

## International Union of Crystallography

### Report of the Executive Committee for 1985

#### Meetings

The Union sponsored the following meetings held during 1985: Course on Static and Dynamic Implications of Precise Structural Information, Erice, Italy, 24 May-6 June; Sagamore VIII, Sanga-Saby, Sweden, 28 July-3 August; Sixth International Meeting on Ferroelectricity, Kobe, Japan, 12-16 August; Symposium on Steric Aspects of Biomolecular Interactions, Sopron, Hungary, 26-29 August; Crystal Deposition and Dissolution in Tissues, Lugrin, France, 29-31 August; Pre-meeting Workshop on Direct Methods and their Application to Structures showing Superstructure Effects, Torino, Italy, 29-31 August; Ninth European Crystallographic Meeting, Torino, Italy, 2-6 September; School on Direct Methods, Macromolecular Crystallography and Crystallographic Statistics, Madras, India, 9-19 December.

The Executive Committee met at Rowton, near Chester, England, 24-27 July. The most important items of business dealt with were (1) approval of the audited accounts for 1984; (2) subscription rates and other matters concerning the Union's journals; (3) other publications of the Union, including the new Volumes of *International Tables for Crystallography*; (4) seventh edition of the *World Directory of Crystallographers*; (5) sponsorship of meetings; (6) arrangements for the XIV General Assembly and Congress; (7) XV General Assembly and Congress; (8) creation of an IUCr Award entitled the Ewald Prize; (9) establishment of a new Commission; (10) office technology.

The Finance Committee met at the Chester Office in March and then at Rowton immediately prior to the Executive Committee meeting.

#### Publications

Volume 41 of *Acta Crystallographica* and Volume 18 of the *Journal of Applied Crystallography* were published, as were Volume 46B of *Structure Reports* and the Brief Teaching Edition of Volume A of *International Tables for Crystallography*. Volumes II and III of the earlier series, *International Tables for X-ray Crystallography*, were reprinted.

#### 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.

#### Personal Notes

Professor P. P. Ewald, the last surviving founder of X-ray crystallography, died on 22 August 1985. He conceived and developed the dynamical theory of X-ray diffraction, which led to numerous advances in the field of crystallography. He was the first Editor of *Acta Crystallographica* and was instrumental in founding the International Union of Crystallography. He chaired the first General Assembly and

International Congress in 1948. He was a member of the Executive Committee of the Union from its beginning until 1966. He was Vice-President from 1957 to 1960 and President from 1960 to 1963. The January 1968 issue of *Acta Crystallographica* was dedicated to him on the occasion of his 80th birthday. The November 1986 issue of *Acta Crystallographica* Section A is to be published as the Ewald Memorial Issue. An obituary has been published [*Acta Cryst.* (1986). A42, 1-5].

Professor Herbert A. Hauptman, Director of the Medical Foundation of Buffalo, and Dr Jerome Karle, Chief Scientist at the Laboratory for the Structure of Matter of the Naval Research Laboratory in Washington, DC, were awarded the 1985 Nobel Prize in Chemistry 'for their outstanding achievements in the development of direct methods for the determination of crystal structures'. Dr Karle has served on the Executive Committee of the International Union of Crystallography for many years and was President of the Union between 1981 and 1984.

#### Work of the Commissions

##### Commission on Journals

Volumes 41 of *Acta Crystallographica* (*Acta*) and 18 of the *Journal of Applied Crystallography* (*JAC*) were produced and published in 1985. The total number of papers published in *Acta* decreased 14% compared with 1984, those in *JAC* increased 12%. The total number of manuscripts submitted to *Acta* in 1985 decreased 2% whereas the number accepted decreased 13%, those for *JAC* increased 20% in both categories, compared with 1984.

The average length of all articles in *Acta* has continued to decrease steadily over the last five years from 4.1 pages in 1981 to 3.3 pages in 1985, with largest average decrease in Section A from 5.9 in 1984 to 5.5 pages in 1985; those in *JAC* remained constant at 4.7 pages in 1984 and 1985, see Table 2. Median publication times for full articles, the average elapsed time between published acceptance and nominal publication dates, were 5.0 months for *Acta A*, 5.6 months for *Acta B*, 3.8 months for *Acta C* and 5.1 months for *JAC*. Corresponding publication times in 1984 were 5.1, 5.5, 3.9 and 5.0 months. The publication time for *Acta C* continues to compare favourably with the best publication times of other major monthly scientific journals.

A total of 38 inorganic, 1 organometallic and 25 organic related papers appeared in Section B in 1985, compared with 58, 14 and 24 respectively in 1984. Papers in all categories of structural science continue to be warmly welcomed in Section B. The corresponding totals for Section C in 1985 were 95 inorganic, 198 organometallic and 400 organic crystal structure communications, compared with 94, 240 and 455 respectively in 1984, with substantial decreases in both organometallic and organic categories. It is noted that three papers in Section B report the determination of two structures, one reports three structures and another reports four structures. In Section C, 82 papers

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 Cientificas y Técnicas	M. A. R. DE BENYACAR, División Física del Solido, Comisión Nacional de Energía Atómica, 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, Getriedemarkt 9, A-1060 Vienna
Belgium	II	Académie Royale des Sciences, des Lettres et des Beaux-Arts de Belgique	E. LEGRAND, Materials Sciences Department, Studiecentrum voor Kernenergie, B-2400 Mol
Brazil	III	Conselho Nacional de Desenvolvimento Cientifico e Tecnológico	S. CATICHA ELLIS, DESCM, Instituto de Física, Universidade Estadual de Campinas, Campinas, São Paulo 13100
Canada	III	National Research Council	J. T. SZYMANSKI, CANMET, Department of Energy, Mines and Resources, 555 Booth St, Ottawa, Ontario K1A 0G1
Chile	I	Comision Nacional de Investigacion Cientifica y Tecnologia	D. BOYS, Departamento de Física, Universidad de Chile, Casilla 5487, Santiago
China, People's Republic of	IV	Academia Sinica	XU XIAO-JIE, Department of Chemistry, Peking University, Beijing 100871
Czechoslovakia	I	Československá Akademie Věd	J. GARAJ, Department of Analytical Chemistry, Slovak Technical University, Jánska 1, 812 37 Bratislava
Denmark	I	Royal Danish Academy of Sciences and Letters	B. JENSEN, Chemical Institute BC, Danish School of Pharmacy, Universitetsparken 2, Copenhagen DK-2100
Egypt, Arab Republic of	I	Academy of Scientific Research and Technology	S. A. ABDEL-HADY, Faculty of Engineering & Technology, Cairo Higher Institute of Technology, Helwan, Cairo
Finland	I	Suomen Tiedeakatemiain Valtuuskunta	A. VAHVASELKÄ, Department of Physics, University of Helsinki, Siltavuorenpenger 20 D, SF-00170 Helsinki 17
France	IV	Académie des Sciences (Institut de France)	Y. EPELBOIN, Association Française de Cristallographie, Tour 26, 4 place Jussieu, 75230 Paris CEDEX 05
German Democratic Republic	I	Vereinigung für Kristallographie in der GGW de DDR	P. RUDOLPH, Humboldt-Universität-Berlin, Skt. Physik, Ber. Kristallographie, Invalidenstr. 110, 1040 Berlin
Germany, Federal Republic of	IV	Arbeitsgemeinschaft Kristallographie	H. BURZLAFF, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Universität, Bismarckstr. 10, D-8520 Erlangen
Hungary	I	Magyar Tudományos Akadémia	P. GADÓ, Pagony u.4, Budapest H-1124
India	II	Indian National Science Academy	A. K. SINGH, Materials Science Division, National Aeronautical Laboratory, Kodihalli, Bangalore 560 017
Israel	I	Israel Academy of Sciences and Humanities	M. HAREL, Weizmann Institute of Science, Rehovot
Italy	III	Consiglio Nazionale delle Ricerche	G. FILIPPINI, Centro CNR, Dip. Chim. Fis. Elettrochim, Università di Milano, Via Golgi 19, 20133 Milano
Japan	IV	Science Council of Japan	J. HARADA, Department of Applied Physics, Faculty of Engineering, Nagoya University, Furouchu, Chikusa-ku, Nagoya 464
Mexico	I	Consejo Nacional de Ciencia y Tecnologia	M. SORIANO-GARCIA, Instituto de Quimica, Circuito Exterior, UNAM, Delegacion Coyoacan, 04510 Mexico D.F.
Netherlands	II	Stichting voor Fundamenteel Onderzoek der Materie met Röntgen-en Elektronenstralen	The Executive Secretary, FOMRE, Koningin Sophiestraat 124, 2595 TM's-Gravenhage
New Zealand	I	The Royal Society of New Zealand	J. SIMPSON, Chemistry Department, University of Otago, PO Box 56, Dunedin

\* 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 1 (cont.)

Country	Category*	Adhering Body	Secretary of National Committee
Norway	I	Det Norske Videnskaps-Akademi	B. F. PEDERSEN, Institute of Pharmacy, University of Oslo, PO Box 1068, Blindern, 0316 Oslo 3
Poland	I	Polska Akademia Nauk	A. PIETRASZKO, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, PO Box 937, 50-950 Wrocław 2
Portugal	I	Sociedade Portuguesa de Fisica	M. M. R. R. COSTA, Departamento de Fisica, Universidade de Coimbra, 3000 Coimbra
South Africa	I	South Africa Council for Scientific and Industrial Research	E. P. DU PLESSIS, International Relations Division, CSIR, PO Box 395, 0001 Pretoria
Spain	III	Consejo Superior de Investigaciones Cientificas	M. MARTINEZ, Instituto de Quimica Fisica 'Rocasolano', Consejo Superior de Investigaciones Cientificas, Serrano 119, 28006 Madrid
Sweden	II	Kungliga Vetenskapsakademien	P. KIERKEGAARD, Arrhenius Laboratory, University of Stockholm, S-106 91 Stockholm
Switzerland	II	Schweizerische Gesellschaft für Kristallographie	H.-B. BÜRGI, Universität Bern, Laboratorium für Chemische und Mineralogische Kristallographie, Freiestrasse 3, CH-3012 Bern
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	C. T. PREWITT, National Research Council, Commission on Physical Sciences, Mathematics and Resources, 2101 Constitution Avenue, Washington, DC 20418
USSR	V	Akademija Nauk SSSR	V. I. SIMONOV, Institute of Crystallography, Academy of Sciences of the USSR, Leninsky prospekt 59, Moscow 117333
Yugoslavia	I	Jugoslavenska Akademija Znanosti i Umjetnosti	B. KAMENAR, Laboratory of General and Inorganic Chemistry, Faculty of Science, The University, Ulica Soc. Revolucije 8, 41 000 Zagreb

\* See footnote on preceding page.

report the determination of two structures, nine report three structures, two report four structures and one reports five structures.

The distribution of papers and authors by country, for all sections of *Acta* and for *JAC*, is given in Table 3. The allocation method is shown in the notes to the table. Three countries contributed papers in 1984 but not in 1985, while four others contributed in 1985 but not in 1984. The single largest change is found in the reduced contribution by the USA to Section C in 1985. The total contribution from Poland and Spain increased, whereas that from the Federal Republic of Germany, India, Italy, Japan, the UK and the USA each decreased by more than fifteen papers in 1985.

Publication of the *Index* to Volume 40 of *Acta* was again very late, due to software problems that have now been fully resolved. The computer-prepared *Index* to Volume 18 of *JAC* appeared on time, bound in with the final issue.

The Commission records with deep sorrow the death of John E. Derry, Deputy Technical Editor, on 2 September 1985 [obituary in *Acta* (1986). B42, 120]. Michael H. Dacombe was appointed acting Deputy Technical Editor. Following the resignation of David W. Penfold as Technical Editor, effective 31 December 1985 [an appreciation of his services to the IUCr and details of all the resultant staff changes are given in *Acta* (1986). A42, 288], M. H. Dacombe was appointed Technical Editor. The Commission records its gratitude to the members of the technical

editing staff in Chester for their devoted service during a period of anguish and understaffing. G. Will was appointed Co-editor of *JAC*.

#### Commission on Structure Reports

Volume 46B (Organic Compounds for 1980, 1452 pages in two volumes) was published in 1985. Volume 48B (Organic Compounds for 1981, 1852 pages in two volumes) is with the publisher and will appear in 1986. Co-editorial work is nearing completion for Volume 49B (Organic Compounds for 1982), is well in hand for Volumes 50B and 51B and is in progress for Volume 52B (Organic Compounds for 1983, 1984 and 1985 respectively). The manuscripts for the Inorganic Sections of Volumes 49A, 50A and 51A (Metals and Inorganic Compounds for 1982, 1983 and 1984 respectively) have been completed and await completion of the relevant Metal Sections: these sections are being worked on. Work is also in progress on Volume 52A (Metals and Inorganic Compounds for 1985).

#### Commission on International Tables

The Editors of the volumes and the members of the Commission remain as given in the report for 1984. Work has continued actively throughout the year; the Editors and some Commission members held discussions in Torino at the time of the Ninth European Crystallographic Meeting, and the Editors of Volumes B and C were able to hold

Table 2. Survey of the contents of the Union Journals

*Acta Crystallographica*

Vol.	Year	Number of Pages*	Number of Papers	Full Articles		Short Structural/Short-Format Papers		Short Communications	
				Number	Average Length	Number	Average Length	Number	Average Length
A37 } B37 } †	1981	944 } 2250 } 3194	158 } 630 } 788	136 } 286 } 422	6.4 } 4.9 } 5.4	— 333	— 2.5	22 } 11 } 33	1.1 } 0.6 } 0.9
A38 } B38 }		1982	880 } 3176 } 4056	155 } 905 } 1060	129 } 370 } 499	6.3 } 4.9 } 5.3	— 518	— 2.6	26 } 17 } 43
A39 } B39 } ‡ C39 }	1983		950 } 770 } 1714 } 3434	146 } 121 } 645 } 912	129 } 118 } 636 } 247	6.4 } 6.4 } 2.7 } 6.4	— — —	— — —	17 } 3 } 9 } 29
A40 } B40 } † C40 }		1984	728 } 616 } 2126 } 3470	123 } 99 } 811 } 1033	109 } 99 } 789 } 208	6.2 } 6.2 } 2.7 } 6.2	— — —	— — —	14 } — } 22 } 36
A41 } B41 } C41 }	1985		624 } 456 } 1836 } 2916	114 } 67 } 703 } 884	108 } 66 } 686 } 174	5.4 } 6.4 } 2.6 } 5.8	— — 8	— — 1.5	6 } 1 } 9 } 16

*Journal of Applied Crystallography*

Vol.	Year	Number of Pages*	Number of Papers	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
14	1981	492	118	69	5.7	7	1.7	26	1.5	7	3.1	9	0.9
15 §	1982	676	132	89	6.2	8	1.0	19	1.7	9	2.3	7	0.9
16	1983	661	135	86	6.8	11	1.7	21	0.6	12	2.7	5	1.0
17	1984	488	104	66	6.2	11	1.5	7	0.5	7	2.4	14	0.9
18	1985	546	116	80	5.5	9	1.8	5	0.4	7	3.3	15	0.5

\* Excluding indexes.

† Volume A37 includes, in addition, 428 pages of abstracts communicated to the Ottawa Congress and Volume A40 includes, in addition, 542 pages of abstracts communicated to the Hamburg Congress.

‡ Volume 39 divided into three new Sections in 1983.

§ Volume 15 includes, in addition, 37 pages of 'Current Crystallographic Books 1970 through 1981.'

¶ Excluding Lead Articles

\*\* Excluding Union Announcements, Crystallographers, and Book Reviews.

further discussions in the course of the Winter School in Madras. Detailed progress reports prepared by the Editors of Volumes B and C were discussed by the Executive Committee of the Union at its summer meeting in Chester.

*Volume A (Space-Group Symmetry)*

A Brief Teaching Edition of Volume A of *International Tables for Crystallography* was published in June 1985. It consists of 128 pages with twenty four selected space-group tables and explanatory text Sections 1, 2, 3 and 5 of the full edition. The price has been kept intentionally low in order to make this edition affordable by students.

The first edition of the full Volume A is expected to be sold out in mid-1986, and a second revised edition was sent to the printer in January 1986. It contains corrections of all errors discovered so far, substantial revisions of several portions of text, new diagrams for the plane groups and the trigonal space groups, and two new sections dealing with normalizers of space groups.

*Volume B (Reciprocal Space)*

Many Chapters have reached an advanced stage, and some final drafts were ready before the end of 1985. However, the prospective authors of two Chapters withdrew, necessitating a rearrangement of Part 4 of the Volume.

The question of submitting computer-readable material was discussed with the Technical Editor of the IUCr during the Torino meeting, and a questionnaire was prepared for completion by prospective authors. Many authors appear to be interested in submitting their contributions on floppy disks, and the printers have indicated that many formats can be read and directly transferred to the photocomposing device. This approach is being further investigated, since it holds promise of eliminating many printing errors, particularly in computer-generated tabular material. It is also likely to reduce costs.

*Volume C (Mathematical, Physical and Chemical Tables)*

The state of Volume C is much the same as for Volume B; many authors have submitted final drafts, and several

Table 3. *Distribution of papers and authors, by country, in Acta and JAC for 1984 and 1985*

Country	<i>Acta Crystallographica</i>																<i>Journal of Applied Crystallography</i>			
	Section A				Section B				Section C				Papers		Authors					
	1984	1985	1984	1985	1984	1985	1984	1985	1984	1985	1984	1985	1984	1985	1984	1985				
Algeria	0.8	-	-	-	-	-	-	-	-	0.3	-	2	-	-	-	-				
Argentina	-	-	-	-	-	-	-	-	-	1.8	1.8	4	6	-	1.0	-	2			
Australia	6.1	7.5	11	12	6.9	7.3	21	18	18.0	13.5	45	39	5.0	6.0	10	11				
Austria	3.0	1.0	8	1	-	-	-	-	0.8	0.7	4	2	2.0	-	3	-				
Bangladesh	-	-	-	-	-	-	-	-	1.5	1.5	6	6	-	-	-	-				
Belgium	1.0	2.1	3	5	-	4.9	-	20	19.7	11.4	67	42	-	1.3	-	4				
Brazil	-	0.5	1	1	-	-	-	-	0.8	2.4	3	8	1.0	-	1	-				
Cameroon	-	-	-	-	-	-	-	-	-	0.5	-	1	-	-	-	-				
Canada	2.7	2.1	7	5	4.0	3.3	8	7	38.5	36.5	90	107	2.0	2.0	5	3				
Chile	-	-	-	-	-	-	-	-	4.2	0.9	11	4	-	-	-	-				
China, Peoples' Rep.	2.0	5.0	7	13	2.2	0.7	7	2	2.8	1.2	10	5	-	1.0	2	1				
Czechoslovakia	7.1	0.3	10	2	0.4	-	2	-	7.0	8.0	25	24	4.0	1.4	14	5				
Denmark	2.5	-	6	-	0.5	-	1	-	6.0	6.5	9	11	-	1.1	-	4				
Finland	0.3	-	1	-	-	-	-	1	2.0	3.0	5	9	1.5	1.0	5	1				
France	10.9	6.3	28	18	6.8	8.1	18	39	80.7	75.9	303	262	13.2	11.8	44	35				
German Dem. Rep.	2.1	1.7	5	5	2.0	-	3	-	6.0	0.8	14	3	2.5	3.6	4	8				
Germany, Fed. Rep.	7.3	7.7	16	18	5.8	4.3	9	15	68.3	50.2	187	137	7.5	10.3	18	22				
Greece	-	3.6	3	10	-	-	-	-	4.7	1.3	17	5	-	1.0	-	2				
Hong Kong	-	-	-	-	-	-	-	-	2.0	-	5	-	-	-	-	-				
Hungary	-	-	-	-	-	-	-	-	1.0	1.5	5	6	0.5	-	1	-				
India	2.1	1.0	5	2	3.0	1.0	5	4	60.0	22.8	204	79	3.0	1.0	6	2				
Ireland	-	-	-	-	-	0.4	-	2	1.5	0.5	4	2	-	-	-	-				
Israel	2.3	0.8	4	3	3.0	4.0	4	12	5.4	1.0	10	3	1.0	1.1	3	3				
Italy	3.0	8.3	15	19	4.0	0.1	12	1	48.3	24.6	174	91	2.0	4.0	5	7				
Ivory Coast	-	-	-	-	-	-	-	-	1.8	1.8	10	7	-	-	-	-				
Japan	2.1	3.3	7	9	18.5	7.1	65	18	61.2	48.1	235	173	8.0	3.0	22	8				
Korea, South	-	-	1	-	-	-	-	-	-	0.3	1	1	-	-	-	-				
Malaysia	-	-	-	-	-	-	-	-	1.2	1.0	4	2	-	-	-	-				
Mexico	-	-	1	-	-	-	-	-	6.3	6.7	25	26	-	-	-	-				
Netherlands	8.9	2.6	18	9	1.0	3.0	2	9	25.3	23.0	83	90	7.0	2.0	11	3				
New Zealand	-	-	-	-	-	1.0	-	2	5.0	4.0	14	11	-	-	-	-				
Nigeria	-	-	-	-	-	-	-	-	-	-	2	1	-	-	-	-				
Norway	1.0	1.0	1	1	1.2	-	4	3	0.5	3.7	1	9	-	-	-	-				
Poland	2.0	2.0	7	4	1.5	-	2	-	15.0	29.7	51	71	-	1.5	-	3				
Portugal	1.0	-	1	-	-	-	-	-	0.7	-	2	-	-	-	-	-				
Puerto Rico	-	-	-	-	-	0.2	-	1	-	-	-	1	-	-	-	-				
Romania	-	-	-	-	-	-	-	-	-	-	-	-	1.0	-	2	-				
Saudi Arabia	-	-	-	-	-	-	-	-	3.0	2.0	10	6	-	-	-	-				
Sierra Leone	-	-	-	-	-	-	-	-	-	0.3	-	1	-	-	-	-				
South Africa	0.5	-	1	-	1.0	-	2	-	4.9	3.5	16	9	1.0	2.0	3	6				
Spain	1.0	3.0	3	9	-	0.3	-	1	19.3	32.8	64	123	0.5	2.1	2	10				
Sweden	1.0	-	2	-	2.8	1.0	6	1	11.7	5.4	25	12	1.5	1.0	2	3				
Switzerland	3.0	2.3	4	5	5.0	2.0	13	3	11.9	9.0	36	26	1.0	1.0	1	2				
Taiwan	-	-	-	-	-	0.8	-	3	9.0	7.7	31	31	-	-	-	-				
Tunisia	0.8	-	2	-	-	0.4	-	2	0.6	-	3	1	-	-	1	-				
UK	18.6	11.8	26	28	8.7	10.5	19	33	81.7	68.5	240	214	13.0	13.9	28	52				
USA	19.9	28.7	46	56	19.2	21.0	51	69	179.4	107.5	590	344	24.8	24.0	54	62				
USSR	5.1	8.5	16	28	0.6	1.5	3	5	3.0	8.5	16	43	-	1.7	1	11				
Venezuela	-	-	-	-	-	-	-	-	-	2.0	-	8	-	-	-	-				
Yugoslavia	-	-	-	-	-	-	-	-	6.2	7.6	22	23	1.0	1.0	4	2				

**Notes:**

1. Errata have been excluded.
2. The papers have been allocated to the country or countries where the work was done, directly proportional to the number of authors per country for each paper.
3. The authors' nationalities have been given where known. If an authors' nationality is not known to be otherwise it is given as that of the country in which the work was done.

have offered to provide floppy disks if requested. Withdrawal of authors has posed similar problems, several authors have failed to meet their promised deadlines, and it has not yet been possible to find willing authors for all Chapters. In some cases editorial updating of the corresponding parts of the old Volumes II-IV would suffice to fill the gaps, but it may be found desirable to omit certain planned sections if they cannot be provided before the technical editing of Volume B is completed.

**Commission on Biological Macromolecules**

Major changes in the membership of this Commission took place at the Hamburg General Assembly. During the Hamburg Congress the Commission held one closed meeting. The major issues that were discussed during this meeting were problems connected with commercialization of software and the delay in deposition of protein structure coordinates.

There has been no formal meeting of the Commission since the Hamburg Congress. The activities of the Commission were thus restricted to correspondence by mail. The Commission has endorsed the Protein Data Bank at Brookhaven National Laboratory in the USA as the official repository for structural data obtained by diffraction studies of biological macromolecules. The Commission has also been actively engaged in suggestions for the scientific programme at the next International Congress of Crystallography in Perth, Australia.

#### *Commission on Charge, Spin and Momentum Densities*

The highlight of the year for the Commission was the VIII Sagamore Conference on Charge, Spin and Momentum Densities held from 28 July to 3 August at the Sanga conference centre in Sweden under the able chairmanship of I. Olovsson. The theme of the meeting was the relevance of charge, spin and momentum density studies to chemical bonding. This meeting provided a useful forum for discussion of the current status of research in the interest areas of the Commission. The invited papers set the framework within which lively discussion of current problems took place. Well filled poster sessions gave a good coverage of research work in progress. The Commission extends its warm thanks to Professor Olovsson for organising this very successful meeting.

The Commission held two closed meetings during the conference in which its future activities were discussed. Projects which are being considered are one for the computation of form factors from correlated wave functions and one on comparison of charge, spin and momentum densities in simple solids. The future of the Sagamore conferences was discussed in both the closed and an open meeting. It was generally agreed that they were useful and should be continued. A proposal from the Solid-State Physics group at the University of Coimbra, Portugal, to host the IX Sagamore conference was accepted.

#### *Commission on Crystal Growth and Characterization of Materials*

During the Ninth European Crystallographic Meeting held in Torino, Italy, 2-6 September, the Commission organized the open meeting on 'Physical Properties, Structural Assessment and Applications of Advanced Materials', which was well attended. The speakers, all invited, were able to illustrate the ever closer connections developing between crystallographic methods and the sophisticated cross-disciplinary procedures on which growth and processing of advanced (mainly electronic) materials are based.

Work is also being carried out by the Commission for the organization of two international schools mainly devoted to young scientists of developing countries. The first one will be held in Trieste, Italy, (January 86) on 'Technology, Characterization and Properties of Epitaxial Electronic Materials' and the second one in Fayoum, Egypt, (October 86) on 'Solar Cell Materials and Applications'.

Other possible schools in developing countries, to be submitted to the IUCr for sponsorship, are presently being considered by the Commission.

#### *Commission on Crystallographic Apparatus*

During 1985 much of the attention of the Commission has been focused on the production of sections for *Inter-*

*national Tables for Crystallography*, Volume C. No new projects have been undertaken. Of the existing projects:

(i) The *X-ray Attenuation Project* (D.C. Creagh) has been completed and the results for silicon have been submitted to *Acta Crystallographica* for publication [Creagh & Hubbell (1987). A43, 102-112]. Because some laboratories have still to provide data for both the pyrolytic graphite and the copper specimens it has not been possible to complete the assessment of the data. When all the relevant information is to hand papers will be submitted to *Acta Crystallographica* for publication.

(ii) The *Radiation Safety Project* (S. Martinez-Carrera) has been completed and has culminated in the production of Chapter 10: *Radiation Safety* (D.C. Creagh and S. Martinez-Carrera) for *International Tables for Crystallography*, Volume C. The final draft of this chapter is in the hands of the Editor. In its final revision cognisance has been taken of recent changes in both British and Australian Ordinances relating to radiation protection.

(iii) The *Profile Analysis Project* (M. Zocchi) has however not proceeded well owing to the ill-health of Professor Zocchi. It is regretted that his ill-health has forced him to resign from his membership of the Commission. Whether or not this project can proceed will depend to some extent on the success of the Open Commission Meeting which will be held at the Fourteenth Congress. It will address the topic 'Recent Advances in X-ray Powder Diffractometry' and a substantial section of the meeting will deal with techniques for the profile analysis of diffraction patterns.

No new projects have been suggested to the Commission for evaluation. During 1986 its principal activities will centre on the production of sections for *International Tables for Crystallography*, Volume C and the organization of the Open Commission Meeting for the forthcoming IUCr Congress.

#### *Commission on Crystallographic Computing*

In 1985 the *Guidelines for Computer Program Abstracts* which are to be published in the *Journal of Applied Crystallography* were finalized. [*J. Appl. Cryst.* (1985). 18, 189-190.] It is a way of distributing up-to-date information on programs to the whole crystallographic community. H. D. Flack and other members of the Commission also took part in revisions of the Standard Crystallographic File Structure in close cooperation with the IUCr Commission on Crystallographic Data.

However, the main activities of the Commission were the organization of Schools and open meetings. During 29-31 August 1985 the Workshop on 'Direct Methods and their Application to Structures Showing Superstructure Effects' was held in Torino immediately before the Ninth European Crystallographic Meeting, under the auspices of the Commission. The Workshop was divided into lectures, discussions and practical sessions with computing facilities; there were approximately 37 participants, including ten lecturers. Lectures were published as a booklet of 81 pages. R. Böhme and D. Viterbo were the chief organizers of that successful event.

By the end of 1985, work on the School on Crystallographic Computing planned for Summer 1986 (11-20 August) in Leipzig, German Democratic Republic, had progressed. Responses to the first circular from more than one hundred students reached the organizers, H. Schenk

(Chairman of the Programme Committee) and P. Paufler (Chairman of the Local Committee).

Simultaneously, a great effort was paid to preparation for the School in Adelaide (22–29 August 1987), where N. Isaacs is Programme Committee Chairman and M. R. Taylor Local Organizing Committee Chairman.

Finally, an Open Meeting of the Commission will be held during the Fourteenth IUCr Congress in Perth, Australia. It will be a joint meeting together with the IUCr Commission on Crystallographic Teaching and will focus on 'Crystallographic Micro-computing'.

#### *Commission on Crystallographic Data*

A questionnaire to the National Committees concerning the 'Accessibility of Databases' was returned in the course of the year from 11 countries. The main conclusions are: Databases are highly acknowledged instruments to handle crystallographic data. Not all potential users are familiar with the scientific possibilities of databases and the technical conditions to access them. High standards for contents of databases and for programs to handle them are expected.

In September the Commission met in part at Torino during the Ninth European Crystallographic Meeting. Standardization on the unit cell and the quality of deposited data have been discussed. Reports on these items will be published.

I.D. Brown prepared and distributed a revised version of the 'Standard Crystallographic File Structure'.

#### *Commission on Crystallographic Nomenclature*

The work of the Commission in 1985 was largely carried out by correspondence and the devoted efforts of its several committees. The *ad hoc* Committee on the Nomenclature of Symmetry [see *Acta Cryst.* (1986). A42, 64 for the committee membership] has reached an advanced stage in formulating a proposed definition of symmetry elements and their loci.

Members of the new Subcommittee on Statistical Descriptors in Crystallography appointed in early 1985 [see *Acta Cryst.* (1986). A42, 64 for the terms of reference], with D. Schwarzenbach as Chairman, include H. D. Flack, W. Gonschorek, R. E. Marsh, E. Prince, B. E. Robertson and J. S. Rollett. The Subcommittee has generated vigorous correspondence and is moving toward preparation of a preliminary report.

The provisional Subcommittee on the Nomenclature of Inorganic Structure Types [see *Acta Cryst.* (1986). A42, 64 for the subcommittee membership] met in Lisbon 17–24 April 1985 and produced a useful preliminary report. The progress achieved was encouraging enough that the Commission reappointed all members to regular Subcommittee membership, charged with the formulation of a universal notation for structural similarities. A further meeting in person of the Subcommittee is planned.

The Commission has remained in contact over the year with the International Union of Pure and Applied Chemistry, the International Union of Pure and Applied Physics, the International Mineralogical Association, and other national and international bodies on a variety of nomenclature issues.

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

Members of the Commission have agreed to conduct a round-robin study designed to provide a basis for evaluating the accuracy of pressure measurements made at elevated temperatures. High grade zinc sulfide has been purchased and is presently being distributed to various high-pressure laboratories world-wide. The phase transition pressure in ZnS, which is about 15 GPa at room temperature, will be determined at several temperatures including 100, 200 and 300°C. The combined results determined by various calibration methods will be statistically analysed and an evaluation of the accuracy of pressure calibration in this temperature range made.

#### *Commission on Crystallographic Teaching*

The major effort of the Commission went in organizing a Winter School in Bangalore in December 1985, under the Local Chairmanship of S. Parthasarathy. The themes of the school were direct methods, crystallographic statistics and macromolecular crystallography. Approximately 100 students and 17 lecturers made the school highly successful. The proceedings of the school will be published in due course and will be available at a moderate price.

The Commission organized together with the Commission on Small Molecules a one day tutorial just before the Ninth European Crystallographic Meeting in Torino, Italy, which attracted 100 participants.

The Commission will try to organize in the near future more schools on a range of topics, with the common property that at least half of the course content will be devoted to teaching aspects, so that the participants can use the information to improve their own teaching at their home institutions.

The Subcommittee on the History of Crystallography finalized their review on the *Historical Atlas of Crystallography*. The Commission put the proposal to the Executive Committee that it should support the publication of the Atlas financially.

At the Fourteenth IUCr Congress in Perth, the Commission will be involved in organising a microcomputer exhibition and demonstration, a book exhibition and a noncommercial exhibition. C. H. L. Kennard will be the local organizer of these items.

#### *Commission on Electron Diffraction*

The Commission is responsible for advising the Editors of Volumes B and C of *International Tables for Crystallography* on sections dealing with electron diffraction and microscopy, and various members of the Commission have written articles for *International Tables*. There has been considerable correspondence between the Editors of *International Tables*, the Chairman of the Commission and authors of the various sections, and in some cases there have been meetings between the Chairman and authors.

Preliminary correspondence between members of the Commission concerning the Fourteenth IUCr Congress in Perth in 1987 has occurred, focusing on whether or not to hold a satellite meeting organized by the Commission. It was finally decided not to organize such a meeting in view of other satellite meetings being planned. In particular, the Commission is supporting the satellite meeting 'Validity of Structures from Electron Microscopy' being organized by

J. Sanders, and the Chairman is a member of the International Programme Committee. The Commission is also supporting the symposium on 'Accuracy in Structure Factor Measurements', being organized by S. W. Wilkins.

The Commission has helped various scientists to locate and borrow computer programs for simulating electron diffraction patterns and images from different types of crystals.

#### *Commission on Neutron Diffraction*

The Symposium on Neutron Scattering at Sydney, Australia, has been rescheduled for 8-10 August 1987. (The symposium is a satellite meeting of the Fourteenth IUCr Congress at Perth which opens immediately afterwards.) Topics for discussion will include structure analysis, magnetic neutron diffraction and industrial applications of neutrons.

The Newsletter appears twice annually and is distributed to over 700 addresses. An Asian issue (edited by R. Chidambaram of Bombay) was sent out in April 1985, and a European issue (edited by K. Hennig of Dresden) in October 1985.

The Commission has given assistance to G. E. Bacon in editing the book *Fifty Years of Neutron Diffraction: the Advent of Neutron Scattering*. Publication of this book is scheduled for early 1987 (publishers Adam Hilger Ltd). This book forms a trilogy with the earlier volumes: *Fifty Years of X-ray Diffraction*, edited by P. P. Ewald, and *Fifty Years of Electron Diffraction*, edited by P. Goodman.

Other projects pursued by the Commission include the compilation of Debye-Waller factors of elements and simple compounds (N. M. Butt), and the planning of future international summer schools on neutron scattering (B. T. M. Willis).

#### *Commission on Small Molecules*

The Commission on Small Molecules (CSM) had a productive year in 1985. The Commission organized a tutorial entitled 'Molecular Systematics: Recognition, Analysis and Presentation'. The tutorial was co-sponsored by the Commission on Crystallographic Teaching and was held the day before the Ninth European Crystallographic Meeting in Torino, Italy. The tutorial, which was very well attended, represented the first activity by CSM in the framework of the crystallographic community. The organizational efforts by F. H. Allen and A. Domenicano were greatly appreciated by the participants and by CSM.

CSM also participated in the organization of the international symposium 'Steric Aspects of Biomolecular Interactions' that was sponsored by the Hungarian Chemical Society and the IUCr. The symposium, held in Sopron, Hungary, brought together scientists of many disciplines whose common interest was the study of interrelationships between structure and biological properties. The programme provided the numerous participating crystallographers with an opportunity to interact closely with colleagues with expertise in solution and theoretical studies.

With encouragement from CSM, P.W. Codding organized a microsposium entitled 'X-ray Crystallographic Studies of Biologically Active Heterocycles' in the framework of the Tenth International Congress of Heterocyclic Chemistry held in Waterloo, Ontario, Canada. The lectures in the microsposium were well attended,

obviously by chemists as well as crystallographers even though there were a number of parallel sessions. The success of the microsposium demonstrated that systematic crystallographic studies of small molecules are of interest to a broad audience.

W. L. Duax, CSM Secretary, put out two issues of the CSM Newsletter. The Newsletter is intended to provide information of interest to small-molecule crystallographers, including CSM activities and a calendar of meetings of potential interest. Distribution is intended primarily for editors of national crystallographic newsletters, but individual inquiries are welcomed with the understanding that the Newsletter will be circulated.

During 1985, the organization of two major symposia was pursued. One, entitled 'Molecular Structure: Chemical Reactivity and Biological Activity', will be held with IUCr sponsorship in Beijing, China, 15-21 September 1986. The symposium is international in character and consists of invited lectures and contributed papers. Considerable effort is being made to include a broad spectrum of topics of interest to small-molecule crystallographers.

The second symposium, also with IUCr sponsorship, will be held at Schloss Elmau, near Garmisch Partenkirchen, Federal Republic of Germany, 20-24 October 1986. The theme of the symposium is 'Computational Methods in Chemical Design: Molecular Modelling and Computer Graphics'. The main purpose is to bring together crystallographers, solution spectroscopists and theoreticians in an effort not only to improve interdisciplinary communication, but also to increase their awareness of the applicability of modern technology to structural research.

#### **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 1985 the Executive Committee approved sponsorship of the following schools and meetings, mostly with financial support:

1. Symposium on Steric Aspects of Biomolecular Interactions, Sopron, Hungary, 26-29 September 1985.
2. Winter School on Technology, Characterization and Properties of Epitaxial Electronic Materials, Trieste, Italy, 13-24 January 1986.
3. First International Symposium on Shaped Crystal Growth, Budapest, Hungary, 22-25 July 1986.
4. Tenth European Crystallographic Meeting, Wrocław, Poland, 5-9 August 1986.
5. Summer School on Crystallographic Computing, Leipzig, German Democratic Republic, 11-20 August 1986.
6. International School of Solar Cell Materials and Applications, Fayoum, Egypt, 19-30 October 1986.
7. International Winter School on Crystallographic Computing, Bedford Park, Australia, 22-29 August 1987.

During 1984 the Executive Committee approved sponsorship of the following schools and meetings, mostly with financial support (this list was given incorrectly in the Report of the Executive Committee for 1984 and is therefore given now for completeness):

1. Course on Static and Dynamic Implications of Precise Structural Information, Erice, Italy, 24 May-6 June 1985.

2. Sagamore VIII, Sanga-Saby, Sweden, 28 July-3 August 1985.

3. Sixth International Meeting on Ferroelectricity, Kobe, Japan, 12-16 August 1985.

Other meetings which received Union support have been listed earlier in this Report. Organizers of meetings wishing to seek Union sponsorship should write as early as possible to the Chairman of the Sub-Committee: Professor M. Nardelli, Istituto di Chimica Generale ed Inorganica, Università di Parma, Viale delle Scienze, 43100 Parma, Italy.

#### Representatives on Other Bodies

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

The International Council for Scientific and Technical Information and its associated committees met in the Kongresshaus, Baden-Baden, from 29 May to 2 June 1985. Four new members were admitted: Centre National de l'Information Chimique (CNIC), France, in Class B; CODATA in Class A; European Physical Society in Class A; National Institute for Informatics, South Africa, in Class B. The Classes of membership are in accordance with the new Statutes adopted in 1984; the Sub-committee on Statutes and By-Laws reported that minor amendments necessitated by the laws of Belgium and the USA had been successfully adopted by postal ballot. (The new membership arrangements have proved popular, and several applications in Classes A and B are pending.)

Recently the interests of ICSTI members have tended to be interdisciplinary, and the activity of the working groups by discipline has declined. It was therefore proposed that the working groups should be dissolved, and that ICSTI should operate through Special Interest Groups; two of these (Legal Aspects of Information Transfer; Document Delivery) were already in existence. The Working Group in Geology was dissolved, at its own request; the Working Groups in Physics and Chemistry will be continued for at least one further year; the Working Group in Life Sciences had requested dissolution, but the Council did not act on the request, as the Group still had questions of terminology under discussion. The Representative of the IUCr was asked to ascertain the degree of interest of Members in a Special Interest Group on Education and User Needs.

The next Council meeting (which will be a General Assembly, with elections for the Executive Board) and the associated committee meetings will take place in York in May 1986. The main theme is expected to be legal aspects of information transfer.

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

The Executive Committee of CODATA decided to form a strong collaboration with ICSTI (International Council for Scientific and Technical Information). In the long term this could help to bring crystallographic results to scientists of other fields. This is a continuation of the main activities of CODATA which tries to transfer experience in and results of modern data handling - this means computerized data management - from one scientific field to others. For the IUCr the following plans to be started in 1985 could be interesting:

1. *Ad hoc* group to discuss data dissemination and/or training activities;
2. *Ad hoc* group to deal with the broad problems of computer handling of data;
3. Working group to prepare a glossary of terms and acronyms used in scientific and technical data handling;
4. Workshop on nucleic acid and protein sequence data banks;
5. Preparation of computer-searchable directories of data sources.

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

In 1985 there was no meeting of COSPAR. However, two very important events in the field of materials science in space took place, which will be discussed at the next COSPAR meeting in Toulouse (30 June-12 July 1986). The first was the NASA Spacelab-3 flight which, in spite of technical defects in many experiments, gave clear support for vapor growth experiments in space. An  $\alpha$ -HgI<sub>2</sub> crystal grown in space gave grade A (spectrometer quality) detectors. The second important event was the D-1 Mission, a flight of Spacelab chartered by the Federal Republic of Germany. More than 70 materials and life sciences experiments were performed, most of them successfully. Unfortunately for protein crystallography, owing to a dramatic error the crystallization of proteins could not be activated. In the meantime, after the success of protein crystallization during the European SL-1 mission, NASA has performed similar experiments in a crush programme, some of which were quite successful. With the delays of the shuttle programme it is not clear, at present, when the next protein crystallization experiment will take place.

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

CTS organized in August 1985 a very successful meeting on the theme 'Science and Technology Education for Future Human Needs' in Bangalore, India. The CTS also met in India: however, the IUCr Representative was not present.

##### *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 1985.

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

IDCNS is the central committee through which provisional recommendations on nomenclature and symbols generated by all IUPAC divisional committees and commissions pass for approval. The IUCr appointed S. C. Abrahams its first representative to IDCNS in 1984 [see *Acta Cryst.* (1986). A42, 67] with A. J. C. Wilson as alternate. They now receive copies of all recommendations. Typical of those requiring a crystallographic input are the current revisions of IUPAC's 'Green Book' (*Nomenclature of Physical Chemistry*), 'Red Book' (*Nomenclature of Inorganic Chemistry*), and the IUPAC nomenclature report *Terminology Relating to Crystalline Polymers*.

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

The Commission works in a way similar to that followed by the IUCr Calendar Sub-Committee. This means that all the applications for sponsorship and financial support for International Conferences are examined first by the Commission and then are considered for the final decision by the IUPAP Council. The criteria used to evaluate the applications are similar to those used by the IUCr.

All the work of the Commission is by mail. In 1985, after the appointment of M. Nardelli as IUCr Representative on that Commission, two applications were examined. In 1986 (up to July 1986), ten applications for meetings to be held in 1987 have been considered and a priority list had to be suggested. Many of the considered meetings are on subjects more or less related to crystallography.

One meeting for 1986 and one for 1987 have been approved by the IUPAP Council.

*Conference Committee of the European Physical Society*

The Committee held its annual meeting on 13 September 1985 in Bucharest. During the meeting many aspects of EPS conferences were discussed. In particular, organizers of EPS Conferences often face the uncertainty that invited scientists from some countries may not get their visas in time. It was confirmed that the NATO-supported EPS sponsored conferences have to follow the EPS rules; that is, invited participants from all EPS countries are treated in the same way.

The opportunity that young scientists have for open discussion with leading scientists during conferences was discussed. The IUCr Representative illustrated the policy the Union follows to increase the participation of young scientists in IUCr-sponsored meetings.

Concerning invited speakers, it was considered advisable to differentiate between outstanding speakers for plenary sessions and outstanding scientists who are sometimes not such brilliant speakers and are more effective in special sessions.

In 1985 the committee approved nine EPS-organized Conferences, 25 EPS-sponsored Conferences, 11 Schools (including three organized by EPS) and four Study Conferences.

*International Organization for Crystal Growth*

During 1985, the IOCG has carried out formal activity only concerned with its main events due in 1986 in Edinburgh, Scotland (International Summer School on Crystal Growth: ISSCG-6), and York, England (International Conference on Crystal Growth: ICCG-8).

According to the IOCG statute, a nomination committee, chaired by E. Kaldis, has been appointed in order to organize a ballot among the eligible members with a view to (partly) renew the Executive Committee.

Important points which are expected to be debated in 1986 in York during the General Assembly of the IOCG include the following:

(a) The creation of two prizes for the best papers on crystal growth, to be distributed at each ICCG starting with ICCG-9, Japan, August 1989.

(b) Whether communication has been improved between members of the crystal growth community *via* the national

organizations of crystal growth. (Presently there are nine national associations officially recognized by the IOCG.)

(c) Methods of improving in practice the status of the IOCG.

*European Crystallographic Committee*

A meeting of this Committee was held on 5 September 1985 during the Ninth European Crystallographic Meeting in Torino. A. Kálmán was appointed the *ad interim* IUCr Representative as M. Nardelli was Chairman of the ECM-9 Programme Committee.

A progress report was received on ECM-10 to be held in Wrocław, Poland, 5-9 August 1986.

The decision to hold ECM-11 in Vienna, Austria, in 1988 was confirmed.

The invitation to hold ECM-12 in Leningrad, Russia, was accepted provisionally.

It was agreed that no sponsorship would be given to the Conference on 'Small-Angle Scattering and Related Methods' to be held in Prague, Czechoslovakia, on 13-16 July 1987.

**International Council of Scientific Unions**

The General Committee of the International Council of Scientific Unions met in Munich, Germany, 14-15 October 1985. Among the matters discussed were the establishment of a Scientific Committee on Biotechnology which was supported and plans for a future programme on Global Change (International Geosphere-Biosphere Programme). 'The central focus of the IGBP would be to describe and understand the interactive physical, chemical and biological processes that regulate the total Earth system, the unique environment for life, the changes that are occurring in this system and the manner in which they are influenced by human actions'. There were also some discussions of a preliminary report of a three-day Conference at Schloss Ringberg, near Munich, 7-9 October 1986, concerning the future role of ICSU in international science cooperation.

**Finances**

The audited accounts for the year 1985 are given at the end of this Report. For comparison, the figures for 1984 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 1985 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 loss has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 148 057. This loss has been divided amongst the ten Fund Accounts with credit balances in direct proportion to the balances on these accounts at 31 December 1985.

As on previous balance sheets, the investments have been valued according to their quotations at the end of the year. Their depreciation in value, together amounting to SwFr 1864, 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 1985 the Union held investments of SwFr 25 000, £100 000 and ECU 100 000 in bonds.

The total of SwFr 2 843 919 with the banks at the end of the year was represented by Dfl 3124, \$459 709 and ECU 54 648 with the Amsterdam–Rotterdam Bank, \$1128 with the First American Bank of New York, \$24 652 with the National Westminster Bank USA, £528 351 with the National Westminster Bank and SwFr 84 093 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, excluding stocks of unsold publications but including the loss of SwFr 148 057 resulting from fluctuations in rates of exchange, have increased during the year, from SwFr 2 806 867 to SwFr 3 630 368.

Three new fund accounts were established in 1984, namely the Book Fund, the Publications and Journals Development Fund and the Research and Education Fund, whilst five fund accounts were closed. Of these three new fund accounts, there were only transactions in the Book Fund in 1985 and there were no transfers from other fund accounts.

The General Fund account shows a surplus of SwFr 283 742 as compared with a surplus of SwFr 145 119 before the transfer of SwFr 50 000 to the new fund accounts in 1984. The administrative expenses were SwFr 170 867 in 1985 as compared with SwFr 140 652 in 1984. Of this amount, SwFr 52 190 was charged to the publications of the Union. SwFr 65 352 was spent on supporting scientific meetings, and SwFr 1157 was required for travel expenses of Union representatives on other bodies. The Executive Committee Meeting cost SwFr 30 956 and the Finance Committee SwFr 11 065. The Union received SwFr 32 565 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 130 830. Interest on bank accounts and investments was SwFr 352 211.

The President's Fund account received SwFr 1252 in donations during 1985. No payments were made from the fund.

The *Acta Crystallographica* account for 1985 shows a surplus of SwFr 542 521 as compared with a surplus of SwFr 420 540 before the transfer of SwFr 250 000 to the new fund accounts in 1984.

The subscription rates were determined to yield a small surplus. However the number of pages printed in 1985 was much less than estimated, and the expected fall in the number of subscriptions did not materialise. In fact, the number of subscriptions increased slightly.

The number of paid subscriptions to all sections of the journal increased from 1170 in 1984 to 1182 in 1985 including 140 personal subscriptions in 1984 and 139 in 1985. There were also 243 paid subscriptions to Section A and

128 paid subscriptions to Sections B and C in 1985, compared with 249 and 133 respectively in 1984. 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 1985. The technical editing costs for *Acta Crystallographica* were SwFr 297 177 in 1985 as compared with SwFr 273 044 in 1984. 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 109 355, as compared with a surplus of SwFr 132 698 before the transfer of SwFr 200 000 to the new fund accounts in 1984. The number of pair subscriptions increased from 1061 in 1984 to 1070 in 1985, including 115 personal subscriptions in 1984 and 118 in 1985.

The *Structure Reports* account shows a deficit of SwFr 21 842 as compared with a deficit of SwFr 9120 in 1984. Sales were rather low since no A series volume was published, and there were still considerable editorial expenses for new volumes to be published in the near future. Publishing and editorial expenses in 1985 were SwFr 34 174 and SwFr 106 161 respectively, as compared with SwFr 56 661 and SwFr 85 105 in 1984. The net income from sales was SwFr 118 859 in 1985 as compared with SwFr 133 107 in 1984.

The *International Tables* account shows a surplus of SwFr 52 312, as compared with a surplus of SwFr 51 842 before the transfer of SwFr 41 208 from the General Publications Fund on its closure in 1984. The Teaching Edition of Volume A was first published in 1985, at a cost of SwFr 11 894. Reprinting Volume II and Volume III cost SwFr 18 714 and SwFr 16 123 respectively. Editorial expenses were SwFr 7440. The net income from sales of SwFr 106 483 derived mostly from the sale of 481 copies of Volume A.

The newly established Book Fund includes the sales of the remaining publications of the Union. SwFr 356 was received from the sale of 20 copies of *Fifty Years of X-ray Diffraction*. SwFr 706 was received from the sale of 45 copies of *Symmetry Aspects of M. C. Escher's Periodic Drawings*, as well as SwFr 387 royalties for the Japanese edition of this book. SwFr 588 was received from the sale of 19 copies of Volume I and 20 copies of Volume II of *Early Papers on Diffraction of X-rays by Crystals*. SwFr 1955 was received from the sale of 38 copies of *Fifty Years of Electron Diffraction*. Sales of the Sixth Edition of the *World Directory of Crystallographers* and of the sundry publications yielded SwFr 181 and SwFr 45 respectively.

The *Molecular Structures and Dimensions* account shows no surplus for 1985, because this account was charged with a contribution of SwFr 9092 towards the publication costs of Volume 15, the volume published in 1984. No other volume was published in 1985 and hence the sales income was very low, SwFr 10 022, as compared with SwFr 36 785 in 1984.

**International Union of Crystallography**  
**Balance Sheet as at 31 December 1985**

	1985		1984		1984		1985		1984	
	As at 1 January 1985	Fluctuations in rates of exchange	Excess of income over expenditure for the year	Balance at 31 December 1985	1984	Swiss Francs	Swiss Francs	1985	Swiss Francs	1984
<b>FUND ACCOUNTS</b>										
General Fund	668,686	-37,345	283,742	915,083	668,686			164,181	128,902	
President's Fund	17,495	-734	1,252	18,013	17,495			2,679,738	2,177,678	2,306,580
<i>Acta Crystallographica</i>	1,092,044	-64,036	542,521	1,570,529	1,092,044			2,843,919	2,177,678	
<i>Journal of Applied</i>										
<i>Crystallography</i>	181,382	-11,390	109,355	279,347	181,382			5,823	5,823	10,780
<i>Structure Reports</i>	134,946	-4,431	-21,842	108,673	134,946			358,231	358,231	250,331
<i>International Tables</i>	132,514	-7,241	52,312	177,585	132,514					
Book Fund	9,616	-542	4,218	13,292	9,616			5,340	5,340	9,352
<i>Molecular Structures</i>										
<i>and Dimensions</i>	7,220	-283	—	6,937	7,220			3,213,313	3,213,313	2,577,043
Publications and										
Journals										
Development Fund	299,313	-11,726	—	287,587	299,313					
Research and										
Education Fund	263,651	-10,329	—	253,322	263,651					
	<u>2,806,867</u>	<u>-148,057</u>	<u>971,558</u>	<u>3,630,368</u>	<u>2,806,867</u>			<u>523,316</u>	<u>320,164</u>	<u>322,761</u>
								-1,864	2,597	
								521,452		
								7,222	9,142	
								<u>3,630,368</u>	<u>2,806,867</u>	<u>2,806,867</u>

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

We have audited the financial statements on pages 148-155 in accordance with approved Auditing Standards.

We have not been requested by the Union to consider the requirements of Swiss Company Law as regards these financial statements.

In our opinion, the financial statements give a true and fair view of the state of affairs of the Union at 31 December 1985 and of its excess of income over expenditure and source and application of funds for the year then ended.

Manchester, England  
 11 August 1986

Signed TOUCHE ROSS & CO

*Chartered Accountants*

## General Fund Account for the year ended 31 December 1985

	Swiss Francs			Swiss Francs	
	1985	1984		1985	1984
Subscriptions to ICSU and ICSU bodies		5,645	Grant received from Unesco subvention to ICSU	32,565	37,905
Administration expenses:			Grant received from ICSU	12,749	—
General Secretary and Treasurer: honorarium and secretarial assistance	9,856		Subscriptions from Adhering Bodies	130,830	132,610
Audit and accountability charges	14,729		Interest on investments	43,999	32,563
Legal and professional fees	2,699	6,002	Interest on bank accounts	308,212	178,648
Postage and sundries	695	12,107	Commission expenses refund	—	4,528
Travelling expenses	2,916	1,284	Amounts charged to the following journals and publications:		
Bank charges	1,246	1,231	<i>Acta Crystallographica</i>	38,445	31,647
Executive Secretary's office: Salaries and expenses	138,137	2,677	<i>Journal of Applied Crystallography</i>	12,815	10,549
Computer expenses	—	570	<i>Molecular Structures and Dimensions</i>	930	908
Depreciation of office equipment	589	109,785		52,190	43,104
		6,575			
		421			
		170,867			
		140,652			
Thirteenth General Assembly and Congress:					
Executive Committee	—	47,243			
Travel grants	—	43,602			
		90,845			
Meeting of the Executive Committee					
Finance Committee expenses	30,956	—			
Travel expenses of IUCr	11,065	14,419			
Representatives on other bodies	1,157	7,034			
Commission expenses	8,673	420			
Sponsorship of meetings	65,352	24,951			
Donation to COSTED	2,090	—			
Preparation of a history of the Union	998	—			
Loss on sale of investments	—	537			
Transfers to other Funds:					
Publications and Journals Development Fund	—	25,000			
Research and Education Fund	—	25,000			
Excess of income over expenditure carried to balance sheet	283,742	95,119			
	580,545	429,358		580,545	429,358





**Structure Reports Account for the year ended 31 December 1985**

	Swiss Francs	
	1985	1984
Publication expenses:		
Printing and binding Volume 46B (1984 Volumes 45B and 48A)	27,231	40,039
Typing of manuscripts	6,943	34,174
		16,622
		56,661
Depreciation	366	461
Editorial expenses:		
Editorial honoraria	106,161	85,105
		142,227
	140,701	142,227
		161,258
		180,503
	42,399	47,396
		133,107
	21,842	9,120
	140,701	142,227

Swiss Francs  
1985

Sale of copies  
Volume 46B  
(1984 Volumes 45B and 48A)  
Earlier volumes and indexes  
Less Publisher's commission  
on sales  
Excess of expenditure over income  
carried to balance sheet

Swiss Francs  
1984

**International Tables Account for the year ended 31 December 1985**

	Swiss Francs	
	1985	1984
Publication expenses:		
Printing and binding Volume A	—	34,076
Printing and binding Teaching Edition of Volume A	11,894	—
Reprinting Volume II	18,714	—
Reprinting Volume III	16,123	—
	46,731	34,076
Editorial expenses:		
Editorial honoraria	6,270	7,500
Secretarial assistance and postage	1,170	6,736
		14,236
	52,312	93,050
	106,483	141,362
		141,244
	43,842	41,090
		100,154
	—	41,208
	106,483	141,362

Swiss Francs  
1985

Sale of copies  
Volume A  
Teaching Edition of Volume A  
Volumes II, III and IV  
Less Publisher's commission  
on sales  
Transfer from General  
Publications Fund

Swiss Francs  
1984

Excess of income over expenditure  
carried to balance sheet

**Book Fund Account for the year ended 31 December 1985**

	Swiss Francs 1985	1984	Swiss Francs 1985	1984
<i>Excess of income over expenditure carried to balance sheet</i>				
	4,218	9,118		
	<u>4,218</u>	<u>9,118</u>		
			356	335
Sales of copies, net of Publisher's commission on sales			706	357
<i>Fifty Years of X-ray Diffraction</i>			588	99
<i>Escher Drawings</i>			1,955	1,956
<i>Early Papers</i>				
<i>Fifty Years of Electron Diffraction</i>			181	185
<i>World Directory of Crystallographers</i> , 6th Edition			45	103
Sundry Publications				
Royalties			387	203
<i>Escher Drawings</i>				
Opening balance at 1 January 1984			—	5,880
from a combination of other Funds*			<u>4,218</u>	<u>9,118</u>

\* The balances on the following Fund accounts were combined on 1 January 1984 to form a new fund—the 'Book Fund'.

	Swiss Francs
<i>Fifty Years of X-ray Diffraction</i>	5,127
<i>Escher Drawings</i>	21,095
<i>Early Papers</i>	-9,827
<i>Fifty Years of Electron Diffraction</i>	-10,515
	<u>5,880</u>

**Molecular Structures and Dimensions Account for the year ended 31 December 1985**

	Swiss Francs 1985	1984	Swiss Francs 1985	1984
<i>Publication expenses:</i>				
Printing and binding Volume 15		24,513	6,725	36,569
Carriage and miscellaneous expenses		3,191	7,078	13,508
Salaries	9,092	8,173	<u>13,803</u>	<u>50,077</u>
Administration expenses				
<i>Excess of income over expenditure for the year:</i>	930	908	3,781	10,022
University of Cambridge				
IUCr carried to balance sheet			10,022	36,785
	<u>10,022</u>	<u>36,785</u>	<u>10,022</u>	<u>36,785</u>

**Statement of Source and Application of Funds**  
**Year ended 31 December 1985**

	Swiss Francs	
	1985	1984
Source of funds		
Excess of income over expenditure for the year	971,558	744,317
Loss/gain on fluctuations in rates of exchange	-148,057	+145,333
	823,501	889,650
Adjustment for items not involving the movement of funds:		
Depreciation	3,499	3,294
Loss on sale of investment	—	537
Loss/gain on fluctuations in rates of exchange on office equipment and investments	-7,367	+15,988
	819,633	909,469
Total generated from operations	819,633	909,469
Proceeds on sale of investment	—	18,000
Decrease in debtors and accrued income (including subscriptions)	—	178,734
Increase in creditors, accrued charges and income received in advance	9,540	—
	829,173	1,106,203
Application of funds		
Increase in debtors and accrued income (including subscriptions)	-103,888	—
Decrease in creditors, accrued charges and income received in advance	—	-19,322
Purchase of office equipment	-1,515	-7,922
Purchase of investment	-191,388	-24,615
	532,382	1,054,344
Increase in net liquid funds	532,382	1,054,344

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.

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) The office computer was fully depreciated in the year of purchase.

### 2. Rates of Exchange

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

	1985	1984
Netherland Guilders	1·3397	1·3800
Danish Crowns	4·3541	4·4000
Pounds Sterling	0·3225	0·3304
US Dollars	0·4785	0·4000
Canadian Dollars	0·6603	0·5240

**3. Taxation**

As an association incorporated in Switzerland, the Union is exempt from Swiss Federal and Geneva Cantonal tax. Under the terms of the United Kingdom/Switzerland Double Taxation Agreement dated 8 December 1977,

investment income arising within the United Kingdom under present circumstances will not be subject to United Kingdom tax.

Other investment income received from countries with which Switzerland has a Double Taxation Agreement is exempt from tax.

**4. Investments**

	Holding at cost 1 January 1985	Swiss Francs			Holding at cost 31 December 1985
		Additions during the year	Disposals during the year	Fluctuations in rates of exchange	
Deposited for safe custody with the Union Bank of Switzerland Sw Fr 25,000 (4.5% Swiss Federal 1983-1995)	24,615	—	—	—	24,615
Deposited for safe custody with National Westminster Bank PLC, Manchester £100,000 (10.5% Treasury Stock 1989)	298,146	—	—	7,303	305,449
Deposited for safe custody with Amsterdam-Rotterdam Bank NV ECU 100,000 (9.5% New Zealand 1985-1992)	—	191,388	—	—	191,388
	<u>322,761</u>	<u>191,388</u>	<u>—</u>	<u>7,303</u>	<u>521,452</u>

Investments are noted in the balance sheet at their market value at 31 December 1985. The difference between cost and market value has been shown as an adjustment in order that the investments can be stated at cost.