscences from many centres of research), and the present status in several fields of electron diffraction. It is being edited by P. Goodman and a number of co-editors, and should be with the printer before the end of 1980.

2. *Structure Factor Project*. This project is designed to compare data from many laboratories: to check the reliability of several methods of electron diffraction measure-

ment, and to provide valuable data on key substances. So far between 15 and 20 specimens of high-purity GaAs and Cu have been distributed to laboratories in Australia, Japan and the UK. The GaAs samples were all cut from one single crystal. A third sample, of a key silicate mineral, is yet to be distributed. The first data from these samples are to be expected during the next 12 months.

3. *Space Group Project*. The aim of the project is to collect and collate electron diffraction data and methods for space-group determination. Initially three laboratories were contributing to this project, but the interest in this subject has grown to include several laboratories employing high-resolution lattice imaging. The main laboratory active in this area is at Bristol University and has supplied information on 30 space groups belonging to all six crystal systems (trigonal and cubic). It is planned to receive and distribute information at regular intervals so that crystallographers can readily keep in touch with work in progress.

4. *Gas Electron Diffraction Information Service Project*. The project was started in 1977. The third issue (24 pages), organized by K. Hedberg and compiled by B. Starck, was distributed in February 1979. For details of the earlier issues see the Commission reports for 1977 and 1978 [*Acta Cryst.* (1978), **A34**, 1036; (1979), **A35**, 1073].

#### *Commission on Neutron Diffraction*

There has been extensive correspondence within the Commission concerning the Twelfth Congress in Ottawa in 1981 and the associated symposium on neutron scattering. Arrangements have now been made to hold the symposium at Argonne National Laboratory, 12–13 August 1981, with M. H. Mueller as local chairman. It will cover all aspects of neutron scattering, with emphasis on pulsed neutron research and techniques.

Other activities of the Commission have continued. These include the *Magnetic Structure Data Sheets* edited by D. E. Cox, of which the latest batch was sent out in the spring, the compilation of coherent scattering amplitudes by G. E. Bacon, and the bibliography of neutron scattering literature at the Japanese Atomic Energy Research Institute under the direction of S. Hoshino. Two other projects are in a preliminary stage: a compilation of coherent and absorption cross sections by T. M. Sabine and W. B. Yelon, and a compilation of diffractometers and software by M. S. Lehmann and H. Dachs. Unfortunately, there was insufficient material for an issue of the *Neutron Diffraction Newsletter*. All diffractionists are strongly urged to supply items for this Newsletter, to ensure its continued publication.

#### **Sub-Committee on the Union Calendar**

The Sub-Committee receives and considers requests for Union sponsorship and nominal financial support, and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-Committee, during 1979 the Executive Committee approved sponsorship of the following school and meeting, with financial support to the school:

1. Spring School on New Crystallographic Perspectives in Materials Science (Erice, Italy, 8–22 April 1980).

2. Sixth European Crystallographic Meeting (Barcelona, Spain, 28 July–1 August 1980).

Meetings held in 1979 which received Union support are listed at the beginning of the Report of the Executive Committee, under the heading *Meetings*. Organizers of meetings wishing to seek Union sponsorship should write, as early as possible, to the Chairman of the Sub-Committee, Professor J. Karle, Code 6030, Naval Research Laboratory, Washington DC 20375, USA.

#### **Representatives on Other Bodies**

##### *Abstracting Board of the International Council of Scientific Unions*

The Abstracting Board held a series of meetings in Versailles and Paris during the week beginning 19 October 1979. There was only one candidate for membership, the National Technical Information Service, a US government agency. It was elected without dissent, in the category of Member Services. It was gratifying to learn that the reorganization of the Board reported last year, together with a reduced programme of current activities, had cleared the accumulated deficit. A moderate increase in activity could be undertaken in the coming year. Because of teaching duties, the Union representative was unable to attend a consultation meeting with experts from developing countries at Unesco, 25–26 October.

Much of the Full Board meeting was taken up with reports from the Technical Planning and Steering Committee and its various sub-committees. The Chemistry Working Group had undertaken to compare the vocabularies used in chemistry and physics, and work would be undertaken on the changes made by abstracting services in the abstracts, and even in the titles, printed in the primary journals. The Physics Working Group and the Geology Working Group had both made great progress with internationally agreed nomenclature.

Two publications produced by the Board, the *International Serials Catalogue*, and the *Barwise Report* on the impact of on-line search facilities, were thought to be of interest to many organizations outside the Board, and it was decided to mount a publicity campaign, in the hope of producing a substantial income from sales. Recommendations on copyright were agreed, with some reservations. That of chief interest to the Union relates to the use of abstracts by secondary services; the Board recommends that reproduction of these should be freely permitted without charge.

Other matters discussed were the education of users; the delivery to users of copies of the primary documents abstracted by the secondary services; economies through sharing of resources between secondary services; the role of the National Members; and the role of Member Unions. The IUCr representative has been charged with convening a meeting of the representatives of Member Unions at the next General Assembly, which will be held in Sevilla, Spain, in May 1980.

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

During 1979 there has been a major change at the Secretariat in Paris. M. B. Dreyfus, the Executive Secretary,

died after a lengthy illness and his successor is Mme P. Glaeser.

17 countries, 15 Unions and 2 co-opted organizations are represented in the General Assembly. The work of CODATA is being undertaken by the following Task Groups:

- Accessibility and Dissemination of Data.
- Chemical Kinetics.
- Computer Use.
- Data for the Chemical Industry.
- Fundamental Constants.
- International Training Course in the Handling of Experimental Data.
- Internationalization and Systematization of Thermodynamic Tables.
- Key Values for Thermodynamics.
- Space- and Time-Dependent Data.
- Transport Properties for Solids.

In addition there are three advisory panels, on biosciences, geosciences and industrial data.

The work of the World Data Referral Centre has continued and CODATA is under contract to Unesco to prepare lists of referral sources, of particular importance to developing countries.

The Sourcebook on *Data Handling for Science and Technology* has suffered various delays but the text has now been submitted to the publisher. This should provide a useful set of basic references to a multitude of data handling problems.

Plans have been formulated to conduct a training course in data dissemination in Japan in 1980. The course will be scheduled to take place just prior to the next CODATA Conference and General Assembly to be held in Kyoto in October 1980. The Union representative is in charge of the organization of the course.

The following issues of the *CODATA Bulletin* appeared in 1979:

- No. 31 *Data Needs for Energy.*
- No. 32 *Guide for the Presentation in the Primary Literature of Numerical Data Derived from Observations in the Geosciences.*
- No. 33 *Evaluated Kinetic and Photochemical Data for Atmospheric Chemistry.*
- No. 34 *Interactive Computer Graphics: An Overview.*
- No. 35 *CODATA Directory of Data Sources for Science and Technology, Chapter 2: Hydrology.*
- No. 36 *CODATA Directory of Data Sources for Science and Technology, Chapter 3: Astronomy.*

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

A reorganization of COSPAR was discussed and accepted at the plenary meeting of COSPAR in May 1979, in Bangalore, India. It included the formation of interdisciplinary scientific commissions and the definition of their fields of activity. It was also decided that, after 1980, COSPAR meetings would be held biennially instead of annually.

The discussions about the future activities of the various commissions, and particularly that on Materials Science in

Space (MSS), lead to the following conclusions of interest to the Union:

(1) After the Apollo missions the activities of MSS are again in a stage of preparation, with numerous experiments being developed in several countries for the flights of the space shuttle. The performance of these experiments in space is expected to bring important contributions to the development of science and technology of materials.

(2) The main activities in this field appear to be taking place in Europe. The European Space Agency has chartered the second flight of the space shuttle for materials research. The absence of active scientific collaboration of the USSR and the USA in the work of MSS is probably due to a lack of suitable representation in COSPAR of materials research in both these countries. Unfortunately it seems very difficult to change this situation at present.

(3) Most national space agencies have started a scientifically based critical reviewing system of the projects for materials investigations in space. In this way, the quality of the planned space experiments accepted by the European Space Agency has increased considerably. It seems, therefore, that the demands of the Union representative that COSPAR should support only high quality fundamental experiments have contributed to an important development. Only after the fundamental phenomena have been clearly understood will applications become possible.

#### *Committee on the Teaching of Science of the International Council of Scientific Unions*

The Committee met in Paris in March 1979 under the chairmanship of C. A. Taylor. The topics which were discussed included: integrated science education, the interface between mathematics and science, technicians and technical training, science and society, the transition from school to university and post-graduate education. In addition, reports were received about the educational activities of each Union.

The newsletter continues to be published regularly, giving information on the activities of the Teaching Commissions of the various Unions. It appears to be a very useful means of communication. The pamphlets in the series *Learning Strategies in University Sciences* have been published and are available from University College Cardiff Press.

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

COSTED continues to provide financial support to help scientists from developing countries attend scientific meetings or schools. However, the Union representative on COSTED has not received any direct information on the activities of this body.

#### *Scientific Committee on Problems of the Environment (SCOPE) of the International Council of Scientific Unions*

The Fourth General Assembly of SCOPE was held in Stockholm, 11–15 June 1979. It was attended by delegates from 24 countries and 10 Unions and Scientific Committees, together with representatives of other international



organizations. Besides the election of an Executive Committee and the discussion of reports, publications and financial matters, one of the principal tasks during the meeting was to elaborate on the future SCOPE programme.

The concentration of SCOPE activities in the period 1977–1979 on a small number of important topics was approved by the Assembly. The studies of the global biogeochemical cycles will also continue to play a major part in the approved future programme and will mainly be confined to C, N, S and P. Other projects including processes in ecosystems, a groundwater modelling clearing-house, ecotoxicology, land transformation and a climate impact study and risk assessment were discussed. For most of these projects it was recommended or suggested that the Executive Committee should seriously consider establishing new projects or obtaining more detailed proposals.

#### *Commission on the Solid State of the International Union of Pure and Applied Physics*

The Commission continued to deal with applications for sponsorship of conferences. Most of its work was devoted to problems of reorganization of the various Commissions within IUPAP which are concerned with condensed matter.

#### *Conference Committee of the European Physical Society*

The Committee approved various European conferences dealing with physics on the high scientific level, on the condition that these conferences were open to participants from all European countries. The Committee collected statistical data concerning various physics conferences, for the purpose of providing technical information to the organizers of future conferences.

The Union representative continued to work to avoid clashes in dates or topics of conferences which were of interest both to crystallographers and physicists.

#### *International Organization for Crystal Growth*

The scientific collaboration between the International Organization for Crystal Growth (IOCG) and the Union continues to improve because of the close exchange of ideas between members of the Commission who have responsibilities in both organizations and the officers of IOCG. In particular there was collaboration in the preparation of the programme for the Sixth International Crystal Growth Conference and for the International Specialists School on Crystal Growth, to be held in Moscow and Suzdal respectively in September 1980.

#### *European Crystallographic Committee*

The Union representative attended the meetings of the European Crystallographic Committee held on 14 and 17 August 1979, during the Fifth European Crystallographic Meeting in Copenhagen. His role at the meetings was to be responsive to matters that concerned the affiliation of the European Crystallographic Committee with the Union. His duties also involved the making of a report to the Executive Committee of the Union concerning such matters and the main agenda items. No significant issues arose concerning the affiliation of the European Crystallographic Committee with the Union.

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

The Union was represented at the meeting of the ICSU General Committee held in Brussels, 4–5 July 1979, by the Immediate Past President, Professor A. Magnéli.

At the opening of the meeting the President of ICSU pointed out that sixty years ago, in July 1919, the International Research Council (IRC), ICSU's immediate predecessor, had been created in Brussels. It began as a small organization with 12 National Members and 3 Scientific Unions. In 1931, when the IRC was dissolved and ICSU was created, there were 40 National Members and 8 Scientific Unions. Now there are 68 National Members and 18 Scientific Unions, and 18 National and Scientific Associates. Throughout these sixty years the basic objective of the IRC and ICSU has been to improve international scientific cooperation for the benefit of mankind. In his report the President stressed the importance of ICSU in international scientific affairs but also the need to make the work of ICSU better known, particularly to the younger scientists.

In their reports the President and the Secretary General emphasized that ICSU is now developing a whole new range of projects. Work with and for developing countries is greatly increasing. The Singapore Symposium on Science and Technology for Development had meant considerable progress and might lead to major activities in the future.

Decisions and recommendations by the General Committee covered matters such as undisturbed radiofrequencies for radioastronomy and space research, cooperation with the United Nations Development Programme (UNDP) in the period immediately following the UN Conference on Science and Technology for Development, cooperation with the United Nations Environmental Programme (UNEP) concerning an assessment of the extent of increase of carbon dioxide in the atmosphere and of the sensitivity of climate to such an increase, establishment of a steering committee with ICSU representation to carry out a feasibility study of an International Biosciences Centre, and support of an initiative by the International Union of Biological Sciences concerning action to deal with population problems.

Much of the meeting was concerned with reports of the scientific activities of the Unions and other international organizations.

### **Finances**

The Union's auditors, Mann Judd, merged with Touche Ross in 1979 and now practice under the name, Touche Ross & Co. The audited accounts for the year 1979 are given at the end of this Report. For comparison, the figures for 1978 are provided in italics. Negative quantities are indicated by parentheses.

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 US dollars at 31 December 1979 have been translated into US dollars in the Balance Sheet at the rate operative at that date. For the Income and Expenditure Accounts, transactions have been translated into US dollars by applying the rates of exchange appropriate to the individual dates of these transactions. As a consequence of

the fluctuations in exchange rates, a surplus has arisen on the assets of the Union, in terms of US dollars, amounting to \$25 808. This surplus has been divided amongst the nine Fund Accounts with credit balances, in direct proportion to the balances on these accounts at 31 December 1979.

The General Fund account shows a surplus of \$29 433 as compared with a surplus of \$12 033 in 1978. The administrative expenses were \$63 875 in 1979 as compared with \$44 169 in 1978. Of this amount, \$19 858 was charged to the publications of the Union. \$3000 was spent on supporting a scientific meeting and providing additional travel grants, whilst \$2650 was required for travel expenses of Union Representatives on other bodies and \$7037 was allocated to assist Commission meetings. A charge of \$5496 was made to the General Fund for the publication of the Report of the Eleventh General Assembly and Congress. The Executive Committee meeting cost \$10 371. The Union received \$6000 from the Unesco subvention to ICSU, \$4000 under a Unesco Contract towards the cost of the teaching pamphlets prepared by the Commission on Crystallographic Teaching, and a donation of \$2500. The subscriptions from Adhering Bodies increased to \$44 400 as a result of the increase of the unit contribution to \$300. \$842 was received from sales of the Fifth Edition of the *World Directory of Crystallographers*.

Investments of Dfl 120 000, DM 256 000 and Swiss F 90 000 were purchased during the year, and the income from investments rose to \$36 761 compared with \$25 267 in 1978. Interest from banking accounts rose to \$6921, whilst a gain of \$2310 arose from the redemption of Dfl 27 000, \$8000 and DM 5000 of investments during 1979.

The President's Fund account received \$526 in donations during 1979, whilst a travel grant of \$156 was paid from the fund.

The *Acta Crystallographica* account for 1979 shows a surplus of \$1926 as compared with a surplus of \$75 778 in 1978. The subscription rates were increased by about 5% in 1979.

The number of paid subscriptions to both sections of the journals dropped from 1503 in 1978 to 1453 in 1979, including 168 personal subscriptions in 1978 and 152 in 1979. There were also 253 paid subscriptions to Section A and 131 paid subscriptions to Section B in 1979, compared with 248 and 108 respectively in 1978. As in previous years, the total 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; 87 and 13% respectively for 1979. The technical editing costs for *Acta Crystallographica* were \$108 477 in 1979 as compared with \$63 726 in 1978, but still form only a small part of the overall production costs. The increase in costs is attributable to the increase in the technical editing staff, the overall salary increases as a result of increases in the cost of living in the UK, \$11 887 expenses incurred in preparation for the move to larger premises in Chester and an increase in the value of sterling with respect to the US dollar. The journals accounts have also been charged with administrative expenses as in previous years and as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a deficit of \$2996 as compared with a surplus of \$5903 in 1978. The subscription rates were increased by about 4% for 1979. The number of paid subscriptions increased slightly

from 1178 in 1978 to 1180 in 1979, including 106 personal subscriptions in 1978 and 107 in 1979.

The *Structure Reports* account shows a surplus of \$30 992 as compared with a surplus of \$2835 in 1978. Publishing expenses and editorial expenses in 1979 were \$40 491 and \$20 570 respectively.

The *International Tables* account shows a surplus of \$7345 as compared with a surplus of \$8037 in 1978. No publication expenses were incurred in 1979 in connection with the present series of *International Tables*, and the net sales income from this series was \$14 182. The expenses for the new volume on direct space were \$6837, including the preparation of artwork and general editorial expenses.

\$102 was received from the sale of seven copies of *Fifty Years of X-ray Diffraction*. \$872 was received from the sale of 66 copies of *Symmetry Aspects of M. C. Escher's Periodic Drawings*, as well as \$250 royalties for 416 copies of the North American edition of this book sold by Harry Abrams Inc. in 1978 and further royalties of \$82. The sale of 17 copies of Volume I and 19 copies of Volume II of *Early Papers on Diffraction of X-rays by Crystals* yielded \$424, reducing the deficit on this fund account to \$7137.

The *Molecular Structures and Dimensions* account shows a surplus for 1979, because delays at the publishers prevented the distribution of Volume 9 to subscribers until early in 1979, although the publication expenses for this volume were paid in 1978. Volume 10 was also published in 1979. The account was charged with a contribution of \$8752 towards the salary expenses incurred by the Crystallographic Data Centre in the production of volumes prepared in 1979. 445 copies of Volume 9 and 428 copies of Volume 10 were sold in 1979, as well as some copies of the volumes published in previous years. The excess of income over expenditure, \$24 174, was shared between the University of Cambridge and the Union in the ratio 19:1, so that the Union's share was \$1209.

As on previous Balance Sheets, the investments have been valued according to their quotations at the end of the year. Their appreciation in value, together amounting to \$16 537, has not been entered in the General Fund but has again been included in the assets on the Balance Sheet, to avoid annual fluctuations in value influencing the General Fund Account. At the end of 1979 the Union held investments in government bonds with a total maturity value of £30 000, plus Dfl 314 000, plus \$45 000, plus DM 451 000, plus Swiss F 158 000.

The total of \$130 220 with the Banks at the end of the year was represented by Dfl 24 611 and \$1827 with the Amsterdam-Rotterdam Bank, \$31 077 with the Bankers Trust Company, £14 100 with the National Westminster Bank, Swiss F 83 640 with the Union Bank of Switzerland and Dkr 7617 with the Handelsbanken i Aarhus. The amounts shown in the Balance Sheet for debtors and creditors relate to sums, principally on the publishing accounts, due at 31 December 1979. Where appropriate, these amounts have now been settled.

The Balance Sheet shows that the assets of the Union, expressed in US dollars, have increased during the year, from \$742 736 to \$838 553, after including a gain of \$25 808 resulting from fluctuations in rates of exchange but excluding stocks of unsold publications. This level of assets is necessary if a satisfactory financial backing is to be maintained for the Union's large and costly publication activities.

*Acta Cryst.* (1980), A 36, 1082–1088

## International Union of Crystallography

### Balance Sheet as at 31 December 1979

	US Dollars		US Dollars	
	1979	1978	1979	1978
<b>FUND ACCOUNTS</b>				
General Fund	As at 31 December 1978	Balance at 31 December 1979	CURRENT ASSETS	
President's Fund	135,496	169,898	Cash at Banks	70,107
<i>Acta Crystallographica</i>	3,789	4,284	Current Accounts	91,831
<i>Journal of Applied</i>	386,395	400,020	Deposit and Savings Account	101,461
<i>Crystallography</i>	70,544	69,583	Cash with Union Officials	930
<i>Structure Reports</i>	125,573	161,282	Debtors	225,407
<i>International Tables</i>	(44,096)	(36,751)	Subscriptions from Adhering Bodies, due for 1979 to 1980	580
General Publications	56,465	58,166	Deduct Creditors	357,137
<i>Fifty Years of X-ray</i>	2,454	2,633		95,224
<i>Diffraction</i>	9,733	11,267	NET CURRENT ASSETS	261,913
<i>Escher Drawings</i>	(7,561)	(7,137)		
<i>Early Papers</i>	3,944	5,308	FIXED ASSETS	
<i>Molecular Structures</i>			Investments on 31 December 1979	586,155
<i>and Dimensions</i>			At market value	(16,537)
	\$742,736	\$838,553	(Appreciation)/Depreciation in value	345,050
			At cost	(13,618)
	\$25,808	\$70,009	Office Equipment at cost, less depreciation	331,432
				6,085
			TOTAL FIXED ASSETS	576,640
				337,517
				\$838,553
				\$742,736

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

In our opinion, the accounts, accounting policies and notes on pages 1082–1088, which have been prepared under the historical cost convention, give a true and fair view of the state of affairs of the International Union of Crystallography at 31 December 1979 and of its income and expenditure for the year ended on that date.

Manchester, England  
2 June 1980

Signed: TOUCHE ROSS & Co.

Chartered Accountants

## General Fund Account for the year ended 31 December 1979

	US Dollars		US Dollars	
	1979	1978	1979	1978
Subscription to ICSU (24% of subscriptions received from Adhering Bodies in 1978)		718		7,000
Subscription to ICSU Abstracting Board	821	360	4,000	—
Subscription to ICSU Committee on the Teaching of Science	360	300	44,400	32,560
Administration Expenses:			36,761	25,267
Honoraria: General Secretary, Treasurer and Secretarial Assistance	2,193		6,921	4,583
Audit and Accountancy Charges	4,503		2,310	1,704
Taxation Services	548		2,500	—
Legal Fees	727		842	37
Postages, Stationery, Printing and Sundries	1,646	1,925	34	451
Travelling Expenses	1,888	2,772	—	56
Bank Charges and Differences on Exchange	987	783	—	—
Executive Secretary's Office: Salaries and Expenses	45,789	558	—	—
Renovation and Refurbishing of Premises	4,555	956	14,400	10,230
Depreciation of Office Equipment	1,039	628	4,800	3,410
		(442)	658	489
	63,875	34,817	19,858	14,129
		1,185		
		987		
		44,169		
Eleventh General Assembly and Congress Executive Committee	—	11,139		
Travel Grants	—	7,680		
Expenses of Commissions	—	324		
Incidental Expenses	—	1,924		
Publication of Report	5,496	—		
Meeting of the Executive Committee	10,371	—		
Travel Expenses of IUCr Representatives on Other Bodies	2,650	2,163		
Expenses of Commissions	7,037	422		
Sponsorship of Meetings	1,000	4,555		
Travel Grants	2,000	—		
Distribution Costs of the Proceedings of the Madrid Conference on Anomalous Scattering	283	—		
Excess of Income over Expenditure carried to Balance Sheet	29,433	12,033		
	<u>\$123,626</u>	<u>\$85,787</u>	<u>\$123,626</u>	<u>\$85,787</u>

Grant received from Unesco Subvention to ICSU  
 Unesco Contract for Pamphlets Project  
 Subscriptions from Adhering Bodies  
 Interest on Investments  
 Interest on Banking Accounts  
 Profit on Redemption of Investments  
 Donation  
 Sale of *World Directory of Crystallographers: 5th Edition*  
 Sale of the Proceedings of the Madrid Conference on Anomalous Scattering  
 Net Sale of Sundry Publications (Bibliographies, *Book List, List of Computer Programs and Index of Crystallographic Supplies*)  
 Amount charged to Journals and Publications:  
*Acta Crystallographica* 14,400  
*Journal of Applied Crystallography* 4,800  
*Molecular Structures and Dimensions* 658

**President's Fund Account for the year ended 31 December 1979**

	US Dollars	
	1979	1978
Travel Grant	156	333
Excess of Income over Expenditure	370	947
carried to Balance Sheet	<u>\$526</u>	<u>\$1,280</u>
	<u>\$526</u>	<u>\$1,280</u>

US Dollars

1978

1979

526

1,280

\$1,280

\$526

**Acta Crystallographica Account for the year ended 31 December 1979**

Publication Expenses:					
Printing and binding Volume 35 (1978 Volume 34)	299,983	273,593		538,084	519,053
Distribution and Postage	33,228	32,451		14,391	26,998
Airfreight Costs	11,742	11,270		8,654	8,887
	<u>344,953</u>	<u>317,314</u>		<u>561,167</u>	<u>554,965</u>
Printing Index to Volume 34 (1978 Volume 33)	8,353	6,396		55,207	54,605
Printing Acta Supplement S4 to Volume A34	-	5,605	329,315	1,434	-
Editorial Expenses:					
Editorial Honoraria	12,746	12,723		215	1,219
Secretarial Assistance	4,035	2,358			
Postages, Telephone and Office Sundries	7,857	5,099			
Travelling Expenses	3,264	423			
Technical Editing:					
Salaries and Expenses	96,590	60,634			
Renovation and Refurbishing of Premises	11,887	3,092			
Depreciation of Office Equipment	1,168	137,547	708	85,037	
	<u>14,400</u>	<u>10,230</u>			
Administration Expenses	1,926	75,778			
Excess of Income over Expenditure	<u>\$507,179</u>	<u>\$500,360</u>		<u>\$507,179</u>	<u>\$500,360</u>
carried to Balance Sheet					

Subscriptions to Volume 35  
(1978 Volume 34)

Sale of Back Numbers and Single Copies

Airfreight Charges to Subscribers

Royalties

Less Publisher's Commission on Sales

Income from Advertisements

Less Advertising Agent's Commission

and Expenses



**Structure Reports Account for the year ended 31 December 1979**

	US Dollars		US Dollars	
	1979	1978	1979	1978
Publication Expenses:				
Printing and Binding Volumes 42B and 43A				
(1978 Volumes 41B and 42A)	34,297	41,937	87,188	94,521
Typing of Manuscripts	2,534	2,639	24,400	94,521
Cost of transferring stocks to new publisher	3,660	—	111,588	77,970
Editorial Expenses:				
Salary and Honoraria: Editors, Abstractors and Assistants	20,570	30,295	19,535	16,551
Office and Travelling Expenses	—	100	—	—
Depreciation of Office Equipment	—	164	—	—
Less Publisher's Commission on Sales	20,570	30,559	92,053	77,970
Excess of Income over Expenditure carried to Balance Sheet	30,992	2,835	\$92,053	\$77,970

**International Tables Account for the year ended 31 December 1979**

Publication Expenses:				
Artwork for Volume on Direct Space	3,892	—	20,206	17,919
Editorial Expenses:				
Secretarial Assistance and Postages	905	972	6,024	5,115
Travelling	1,963	2,740	14,182	12,804
Less Publisher's Commission on Sales	2,868	3,712	—	10,985
Computer Trial Project:				
Salary	—	10,799	—	37
Travelling and Miscellaneous Expenses	77	1,278	—	—
Less Publisher's Commission on Sales	7,345	8,037	—	—
Excess of Income over Expenditure carried to Balance Sheet	\$14,182	\$23,826	\$14,182	\$23,826

**Fifty Years of X-ray Diffraction Account for the year ended 31 December 1979**

	US Dollars	
	1979	1978
Excess of Income over Expenditure carried to Balance Sheet		
	127	79
Sales of Copies	102	102
Less Publisher's Commission on Sales	63	63
	<u>\$102</u>	<u>\$102</u>
		<u>\$63</u>

**Escher Drawings Account for the year ended 31 December 1979**

Excess of Income over Expenditure for the year	1,090	1,019
Sale of Copies	218	204
Less Publisher's Commission on Sales	872	815
Royalties	332	674
	<u>\$1,204</u>	<u>\$1,489</u>
		<u>\$1,489</u>

**Early Papers Account for the year ended 31 December 1979**

Excess of Income over Expenditure carried to Balance Sheet	530	593
Sale of Copies of Volumes I and II	106	119
Less Publisher's Commission on Sales	424	474
	<u>\$424</u>	<u>\$474</u>
		<u>\$474</u>

**Molecular Structures and Dimensions Account for the year ended 31 December 1979**

Publication Expenses:			
Printing and Binding Volume 10 (1978 Volume 9)	8,645	9,957	39,213
Printing and Binding Guide to Literature	—	9,950	4,975
Carriage and Miscellaneous Expenses	483	786	8,382
Salaries	8,752	3,324	30,297
Administration Expenses			5,302
Excess of Income over Expenditure for the year:	1,316	978	24,995
University of Cambridge	22,965	—	—
IUCr carried to Balance Sheet	1,209	—	—
	<u>\$43,370</u>	<u>\$24,995</u>	<u>\$43,370</u>
			<u>\$24,995</u>



### Accounting Policies

#### 1. Rates of Exchange

Unesco rates of exchange as issued by the ICSU Secretariat are used in the preparation of accounts.

Assets and liabilities held in currencies other than US Dollars at the Balance Sheet date are translated into US Dollars at the rates operative on that date.

In each of the Income and Expenditure Accounts, transactions in currencies other than US Dollars 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 Balance Sheet date.

#### 2. Publication Costs

Publication, editorial and administrative expenses of publications are charged in the appropriate Income and Expenditure Account as and when incurred.

#### 3. Stocks of Unsold Copies of Union Publications

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

#### 4. 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.

#### 5. Depreciation

(i) Investments are included in the Balance Sheet at market value. Depreciation or appreciation, calculated as the difference between cost and market value, is added or deducted to bring the Investments back to cost to prevent the fluctuation in value from influencing the General Fund.

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

### Notes on the Accounts

#### 1. Rates of Exchange

The rates of exchange operative at the Balance Sheet date were as follows compared with the US Dollar:

	1979	1978
Netherlands Guilders	1.94	2.08
Danish Crowns	5.32	5.32
Pounds Sterling	0.456	0.511
Swiss Francs	1.60	1.73
German Marks	1.74	1.92

#### 2. 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, income arising within the United Kingdom under present circumstances will not be subject to United Kingdom Tax.