

## International Union of Crystallography

### Report of the Executive Committee for 1983

#### Meetings

The Union sponsored the following meetings held during 1983: International School on Materials Science and Solar Energy, Cairo and Alexandria, Egypt, 18 March-1 April; International School on Teaching Crystallography for Materials Science, Brasilia, Brazil, 18-27 July; Eighth European Crystallographic Meeting, Liège, Belgium, 8-12 August; International Summer School on Crystallographic Computing, Kyoto, Japan, 18-27 August; Fifth International Summer School on Crystal Growth and Materials Science, Davos, Switzerland, 3-10 September; VII International Conference on Crystal Growth, Stuttgart, Federal Republic of Germany, 12-16 September; Fifth European Meeting on Ferroelectricity, Torremolinos, Spain, 26 September-1 October.

The Executive Committee met at Liège, Belgium, 3-5 August. The most important items of business dealt with were (1) approval of the audited accounts for 1982; (2) subscription rates and other matters concerning the Union's Journals, including publication of a cumulative index for *Acta Cryst.* for the years 1973-1982 inclusive; (3) other publications of the Union, including the new Volumes of *International Tables for Crystallography*; (4) arrangements for the XIII International Congress of Crystallography; (5) agenda for the XIII General Assembly, including the establishment of a new commission; (6) seventh edition of the *World Directory of Crystallographers*; (7) sponsorship of meetings; (8) office computer; (9) representation of the Union on other bodies.

The Finance Committee met in Chester early in the year and then in Liège immediately prior to the Executive Committee Meeting.

#### Appointments

The Executive Committee confirmed the appointments of J. Drenth, J. A. Ibers and C. E. Nordman as Co-editors of *Acta Crystallographica*.

#### Publications

Volume 39 of *Acta Crystallographica* and Volume 16 of the *Journal of Applied Crystallography* were published in 1983, as were Volume 36 of *Structure Reports*, Volume A of *International Tables for Crystallography* and Volume 14 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.

#### Work of the Commissions

##### *Commission on Journals*

Volumes 39 of *Acta Crystallographica* (*Acta*) and 16 of the *Journal of Applied Crystallography* (*JAC*) were produced and published in 1983 with *Acta B* divided in two Sections. This was the first major rearrangement of *Acta* since 1968 when the journal was initially split into Sections A and B. The new Section A, subtitled *Foundations of Crystallography*, is concerned with basic developments in all areas of crystallography. Section B, *Structural Science*, welcomes structurally based papers from disciplines throughout the natural sciences. Papers reporting crystal structure determinations are now published in Section C, which incorporates the journal *Crystal Structure Communications*. An editorial giving the reasons for the division was published in *Acta* (1982), A38, 1-2; B38, 1-2: a new edition of *Notes for Authors* was published in *Acta* (1983), A39, 174-186.

The total number of papers published in *Acta A* and in the combined *Acta B* and C decreased by 16% in 1983, those in *JAC* by 2%, see Table 2. The decline may be partially associated with the changed emphasis in *Acta B* from primarily reporting crystal structure determinations to encouraging exciting papers that combine a major structural study with an important experimental or theoretical contribution to one of the natural sciences, and with the introduction of a standard format in *Acta C* designed to facilitate the reader's retrieval of structural information. However, the total number of papers accepted for *Acta* in 1983 is 19% higher than in 1982, those for *JAC* 21% smaller. The average length of all articles in *Acta* remains rather constant at about 3.8 pages, with those in *JAC* about a page longer, of which about one-half is due to starting each paper on a new page.

Median publication times for full articles, the averaged elapsed time in months between the published acceptance and nominal publication dates, were 4.8 months for *Acta A*, 5.3 months for *Acta B*, 4.3 months for *Acta C* and 5.3 months for *JAC*. It may be recalled that only *Acta C* appears monthly, the others bimonthly. Short communications have median publication times one month shorter than full articles in *Acta A* and B, three weeks shorter in *Acta C* and one week shorter in *JAC*.

The informal grouping of papers in *Acta B*, and now in *Acta C*, as inorganic, organometallic or organic was continued in 1983. *Acta C* continues the distribution pattern of Short Structural Papers established in previous volumes of *Acta B* in which organic papers form the majority, whereas the new *Acta B* contains more inorganic papers. A total of 59 inorganic, 15 organometallic and 40 organic related articles appeared in *Acta B*, with 118 inorganic, 188 organometallic and 330 organic articles in *Acta C*.

The distribution of papers and authors by country in all sections of *Acta* and *JAC* is given in Table 3. The method used for allocating papers and authors to countries is given

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 y Técnicas	M. A. R. DE BENYACAR, Division Física del Sólido, Commission 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, Getreidemarkt 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 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	D. BOYS, 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, 180 40 Praha 8
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	II	Vereinigung für Kristallographie in der GGW der DDR	P. PAUFLER, VFK, Invalidenstrasse 43, DDR-104 Berlin
Germany, Federal Republic of	IV	Arbeitsgemeinschaft Kristallographie	H. BURZLAFF, Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Universität, Loewenichstrasse 22, D-8520 Erlangen
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	S. K. SIKKA, Scientific Officer, Neutron Physics Division, Bhabha Atomic Research Centre, Trombay, Bombay 400085
Israel	I	Israel Academy of Sciences and Humanities	G. M. REISNER, Department of Chemistry, Technion, Israel Institute of Technology, Haifa 32000
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. IITAKA, Faculty of Pharmaceutical Sciences, University of Tokyo, Bunkyo-ku, Tokyo
Netherlands	III	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. M. WATERS, Department of Chemistry, Massey University, Palmerston North
Norway	I	Det Norske Videnskaps Akademi	B. F. PEDERSEN, Department of Pharmacy, University of Oslo, PO Box 1068, 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
Portugal	I	Sociedade Portuguesa de Física	M. M. R. R. COSTA, Departamento de Física, Universidade de Coimbra, 3000 Coimbra

\* 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
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. MARTINEZ CARRERA, Instituto de Quimica Fisica 'Rocasolano', Consejo Superior de Investigaciones Cientificas, Serrano 119, Madrid 6
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, 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.

in the footnotes to the table. Two countries, Ghana and Iraq, contributed papers in 1981 but not in 1982 or 1983. Eight countries with no papers or authors in 1981 or 1982, Bulgaria, Camerouns, Colombia, the Arab Republic of Egypt, Hong Kong, Jamaica, Lebanon and Syria, are represented in 1983, with a total of 65 countries listed. The usual relatively large year-to-year fluctuations in the number of papers contributed by several countries may again be noted.

The *Index* to Volumes A38 and B38 of *Acta* was published in 1983 and again consisted of five separate indexes: a subject index, a chemical name index, an inorganic formula index, an organic formula index (organometallic compounds are generally included in both formula indexes) and an author index. The subject and author indexes to *JAC* in 1983 were bound in with the final issue of Volume 16.

#### Commission on Structure Reports

Volume 36 (the ten-year Index covering the years 1961-1970, 337 pages), prepared by W. B. Pearson, was published in 1983. Volume 45B (Organic Compounds for 1979, 1542 pages) and Volume 48A (Metals and Inorganic Compounds for 1981, 420 pages) have been prepared for the publisher and will appear early in 1984. The manuscript of the Inorganic section of Volume 49A (Metals and Inorganic Compounds for 1982) is ready and only awaits completion of the Metals section. Manuscript preparation is at an advanced stage for Volume 46B and continues for Volume 48B (Organic Compounds for 1980 and 1981 respectively). Co-editorial work continues for Volume 50A (Metals and Inorganic Compounds for 1983) and for Volumes 49B and 50B (Organic Compounds for 1982 and 1983 respectively).

#### Commission on International Tables

No Commission was elected in 1981. In 1982 the Executive Committee discussed the problem of producing further volumes, and appointed U. Shmueli as Editor of Volume

B: Reciprocal Space, and A. J. C. Wilson as Chairman of the Commission and Editor of Volume C: Mathematical, Physical and Chemical Tables. No further members of the Commission were appointed, so that during 1983 the Commission has consisted only of the Editors and the *ex-officio* members (the President and General Secretary of the Union).

The Editors began work officially on 1 January 1983, though unofficially a great deal of preparatory work had already been done. This included, in particular, development of much of the software required for automated generation of tables for the Chapter 'Symmetry in Reciprocal Space' in Volume B and correspondence concerning computerized typesetting methods. During April/May 1983 the Editors met in Tel Aviv and prepared a lengthy memorandum, including draft Tables of Contents for the two volumes, which was circulated to the Executive Committee, the National Committees, and widely elsewhere. This circulation generated much constructive criticism and offers of help, particularly from several of the Commissions of the Union.

The Editors met again in Cambridge in August 1983, revised the Tables of Contents, and began issuing invitations to prospective authors of the various Parts, Chapters, and Sections. Discussions by the Editor of Volume B in the course of ECM-8 at Liège were of considerable help in choosing authors. In September, however, the Editors were asked to suspend invitations until the proposed authors had been approved by the Executive Committee; obtaining this approval has introduced delays of some months.

The Commission whose term of office expired in 1981 had completed the editorial work on Volume A, and saw it through the press until it was published in 1983. A great debt of gratitude is owed to Theo Hahn and his colleagues.

#### Commission on Biological Macromolecular Crystallography

There has been no formal meeting of the Commission in 1983. The activities of the Commission were therefore

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
A34	1978	1048	189	158	6.0	—	—	31	1.3
B34		3848	1040	510	5.0	490	2.5	40	1.0
A35	1979	1090	187	162	6.0	—	—	25	1.5
B35		3130	898	412	4.7	457	2.5	29	1.5
A36	1980	1096	194	168	6.1	—	—	26	1.3
B36		3212	877	417	5.0	438	2.5	22	1.3
A37	1981	944	158	136	6.4	—	—	22	1.1
B37		2250	630	286	4.9	333	2.5	11	0.6
A38	1982	880	155	129	6.3	—	—	26	1.5
B38		3176	905	370	4.9	518	2.6	17	0.8
A39	1983	950	146	129	6.4	—	—	17	1.0
B39		770	121	118	6.4	—	—	3	0.6
C39		1714	645	—	—	636	2.7	9	0.9

*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
11§	1978	720	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
13	1980	638	130	81	6.2	6	2.0	25	1.8	7	2.7	11	1.0
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

\* Excluding indexes.

† Volume A34 includes, in addition, 431 pages of abstracts communicated to the Warsaw Congress and Volume A37 includes, in addition, 428 pages of abstracts communicated to the Ottawa Congress.

‡ Volume 39 divided into two new Sections in 1983.

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

¶ Excluding Lead Articles and Conference Papers.

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

restricted to correspondence by mail. They included proposals for sessions at the XIII Congress, representation of biological macromolecular crystallography on the Editorial Board of *Acta Cryst.*, and suggestions for new membership of the Commission. A change in the name of the Commission to 'Commission on Biological Macromolecules' has been suggested. The Commission is pleased with the increased coverage of its field at IUCr Congresses and various international meetings.

*Commission on Charge, Spin and Momentum Densities*

There were no meetings directly sponsored by the Commission in 1983. The oxalic acid project was brought to a successful conclusion with presentation of P. Coppens's report for publication [*Acta Cryst.* (1984), A40, 184–195].

Thermal parameters, positional coordinates and  $X-N$  electron density maps for oxalic acid dihydrate from four X-ray and five neutron data sets are compared with each other and three sets of theoretical calculations. Chemically significant features are reproduced in all experimental density maps, the largest discrepancies between experiment and theory occur in the lone-pair regions.

The date and venue for Sagamore VIII have been settled. The conference will be held 28 July–3 August 1985 at Sanga-Saby, Sweden, under the Chairmanship of I. Olovsson.

The comprehensive study on electron density in vanadium, coordinated by P. J. Brown, has continued. The results will be presented and assessed in a microsposium at the XIII Congress.

Table 3. *Distribution of papers and authors, by country, in Acta and JAC for 1982 and 1983*

Country	Section A				Acta Crystallographica				Section C				Journal of Applied Crystallography			
	Papers		Authors		Papers		Authors		Papers		Authors		Papers		Authors	
	1982	1983	1982	1983	1982	1983	1982	1983	1982	1983	1982	1983	1982	1983	1982	1983
Afghanistan	—	—	—	—	—	—	1	—	—	—	—	—	—	—	—	—
Algeria	—	—	—	—	—	—	1	—	—	—	—	—	—	—	—	—
Argentina	2-0	—	4	1	0-8	0-5	5	1	—	0-5	—	2	1-0	1-0	2	3
Australia	14-0	12-5	21	19	20-0	3-9	42	7	—	24-3	—	66	6-0	5-7	6	5
Austria	—	—	—	—	6-7	0-4	15	2	—	1-9	—	6	—	0-7	—	2
Bangladesh	—	—	—	—	—	—	2	—	—	0-3	—	2	—	—	—	—
Belgium	3-0	5-0	7	10	15-9	1-0	68	3	—	9-2	—	31	—	1-0	—	1
Brazil	1-0	1-0	3	6	1-4	—	5	—	—	1-0	—	4	1-0	2-0	4	6
Bulgaria	—	—	—	—	—	—	—	—	—	—	—	—	—	1-0	—	4
Cameroons	—	—	—	—	—	—	—	—	—	0-3	—	1	—	—	—	—
Canada	2-3	4-3	4	5	59-4	1-2	156	1	—	35-6	—	91	2-0	—	4	—
Chile	—	—	—	—	0-7	—	2	—	—	2-0	—	5	1-0	1-0	2	3
China, Peoples' Rep.	—	1-5	4	7	1-0	—	7	1	—	0-3	—	2	2-0	1-0	8	5
Colombia	—	—	—	—	—	—	—	—	—	0-2	—	2	—	—	—	—
Cuba	—	—	—	—	—	—	—	—	—	—	—	—	1-0	1-0	1	3
Czechoslovakia	—	1-0	—	1	9-7	1-7	36	4	—	3-3	—	11	—	5-0	—	10
Denmark	—	1-0	—	2	9-0	—	18	—	—	8-0	—	22	0-6	—	3	1
Egypt, Arab Rep.	—	—	—	—	—	1-0	—	3	—	—	—	1	—	—	—	—
Finland	4-0	—	7	—	9-4	0-5	22	2	—	2-5	—	5	—	1-0	1	3
France	9-7	13-4	26	21	137-0	14-1	439	41	—	85-7	—	286	19-5	20-6	60	55
German Dem. Rep.	4-0	—	8	—	3-4	0-3	14	1	—	1-0	—	4	—	2-0	—	2
Germany, Fed. Rep.	17-2	12-2	26	17	69-7	13-6	178	37	—	53-3	—	100	10-9	11-3	24	33
Greece	0-3	—	1	—	1-0	1-0	4	3	—	4-7	—	16	—	—	—	—
Hong Kong	—	—	—	—	—	—	—	—	—	1-0	—	3	—	—	—	—
Hungary	—	—	—	—	5-2	—	15	—	—	1-0	—	5	—	—	1	—
India	4-5	1-0	14	3	35-3	—	112	—	—	33-4	—	116	3-0	2-0	6	6
Iran	—	—	—	—	—	—	—	—	—	—	—	—	1-0	0-5	1	1
Ireland	—	—	—	—	2-6	—	3	—	—	0-8	—	2	—	—	—	—
Israel	1-3	2-5	2	4	4-3	3-5	12	9	—	1-5	—	4	2-8	3-5	7	9
Italy	4-0	8-3	11	17	42-4	6-1	130	18	—	44-9	—	142	7-0	1-2	23	3
Ivory Coast	—	—	—	—	2-3	—	10	—	—	—	—	—	—	—	—	—
Jamaica	—	—	—	—	—	—	—	—	—	0-3	—	1	—	—	—	—
Japan	18-0	7-0	49	17	54-2	16-3	214	64	—	39-0	—	164	9-3	7-6	41	19
Kenya	—	—	—	—	0-5	—	2	—	—	—	—	—	—	—	—	—
Korea, South	—	—	—	—	—	—	—	—	—	—	—	1	—	—	—	—
Lebanon	—	—	—	—	—	—	—	—	—	0-3	—	3	—	—	—	—
Malaysia	—	—	—	—	—	—	1	—	—	—	—	—	—	—	—	—
Mexico	—	—	—	—	1-0	—	5	—	—	—	—	1	0-3	—	1	—
Morocco	—	—	—	—	—	—	1	—	—	—	—	—	—	—	—	—
Netherlands	7-2	11-8	15	27	18-3	3-0	59	8	—	24-6	—	79	3-0	3-5	6	8
New Zealand	—	—	1	—	1-5	0-1	3	2	—	4-0	—	12	—	—	—	—
Nigeria	—	—	—	—	1-0	—	4	—	—	1-3	—	3	—	—	—	—
Norway	—	1-0	—	2	4-0	—	7	—	—	1-0	—	4	—	2-0	—	3
Pakistan	0-5	—	2	—	—	—	—	—	—	—	—	—	—	—	—	—
Poland	1-0	—	6	—	19-9	2-0	49	4	—	24-4	—	62	2-0	1-0	5	3
Portugal	—	2-0	—	2	—	1-0	—	1	—	—	—	1	—	1-0	—	1
Romania	—	—	—	—	—	—	—	—	—	—	—	—	1-0	—	4	—
Saudi Arabia	—	—	—	—	1-0	—	1	—	—	6-0	—	11	—	—	—	—
South Africa	—	—	—	—	3-1	—	12	—	—	2-3	—	6	—	—	—	—
Spain	0-4	—	2	—	24-9	1-0	88	4	—	28-0	—	104	2-0	2-8	4	12
Sri Lanka	—	—	—	—	—	—	2	—	—	—	—	—	—	—	—	—
Sweden	1-0	—	3	—	19-0	2-5	38	5	—	14-8	—	27	1-0	2-3	4	7
Switzerland	5-5	2-0	6	1	17-7	6-0	44	16	—	5-5	—	16	1-0	1-0	2	1
Syria	—	—	—	—	—	—	—	—	—	—	—	1	—	—	—	—
Taiwan	—	—	—	—	1-0	—	3	—	—	1-0	—	4	—	—	—	—
Thailand	—	—	—	—	—	—	2	—	—	1-0	—	3	—	—	—	—
Togo	—	—	—	—	0-4	—	1	—	—	—	—	—	—	—	—	—
Tunisia	—	—	—	—	—	—	1	—	—	1-2	—	4	—	1-3	—	5
Turkey	1-0	1-0	2	1	0-5	—	2	—	—	—	—	1	1-0	—	2	1
UK	12-3	18-7	26	35	120-1	10-3	324	37	—	60-7	—	205	9-6	17-2	29	44
USA	31-8	27-5	53	46	152-7	27-3	452	68	—	100-9	—	282	37-7	27-8	89	66
USSR	5-0	6-3	11	13	2-8	0-7	18	4	—	0-3	—	2	1-3	1-2	12	7
Venezuela	—	—	—	—	1-3	—	2	—	—	—	—	1	—	—	—	—
Yugoslavia	—	—	—	—	12-9	—	40	—	—	4-7	—	12	2-0	4-0	6	14
Zimbabwe	—	—	—	—	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 author's nationality is not known to be otherwise it is given as that of the country in which the work was done.

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

The main activity this year was the organization of the International School on Materials Science and Solar Energy, 18 March-1 April 1983 in Egypt. The lectures took place one week in Cairo and one week in Alexandria. A total of 125 participants followed the lectures, including approximately 20 from several African countries, Pakistan and India. 15 lecturers from many countries presented an interesting programme, including important aspects of materials science and crystallography centred round materials for solar energy conversion. Apart from the lectures, several topics were discussed in spontaneous meetings between the participants and the lecturers, the main subject being the method of presenting materials science to an audience from a developing country. The opinions of many participants reflected the idea that in some developing countries the practical aspects should be stressed in the first place. As this was the case for many of the lectures presented, the school was considered quite successful. These discussions outside the lecture hall were appreciated as much as the formal lectures, showing a dramatic need for young scientists to exchange opinions with their colleagues from abroad. One left Egypt with the feeling that a successful school is only the beginning and that a lot of effort should be made to continue these contacts in the future. Materials science is really the best bridge for contacts between the IUCr and developing countries. Egypt desperately needs such contacts.

The success of the school in Cairo was due to the secretary and local organizer Salah Arafa and his committee, who have worked very hard. The advice and help of Fahrid Ahmel to our Commission contributed strongly to the success of the school.

In September 1983 in Davos, Switzerland, the 5th International Summer School of Crystal Growth, which was sponsored by the IUCr and the Commission, took place. An interesting programme with 26 lecturers from the best industrial and university laboratories in the USA and Europe presented the state of the art in the field of electronic materials and their applications. Apart from the lecture notes (236 pages), the proceedings will soon be published by North-Holland as a separate volume. 123 participants from 19 countries followed the 10-day course.

### *Commission on Crystallographic Apparatus*

The Commission mourns the death of its chairman, Sixten Abrahamsson.

Commission activity during 1983 has centred on the elaboration of existing projects. There are still significant problems in communication with members of the Commission, which, it is hoped, will be overcome when the Commission meets at the XIII Congress in Hamburg.

Progress with the various projects undertaken under the auspices of the Commission is outlined briefly below.

1. *Microdensitometer Project* (S. Abrahamsson, P. Kierkegaard, O. Lindquist and L. Sjölin). A manuscript on the second phase of this project, a comparison of microdensitometer and diffractometer data, is being written.

2. *X-ray Attenuation Project* (D. C. Creagh). The production of manuscripts on this project are well advanced, and their submission to *Acta Cryst.* is imminent. Their production has been retarded somewhat by the arrival recently of

new data from laboratories and the need to recalculate some theoretical values. Expressions of interest in the project are still being received and sample kits are still being sent to interested laboratories.

3. *Polarization Ratio Survey* (L. D. Jennings). The results of this survey have been published [*Acta Cryst.* (1984), **A40**, 12-16].

4. *Radiation Safety* (S. Martinez Carrera). A considerable volume of information on the radiation safety regulations and practices for many of the countries adhering to the IUCr have been received. How best to deal with the problem of rationalizing this array of information will be discussed at the meeting of the Commission at the XIII Congress.

5. *Accurate Determination of Diffractometer Intensities* (H. Hope). A preliminary study of the effect of the accuracy of measurement of diffractometer intensities on the determination of crystal structures has been undertaken. The results of this will be reported at a later date.

6. *Profile Analysis Project* (J. Čermák). Some difficulty is being experienced in the organization of this very important project.

7. *Intensity Meeting* (S. Abrahamsson, P. Kierkegaard). An Open Meeting of the Commission has been arranged for the XIII Congress. Its topic will be 'Determination of Accurate Intensities and Structure Factors'.

### *Commission on Crystallographic Computing*

The 1983 International Summer School on Crystallographic Computing was held at Kyoto, Japan, 18-26 August 1983. The school was organized by the Commission and the Crystallographic Society of Japan. It was supported financially by a large number of professional and commercial agencies.

This was the first IUCr computing school to be held in the Asian/Pacific area and the second to be run independently from an IUCr Congress. The lecture programme covered a broad range of crystallographic applications, most with a strong macromolecular flavour. Major topics included data measurement and error treatment, solution methodology (direct and indirect), software packages and data-bases, refinement and phase extension, computer graphics, powder analysis, precision electron density studies and electron diffraction.

The programme structure placed particular emphasis on the use of work sessions. The approximately 30 lectures were given in the mornings, leaving most afternoons for parallel 90-minute work periods, which were limited to 10-20 participants. Since English was not the first language of most participants these sessions were of particular importance. The work sessions proved to be the real kernel of the school and the level of effort input by both lecturers and participants ensured their success. Language considerations also necessitated a particularly high level of lecture presentation and documentation. This is reflected in the detailed lecture notes, which are due to be published shortly as *Methods and Applications in Crystallographic Computing* by Oxford University Press.

With over 150 participants and 30 lecturers from 15 different countries, the school organization involved considerable local support. T. Ashida, a Commission member, was the Chairman of the Local Organizing Committee and deserves most credit for the smooth running of the school.

All Commission members are thanked for their assistance in organizing the school programme.

The Commission has also been assisting with the selection of topics and speakers for the 1984 International Summer School on Crystallographic Computing to be held at the Max-Planck-Institut in Mulheim, Federal Republic of Germany, 30 July–8 August. The school is being organized by H. Burzlaff, as Programme Chairman. H. Schenk is acting for the Commission on the programme committee.

#### *Commission on Crystallographic Data*

Most of the activity of the Commission has been directed toward preparation for the 1984 Congress. Two Open Commission Meetings are being planned, one entitled 'Obtaining Structural Data from Computer Databases', the other 'The Role of Crystallographic Data in Systematic Chemistry'.

Other activities involve the preparation of agenda items for the Closed Commission Meeting. Among these are the reports expected from the task forces on the Definition of Keywords, and on the Standard Crystallographic File Structure. There will also be discussions ranging from the systematic reporting of data (standard structure settings, use of the Standard Crystallographic File Structure, reporting of crystal data, the deposition of 'unpublished data') to the accessibility of crystallographic data in data depositories and databases.

#### *Commission on Crystallographic Nomenclature*

The final report on the Nomenclature of Polytype Structures of the IUCr *Ad hoc* Committee on the Nomenclature of Disordered, Modulated and Polytype Structures, with A. Guinier as Chairman, was accepted both by the Commission and the Executive Committee, under ground rules outlined in *Acta Cryst.* (1979), A35, 1072. The report will be published in *Acta Cryst.* (1984), A40, 399–404. The *Ad-hoc* Committee on the Nomenclature of Symmetry, with P. M. de Wolff as Chairman, has nearly completed the final version of their report on the Nomenclature for Bravais Lattice Types, Crystal Families and Arithmetic Classes. Extensive correspondence was exchanged with interested scientists concerning a systematic nomenclature for inorganic structure types, with the Interdivisional Committee on Nomenclature and Symbols of IUPAC concerning a proposed nomenclature of polymer crystallization, and with National Committees concerning Commission membership.

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

The Commission's activities concerned the Open Commission Meeting at the XIII Congress. It was decided to devote the whole session to the use of synchrotron radiation for crystallographic studies at controlled pressures and temperatures. Four invited speakers were selected to review the general problems concerning the use of synchrotron radiation for these studies, as well as the activity in this field around the world.

#### *Commission on Crystallographic Teaching*

The major activity of the Commission during 1983 was centred round the organization of the International School

on Teaching Crystallography for Materials Science, held at the University of Campinas, São Paulo, Brazil, 18–27 July 1983. Seventeen lecturers from ten different countries and 127 students drawn mostly from the Latin American countries participated. The school was organized by the Brazilian National Research Council with S. Caticha Ellis as its Director. It received financial support from the Union, ICSU, and COSTED. The Commission acted as the International Programme Committee for the school. This was the first such school organized in Latin America on the teaching of crystallography and it evinced great interest and enthusiasm among the participants. The Commission is looking for suitable venues for similar schools in Africa and Asia.

Sales of the first ten pamphlets produced by the Commission under its Pamphlet Project (Editor: C. A. Taylor) have been most heartening and the project promises to become self-supporting. An additional set of nine pamphlets on different crystallographic topics are in the press and expected to be available at the XIII Congress.

The Commission is organizing an Open Commission Meeting on 'Teaching Crystallography for Today's Sciences' during the Congress, and helping to set up a non-commercial exhibition of crystallographic books and teaching aids.

#### *Commission on Electron Diffraction*

The activities of the Commission have been dominated by preparing for the XIII Congress and helping with Volumes B and C of *International Tables for Crystallography*. In addition, activities of the three subgroups GED, LEED and HEED have continued and are reported below.

*GED* (Gas-phase electron diffraction). This group continued to be an active and closely knit organization, producing the 11th letter of GEDIS during 1983. This newsletter contained a comprehensive listing of addresses of authors, followed by publications listings for specific molecules separated from those of a more general nature (compiled by Mutter, Seiter and Stark, Ulm/Donau, Federal Republic of Germany).

*LEED*. This group has seen a revival of activity following the appointment of a prominent researcher, P. M. Marcus, to the Commission. In spite of a serious conflict with the International Conference on Surface Structure in San Francisco in 1984, a program has been constructed for an Open Commission Meeting for the XIII Congress, which includes a review of current methods of intensity calculation and relationship to X-ray methods.

*HEED*. Activities of this group continue to be directed towards a better understanding of the role of high-energy electron diffraction methods in crystal structure analysis, and more recently also in surface structure analysis and in electron-energy-loss spectroscopy.

Other Commission activities included:

(a) Circulation of an open letter by B. Zvyagin (USSR), setting out desirable goals for a HEED section in meetings and publications, and including information on the USSR school. Technical information from this has been summarized in an article 'Oriented Texture Pattern Geometry' submitted for Volume C of *International Tables for Crystallography*.

(b) Publication [*Acta Cryst.* (1983), **A39**, 825-837] of tables for space group determination from electron diffraction extinction rules, by M. Tanaka and colleagues (Sendai) (communicated by D. Watanabe). This publication is an important contribution to the Commission's project on space groups.

(c) Collaboration with the Commission on *International Tables* in preparing a joint Open Commission Meeting.

(d) Support for the idea of a Main Lecture at the XIII Congress on Surface Studies by Electron Microscopy.

During the year four Chairman's newsletters were sent out and responses to these have generally been productive. It is hoped that in future newsletters from Commission members will become more frequent.

#### *Commission on Neutron Diffraction*

The planning of the Symposium on Neutron Scattering (Berlin, 6-9 August 1984) was finalized, and a list of invited speakers was set up. The meeting will concentrate on biology, chemistry and materials research, but there will also be a session for magnetism and, as usual, instrumentation and new sources will be discussed.

Two newsletters appeared this year. One issue, occurring in April, was edited by G. H. Lander and M. H. Mueller (Argonne National Laboratory) and dealt mainly with news from Northern America. The second issue, which was edited by T. Hicks (Monash University) came out in October and gave news from Australia, Indonesia, Japan and China.

The Commission has been invited to participate in the preparation of the new Volume C of *International Tables for Crystallography* and has given suggestions of regions where neutron techniques should be specially discussed. Following this it has set up a list of authors for the subchapters in question. The Commission is likewise engaged in organizing an Open Commission Meeting and a Microsymposium at the XIII Congress. The subjects are 'Spallation Sources' and 'Crystal Structure Solution and Analysis by Neutron Techniques'.

Finally, the form factor project, organized by J.-X. Boucherle (Grenoble), has been completed. It contains a 50-page list of literature entries and short comments on magnetic form factors, which have been observed by neutron scattering techniques, and is presently being sent to all the experimentalists concerned for comments and correction. It has, on the other hand, unfortunately not been possible to continue the file on magnetic structures. After discussion in the Commission it was therefore decided to stop this activity.

#### **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 1983 the Executive Committee approved sponsorship of the following schools and meetings, mostly with financial support:

1. International School on Materials Science and Solar Energy, Cairo and Alexandria, Egypt, 18 March-1 April 1983.

2. International School on Teaching Crystallography for Materials Science, Brasilia, Brazil, 18-27 July 1983.

3. Fifth International Summer School on Crystal Growth and Materials Science, Davos, Switzerland, 3-10 September 1983.

4. Fifth European Meeting on Ferroelectricity, Torremolinos, Spain, 26 September-1 October 1983.

5. International Course on Direct Methods of Solving Crystal Structures, Erice, Italy, 7-19 April 1984.

6. Conference on Crystal Growth and Characterization of Polytype Structures, Marseille, France, 3-6 July 1984.

7. International Summer School on Crystallographic Computing, Mulheim/Ruhr, Federal Republic of Germany, 30 July-8 August 1984.

8. Symposium on Neutron Scattering, West Berlin, Federal Republic of Germany, 6-8 August 1984.

9. Symposium on Small-Angle Scattering and Related Methods, Hamburg, Federal Republic of Germany, 20-23 August 1984.

10. Symposium on Metals and Intermetallic Compounds, Aachen, Federal Republic of Germany, 20-24 August 1984.

11. International Summer School on Symmetry-Related Crystal Structures: Group-Subgroup Relations, Marburg, Federal Republic of Germany, 20-24 August 1984.

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 e Inorganica, Università di Parma, Via M. D'Azeglio 85, 43100 Parma, Italy.

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

##### *Abstracting Board of the International Council of Scientific Unions (ICSU AB)*

Two matters have preoccupied the ICSU Abstracting Board during 1983: its restructuring to meet the current needs of the users, producers, and distributors of scientific and technical information; and its relations with ICSU. The Board held its regular triennial General Assembly in Vienna from 23 to 27 May, and both matters received much attention there and at subsequent meetings of the Executive Committee and other bodies within the Board. As a result of these discussions, it has been decided to hold an Extraordinary General Assembly in June 1984 to consider and vote on a new set of Statutes and By-Laws. These would make three major changes from the current situation:

(i) The name of the organization would become the International Council for Scientific and Technical Information (ICSTI).

(ii) There would be two Classes of Full Members, Class A consisting of bodies primarily concerned with the production and utilization of information, and Class B of bodies primarily concerned with the distribution of information. (The IUCr would fall into Class A.)

(iii) In each Class there would be three Categories of dues (on a basis similar to that of the five IUCr categories). On major financial matters the number of votes would depend on the dues Category; on other matters each Full Member would have one vote. The dues for Class B members would be about twice as great as those for Class A in each Category.

In addition to the Full Members, there is provision for Associate Members (organizations) and Honorary Mem-



bers (persons). Such members would have the right to participate in meetings of ICSTI, but would have no vote. Union and Country membership, as such, would disappear, but all existing members in these classes would automatically become members in Class A.

For several years ICSU has been expressing dissatisfaction with the ICSU Abstracting Board, though the reason for the dissatisfaction has never been made clear. At the meeting of the General Committee of ICSU in Warsaw in September 1983 the following resolution was adopted:

'(The General Committee) *recommends* to the 20th General Assembly that the status of the ICSU Abstracting Board as a Permanent Service of ICSU be terminated and further *recommends* that the appropriate modes of cooperation between the Abstracting Board and the ICSU family be determined after the Abstracting Board has established its new structure and objectives.'

The resolution originally proposed was much harsher in tone, and the help given by the IUCr representative on the General Committee of ICSU (A. Magnéli) in obtaining a more moderate wording is greatly appreciated by the Board. The Statutes of ICSU make no provision for the status of 'Permanent Service of ICSU', so the effect of the recommendation, if adopted at the full ICSU meeting in 1984, is not clear. One of the difficulties experienced by the Board in this matter is the reluctance of ICSU to reply to correspondence.

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

1983 fell between two General Assemblies (1982 and 1984) and saw CODATA undertaking a review of its role, particularly in relation to the burgeoning of computer databases.

The IUCr delegate asked that CODATA consider the question of the accessibility of databases. Experiences within the crystallographic community show that there can be different expectations on the part of database publishers and database users regarding the ways in which the databases are made available. The difficulties currently being experienced with this new technology are likely to occur in other disciplines and it seems appropriate that CODATA should address the question in this broader context. It is hoped that the Union will be able to provide advice on these problems in other fields.

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

According to the new regulations COSPAR has a scientific meeting every second year. In 1983 no such meeting took place. This year was, however, very important for materials science in space. In the frame of ESA-NASA collaboration the first space laboratory flight took place in November. The results, as far as they can be evaluated up to now, seem to show a breakthrough for the crystallization of proteins and enzymes. Dr Littke was able to grow under microgravity 1.3 mm single crystals of lysozyme. Compared to earth growth for the same period, these crystals were 1000× larger in volume. For C-galactosides the volume was 27× larger under microgravity conditions. Apart from the practical importance, the strong increase of the rate of crystal growth of proteins under microgravity conditions is very interesting from the point of view of the growth mechanisms.

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

The Committee met 26-27 March 1983 to plan the proposed conference on 'Science and Technology Education and Future Human Needs' to be held in Bangalore, India, 8-15 August 1985, under the auspices of the Indian National Science Academy. The conference is being planned on a large scale and is projected as a major educational event of the decade, with a large number of Unions affiliated to ICSU taking active part in it. Eight major themes were identified: (i) Health; (ii) Food and agriculture; (iii) Energy; (iv) Land, water and mineral resources; (v) Industry and technology; (vi) The environment; (vii) Information technology and transfer; and (viii) Ethics and social responsibility; and a leader nominated for each theme, to prepare the necessary background material for discussion at the conference. All participating Unions have been asked to consider possible contributions they can make under any of the above themes. One of the aims of the conference is to reappraise what should be taught at School and University level in order to promote development.

While crystallography has an important role to play in almost all the above themes the scope of the conference appears much too wide and the duration much too short to enable an in-depth analysis at the conference itself.

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

One of the main activities of COSTED is to provide funds to help participants from developing countries to attend summer schools and, indeed, scholarships were promised to the summer schools organized by the Union in Cairo, Brasilia, Kyoto and Erice. However, there have been extreme difficulties concerning the payment of these scholarships. Not only has the correspondence from and the coordination by COSTED been practically nil with the Union representative and the Union's officers but also with the organizers themselves, creating very great difficulties for them. It is very strongly to be hoped that this situation will improve in the future.

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

The SCOPE activities during 1983 have comprised continuing work on projects of the global biogeochemical cycles, as decided by the Fifth General Assembly of SCOPE in Ottawa, 1982. A workshop on 'Stable Isotopes in the Assessment of Natural and Anthropogenic Sulphur in the Environment' was held in September. During 1983, SCOPE initiated an 'International Assessment of the Environmental Consequences of Nuclear War (ENUWAR)'. A first workshop was held in Stockholm in November; it considered physical and chemical atmospheric effects and climate and also biological impacts.

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

The Commission prepared for the IUPAP Executive Council a priority list of conferences in a given scientific field, together with proposals for financial support. There were no other activities.

*Conference Committee of the European Physical Society*

The Committee met in Nijmegen, The Netherlands. Applications for sponsorship and approval of conferences were discussed. In the period 1983-1984 there are altogether nine conferences organized by EPS divisions, 20 conferences approved by EPS, three so-called 'Study Conferences' and 14 schools under patronage of the EPS. The Union representative passed on information on forthcoming meetings included in *J. Appl. Cryst.*

There was considerable activity in helping to organize scientific meetings for physicists in Europe.

*International Organization for Crystal Growth*

A new council was elected by mail ballot. The new President of the IOCG for 1983-1986 is R. Kern. In the same ballot an amendment of the constitution was accepted, which underlines that the national meetings are subject to the laws and regulations of the host countries. This has been a formal obstacle for the participation of some countries in the IOCG.

IOCG-7 was successfully held in Stuttgart in September 1983. The large European and Japanese participation overcompensated for the decreased participation from the USA and the USSR. The proceedings have been published by North-Holland.

*European Crystallographic Committee*

M. Nardelli attended the meeting of this Committee at Liège, Belgium, on 9 August 1984, in place of the Union representative S. Ramaseshan.

The 8th European Crystallographic Meeting was held at Liège in August. The programme consisted of seven plenary lectures, 43 oral papers and 313 posters. The conference was attended by 410 participants and 40 accompanying members. Plans for ECM-9, to be held in Torino, Italy, 2-6 September 1985, are progressing well. It is hoped to hold ECM-10 in Wrocław, Poland, in 1986. The Committee discussed various methods of helping young crystallographers attend these meetings, and ways of increasing the participation of other countries in the work of the Committee.

**International Council of Scientific Unions**

The 17th Meeting of the General Committee of the International Council of Scientific Unions took place 4-5 August 1983, in the Staszic Palace, ancient site of the Polish Academy of Sciences, in Warsaw. The immediate Past President, N. Kato, was unable to attend because of the simultaneous meeting of the IUCr Executive Committee at Liège, and A. Magnéli therefore represented the Union in Warsaw. Major items treated by the General Committee included the following:

The Seychelles National Environment Commission was accepted as a National Associate of ICSU.

After discussions of the formal links of the ICSU Abstracting Board to ICSU, it was recommended to the 20th General Assembly that the present status of the Board as a permanent service of ICSU be terminated and that appropriate modes of cooperation between the Board and the ICSU family be determined after the Abstracting Board has established its new structure and objectives.

It was decided to establish an *ad hoc* committee to carry out a study of aspects of global change that are not yet

adequately covered, and to make recommendations to the 20th General Assembly for further planning in fields that are interdisciplinary and require international cooperation.

A special committee has been set up by the ICSU Executive Board to make an assessment of the biological, medical and physical effects of large-scale use of nuclear weapons. The Scientific Committee on Problems of the Environment (SCOPE) is also undertaking a study on the environmental consequences of nuclear war. All ICSU adhering bodies were urged to give their full support to this undertaking and to make appropriate additional inputs.

The 20th General Assembly of ICSU will be held in Ottawa in September 1984.

**Finances**

The audited accounts for the year 1983 are given at the end of this Report. For comparison, the figures for 1982 are provided in italics. Negative quantities are indicated by parentheses. As agreed by the General Assembly in August 1981 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 1983 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 27 197. 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 1983.

As on previous Balance Sheets, the investments have been valued according to their quotation at the end of the year. Their appreciation in value, together amounting to SwFr 1031, 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 1983 the Union held investments of SwFr 18 000 and £ 100 000 in government bonds.

The total of SwFr 1 254 695 with the banks at the end of the year was represented by Dfl 14 652 and \$ 317 661 with the Amsterdam-Rotterdam Bank, \$ 19 179 with the Bankers Trust Company, £ 143 786 with the National Westminster Bank and SwFr 52 187 with the Union Bank of Switzerland. The amounts shown in the Balance Sheet for debtors and creditors relate to sums, principally on the publishing accounts, due at 31 December 1983. Where appropriate, these accounts have now been settled.

The Balance Sheet shows that the assets of the Union, excluding stocks of unsold publications but including the loss of SwFr 27 197 resulting from fluctuations in rates of exchange, have increased during the year, from SwFr 1 203 961 to SwFr 1 917 217.

The General Fund account shows a surplus of SwFr 113 114 as compared with a surplus of SwFr 150 041 in 1982. The administrative expenses were SwFr 140 047 in

1983 as compared with SwFr 138 703 in 1982. Of this amount, SwFr 42 969 was charged to the publications of the Union. SwFr 30 247 was spent on supporting scientific meetings, and SwFr 3101 was required for travel expenses of Union representatives on other bodies. The Executive Committee Meeting cost SwFr 17 640 and the Finance Committee SwFr 8557. A charge of SwFr 11 756 was made to the General Fund for the publication of the Report of the Twelfth General Assembly and Congress. The Union received SwFr 30 714 from the Unesco subvention to ICSU and a grant of a further SwFr 4260 from ICSU. The subscriptions from Adhering Bodies were SwFr 129 940. Interest on bank accounts and investments was SwFr 135 672.

The President's Fund account received SwFr 3972 in donations during 1983; no payments were made from the fund.

The *Acta Crystallographica* account for 1983 shows a surplus of SwFr 559 473 as compared with a surplus of SwFr 202 606 in 1982.

The division of *Acta* into three sections in 1983 created large uncertainties in planning the budget. The subscription rates were determined to yield a surplus comparable to that of the previous year. However, the number of pages printed was substantially less than estimated and the fall in the number of subscriptions was also less than expected. A further economy was made in 1983 by terminating the 10% commission given to subscription agencies. The technical editing expenses for 1983 include a charge of SwFr 8194 as a contribution towards the purchase of the office computer, which was made possible by the generous donation from the Japanese crystallographic community.

The number of paid subscriptions to all sections of the journal dropped from 1295 in 1982 to 1197 in 1983, including 132 personal subscriptions in 1982 and 145 in 1983. There were also 271 paid subscriptions to Section A and 142 paid subscriptions to Section B in 1983, compared with 254 and 140 respectively in 1982. 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. The technical editing costs for *Acta Crystallographica* were SwFr 244 671 in 1983 as compared with SwFr 240 492 in 1982. 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 surplus of SwFr 104 696 as compared with a surplus of

SwFr 81 598 in 1982. The number of paid subscriptions decreased from 1105 in 1982 to 1076 in 1983, including 98 personal subscriptions in 1982 and 115 in 1983.

The *Structure Reports* account shows a deficit of SwFr 59 415 as compared with a surplus of SwFr 7239 in 1982, because sales were very low, with no annual volumes being published, and there were still considerable editorial expenses for new volumes to be published in the near future. Publishing and editorial expenses in 1983 were SwFr 20 744 and SwFr 70 373 respectively, as compared with SwFr 52 220 and SwFr 59 435 in 1982. The net income from sales was SwFr 32 131 in 1983 as compared with SwFr 119 356 in 1982.

The *International Tables* account shows a surplus of SwFr 64 746 as compared with a surplus of SwFr 7940 in 1982. It had been expected that Volume A on Space-Group Symmetry would be published in 1982 but there were delays in the final stages of production, and it was not available until late 1983. In addition to the cost of printing, about half the editorial expenses in 1983 related to Volume A (the remainder being for preparatory work for Volumes B and C). There have also been substantial editorial expenses over the many years of preparation of this volume. With the publication of Volume A these expenses have been recovered and the accumulated balance was positive at the end of 1983, for the first time for many years.

SwFr 261 was received from the sale of 17 copies of *Fifty Years of X-ray Diffraction*. SwFr 457 was received from the sale of 32 copies of *Symmetry Aspects of M. C. Escher's Periodic Drawings*, as well as SwFr 326 royalties for the Japanese edition of this book. SwFr 176 was received from the sale of 8 copies of Volumes I and II of *Early Papers on Diffraction of X-rays by Crystals*. The *Molecular Structures and Dimensions* account shows no surplus for 1983, because this account was charged with a contribution of SwFr 38 353 towards the publication costs of Volume 14, the volume published in 1983. The sale of earlier volumes was much lower than for 1982, with 428 copies of Volume 14 and 306 copies of earlier volumes being sold. *Fifty Years of Electron Diffraction* was published in 1981. Net sales of 47 copies yielded SwFr 2254, reducing the deficit on this fund account to SwFr 10 515.

The Special Publications Fund was established in 1981 with the donation from the Japanese crystallographic community. This donation, together with small transfers from the General Fund and the journals accounts, has been used for the purchase of the computer. The fund account has now been closed.

## International Union of Crystallography

## Balance Sheet as at 31 December 1983

	Swiss Francs		1982		1983		1982	
	As at 1 January 1983	(Loss on fluctuations in Rates of Exchange)	Excess of Income over Expenditure for the year	Balance at 31 December 1983	1983	1982	Swiss Francs	1982
<b>FUND ACCOUNTS</b>								
General Fund	433,395	(7,565)	113,114	538,944	433,395			
President's Fund	12,850	(233)	3,972	16,589	12,850			
<i>Acta Crystallographica</i>	317,629	(12,141)	559,473	864,961	317,629			
<i>Journal of Applied Crystallography</i>	137,955	(3,359)	104,696	239,292	137,955			
<i>Structure Reports</i>	198,418	(1,924)	(59,415)	137,079	198,418			
<i>International Tables</i>	(31,685)	(458)	64,746	32,603	(31,685)			
General Publications	76,076	(1,053)	—	75,023	76,076			
<i>Fifty Years of X-ray Diffraction</i>	4,938	(72)	261	5,127	4,938			
<i>Escher Drawings</i>	20,608	(296)	783	21,095	20,608			
<i>Early Papers</i>	(10,003)	—	176	(9,827)	(10,003)			
<i>Molecular Structures and Dimensions</i>	6,942	(96)	—	6,846	6,942			
<i>Fifty Years of Electron Diffraction</i>	(12,769)	—	2,254	(10,515)	(12,769)			
Special Publications	49,607	—	(49,607)	—	49,607			
Fund	<u>1,203,961</u>	<u>(27,197)</u>	<u>740,453</u>	<u>1,917,217</u>	<u>1,203,961</u>			
<b>CURRENT ASSETS</b>								
Cash at Banks								
Current Accounts								134,498
Deposit and Savings Accounts								1,120,197
Treasury Bills								—
								1,254,695
Cash with Union Officials								8,321
Debtors								413,694
Subscriptions from Adhering Bodies, due for 1983								24,723
								<u>1,701,433</u>
Deduct Creditors								<u>121,401</u>
								1,580,032
<b>NET CURRENT ASSETS</b>								1,177,475
<b>INVESTMENTS</b>								
At market value								333,086
(Appreciation)/depreciation in value								(1,031)
At cost								332,055
								18,990
<b>FIXED ASSETS</b>								
Office Equipment at cost, less depreciation								5,130
								<u>7,496</u>
								<u>1,917,217</u>
								<u>1,203,961</u>

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

We have audited the financial statements on pages 102 to 109 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 31st December 1983 and of its excess of income over expenditure and source and application of funds for the year then ended.

Manchester, England  
22 August 1984

Signed: TOUCHE ROSS & CO

Chartered Accountants



## President's Fund Account for the year ended 31 December 1983

	Swiss Francs	
	1983	1982
Travel Grant and Registration Fees	—	582
Excess of Income over Expenditure carried to Balance Sheet	3,972	7,282
	<u>3,972</u>	<u>7,864</u>
	1983	1982
Donations received	3,972	864
Transfer from General Fund Account	—	7,000
	<u>3,972</u>	<u>7,864</u>

## Acta Crystallographica Account for the year ended 31 December 1983

Publication Expenses:				
Printing and Binding Volume 39 (1982 Volume 38)	433,183	579,057	1,511,324	1,239,589
Distribution and Postage	67,061	55,149	24,772	48,810
Airfreight Costs	29,394	25,987	24,517	20,049
	<u>529,638</u>	<u>660,193</u>	<u>198</u>	<u>253</u>
Printing Index to Volume 38 (1982 Volume 37) and sundry printing	30,453	32,098	1,560,811	1,308,701
Cancellation of Computerised Typesetting Facility	—	—	107,527	90,188
Editorial Expenses:				
Editorial Honoraria	31,172	26,627		
Secretarial Assistance	9,179	7,965		
Postages, Telephone and Office Sundries	15,622	8,852		
Technical Editing:				
Salaries and Expenses	236,477	240,492		
Transfer to Special Publications	8,194	—		
Fund re Computer	1,565	2,481		
Depreciation of Office Equipment				
Administration Expenses	31,511			
Excess of Income over Expenditure carried to Balance Sheet	<u>559,473</u>	<u>202,606</u>	<u>1,453,284</u>	<u>1,218,513</u>
	1,453,284	1,218,513	1,453,284	1,218,513
			Less Publisher's Commission on Sales	

*Journal of Applied Crystallography* Account for the year ended 31 December 1983

	Swiss Francs		Swiss Francs	
	1983	1982	1983	1982
Publication Expenses:				
Printing and Binding Volume 16 (1982 Volume 15)	94,368	88,498	287,409	240,429
Distribution and Postage	12,017	10,737	12,402	11,413
Airfreight Costs	5,561	5,374	4,882	4,781
		104,609	136	106
			<u>304,829</u>	<u>256,729</u>
Cancellation of Computerised Typesetting Facility	—	895	20,987	17,629
Editorial Expenses:				
Editorial Honoraria	4,717	3,991	283,842	239,100
Postages, Telephone and Office Sundries	1,846	1,734	892	426
Salaries and Expenses	47,508	35,935		
Transfer to Special Publications	3,311	—		
Fund re Computer	207	361		
Depreciation of Office Equipment		42,021		
			<u>10,503</u>	<u>10,403</u>
Administration Expenses				
Excess of Income over Expenditure carried to Balance Sheet		81,598		
			<u>284,734</u>	<u>239,526</u>
			<u>284,734</u>	<u>239,526</u>

**Structure Reports Account for the year ended 31 December 1983**

	Swiss Francs			Swiss Francs	
	1983	1982		1983	1982
Publication Expenses:			Sale of Copies		
Printing and Binding Volume 36			Volume 36 (1982 Volumes 44B,		
(1982 Volumes 44B, 46A and 47A)	9,982	44,304	45A, 46A and 47A)	19,616	143,110
Typing of Manuscripts	10,762	7,916	Earlier Volumes and Indexes	24,545	19,295
Depreciation		462		44,161	162,405
Editorial Expenses:			Less Publisher's Commission on Sales	12,030	43,049
Salary and Honoraria: Editors,	70,373	59,435	<i>Excess of Expenditure over Income</i>		
Abstractors and Assistants		7,239	<i>carried to Balance Sheet</i>	59,415	—
<i>Excess of Income over Expenditure</i>					
<i>carried to Balance Sheet</i>	91,546	119,356		91,546	119,356

**International Tables Account for the year ended 31 December 1983**

Publication Expenses:			Sale of Copies		
Printing and binding Volume A	84,287	—	Volume A	229,184	—
Reprinting Volume III	13,390	—	Volumes II, III and IV	32,875	12,662
Editorial Expenses:					
Honoraria	19,370	—	Less Publisher's Commission on Sales	262,059	12,662
Secretarial Assistance and Postages	7,330	2,471		72,936	2,251
<i>Excess of Income over Expenditure</i>					
<i>carried to Balance Sheet</i>	64,746	7,940		189,123	10,411
	189,123	10,411		189,123	10,411



**Fifty Years of X-ray Diffraction Account for the year ended 31 December 1983**

	Swiss Francs	
	1983	1982
<i>Excess of Income over Expenditure carried to Balance Sheet</i>		
	261	317
Sale of Copies	373	453
Less Publisher's Commission on Sales	112	136
	<u>261</u>	<u>317</u>
	<u>261</u>	<u>317</u>

**Escher Drawings Account for the year ended 31 December 1983**

11095

<i>Excess of Income over Expenditure carried to Balance Sheet</i>		
	783	717
Sale of Copies	653	573
Less Publisher's Commission on Sales	196	172
	<u>326</u>	<u>401</u>
Royalties	783	717
	<u>783</u>	<u>717</u>

**Early Papers Account for the year ended 31 December 1983**

<i>Excess of Income over Expenditure carried to Balance Sheet</i>		
	176	156
Sale of Copies of Volumes I and II	252	223
Less Publisher's Commission on Sales	76	67
	<u>176</u>	<u>156</u>
	<u>176</u>	<u>156</u>

**Molecular Structures and Dimensions Account for the year ended 31 December 1983**

	Swiss Francs	
	1983	1982
Publication Expenses:		
Printing and binding Volume 14		
(1982 Volume 13)	24,631	21,735
Paper	11,606	8,590
Carriage and Miscellaneous Expenses	886	1,010
Salaries	1,230	14,790
	<u>38,353</u>	<u>46,125</u>
Administration Expenses	955	1,203
<i>Excess of Income over Expenditure for the year:</i>		
University of Cambridge	—	—
IUCr carried to Balance Sheet	—	—
	<u>39,308</u>	<u>47,328</u>
	Swiss Francs	1982
	1983	
Sale of Copies		
Volume 14 (1982 Volume 13)	33,655	31,270
Earlier Volumes	19,949	33,508
	<u>53,604</u>	<u>64,778</u>
Less Publisher's Commission on Sales	14,296	17,450
	<u>39,308</u>	<u>47,328</u>

**Fifty Years of Electron Diffraction Account for the year ended 31 December 1983**

<i>Excess of Income over Expenditure carried to Balance Sheet</i>			
	2,254	10,592	14,314
	<u>2,254</u>	<u>10,592</u>	<u>3,722</u>
	3,046	2,254	10,592
	<u>792</u>	<u>2,254</u>	<u>10,592</u>

**Special Publications Fund for the year ended 31 December 1983**

Purchase of Office Computer	72,617	—	—
	<u>72,617</u>	<u>—</u>	<u>—</u>
Transfers from other funds:			
General Fund	11,505	—	—
Acta Crystallographica	8,194	—	—
Journal of Applied Crystallography	3,311	23,010	—
	<u>23,010</u>	<u>—</u>	<u>—</u>
<i>Excess of Expenditure over Income carried to Balance Sheet</i>	49,607	—	—
	<u>72,617</u>	<u>—</u>	<u>—</u>

**Statement of Source and Application of Funds**  
**Year ended 31 December 1983**

	1983 <i>SwFr</i>	1982 <i>SwFr</i>
Source of funds		
Excess of Income over Expenditure for the year	740,453	468,488
(Loss)/gain on fluctuations in rates of exchange	(27,197)	25,786
	<hr/> 713,256	<hr/> 494,274
Adjustment for items not involving the movement of funds:		
Depreciation	2,623	4,885
Loss on sale of investments	990	—
Loss on fluctuations in rates of exchange on office equipment	526	288
	<hr/> 717,395	<hr/> 499,447
Total generated from operations	717,395	499,447
Proceeds on sale of investments	18,000	—
Increase in creditors	31,175	—
	<hr/> 766,570	<hr/> 499,447
Application of funds		
Increase in debtors (including subscriptions)	(162,336)	(110,395)
Decrease in creditors	—	(101,624)
Purchase of office equipment	(783)	(6,917)
Purchase of investments	(332,055)	—
	<hr/> 271,396	<hr/> 280,511

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

## Notes to the Financial Statements

### 1. Accounting Policies

(a) 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 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) 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.

(iii) 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:

	1983	1982
Netherland Guilders	1.3899	1.29
Danish Crowns	4.4953	4.11
Pounds Sterling	0.3142	0.291
US Dollars	0.4587	0.469
Canadian Dollars	0.5642	0.58

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