### International Union of Crystallography

### Report of the Executive Committee for 1981

### Twelfth General Assembly and Congress

By invitation of the National Research Council of Canada, the Twelfth General Assembly and International Congress of Crystallography were held at Carleton University, Ottawa, Canada, 16–25 August 1981. A report, including a detailed report of the proceedings of the General Assembly, has been published in this journal [*Acta Cryst.* (1983), A39, 425–480] and will be sent to the National Committees for Crystallography.

The meetings were attended by 1330 scientists of whom 116 were from Canada and the remainder from 38 other countries. Professor Dorothy Hodgkin delivered the Congress Discourse, entitled 'Insulin in Crystals', at the Opening Ceremony. There were ten Main Lectures and 43 microsymposia, some of which were organized by Commissions of the Union. In all, 1087 papers were presented, 229 at oral sessions and the remainder at poster sessions. The abstracts of these papers were included in the Congress book of Collected Abstracts, which was reproduced as a supplement to Acta Crystallographica, Section A. Exhibitions of commercial and non-commercial crystallographic equipment, crystallographic books and items relating to the artistic side of crystallography were held during the Congress. Demonstrations were given of various databases. An extensive programme of excursions and social events was arranged. The Congress was organized excellently under the direction of Dr L. D. Calvert, Chairman of the Organizing Committee, and Dr F. R. Ahmed, Chairman of the Programme Committee.

The General Assembly met on the evenings of 17, 18 and 22 August and the afternoon of 25 August. The Portuguese Physical Society was accepted as an Adhering Body in Category I. As a result of reorganization within the Finnish scientific community the Delegation of the Finnish Academies of Science and Letters was accepted as the new Adhering Body in Finland.

The Assembly received the triennial financial report and the reports of the Executive Committee, the Commissions and the Union Representatives on other bodies since the Eleventh General Assembly in 1978. A report was presented on the proposed establishment of an in-house computerized typesetting system, which had been adandoned in mid-1981 mainly because of cash-flow problems, in spite of financial guarantees from various sources and a large donation from the Japanese crystallographic community. A downward trend in the number of manuscripts submitted and reductions in typesetting prices by the Union's printer in the UK made the in-house option less favourable. New Officers of the Union, Chairmen and members of Commissions and Union Representatives were elected, the full list of these people being given as an annex to the published report of the General Assembly. The Assembly changed the currency of the Union's accounts and the unit contribution from US dollars to Swiss Francs, and set the unit contribution for the years 1982–1984 inclusive at SwFr 890.

The General Assembly reaffirmed its decision to hold the Thirteenth General Assembly and Congress in Hamburg, Federal Republic of Germany, in August 1984, and provisionally accepted an invitation from the Australian Academy of Science to hold the Fourteenth General Assembly and Congress in Australia in 1987.

The Executive Committee met for several days before, and most days during, the Congress, mainly to deal with matters directly related to the business of the General Assembly and the work of the Commissions.

### Other Meetings

In addition to its own Congress, the Union sponsored the following meetings which were held during 1981: Applications of the Mössbauer Effect, Jaipur, India, 14–18 December; International Summer School on Crystallographic Computing, Ottawa, Canada, 7–15 August; Neutron Diffraction Conference, Argonne, USA, 12–13 August; Symposium on Crystallography in the Health Sciences; Crystalline Deposits in Human Tissues, Toronto, Canada, 13–14 August; Symposium on Biologically Active Molecules, Buffalo, USA, 26–28 August; V Iberoamerican Congress of Crystallography, Coimbra, Portugal, 20–26 September; International School on Synthesis, Crystal Growth and Characterization of Materials for Energy Conversion and Storage, New Delhi, India, 12–23 October.

### **Executive Committee**

The membership of the Executive Committee, including new members elected by the General Assembly, is as follows:

President: Dr J. Karle (USA); Vice-President: Professor S. Ramaseshan (India); General Secretary and Treasurer: Professor K. V. J. Kurki-Suonio (Finland); Immediate Past President: Professor N. Kato (Japan); Ordinary Members: Professor S. Amelinckx (Belgium), Professor Th. Hahn (Germany, Federal Republic), Professor M. Nardelli (Italy), Professor H. Neels (German Democratic Republic), Dr V. I. Simonov (USSR), Professor M. M. Woolfson (UK). Dr J. N. King continues as Executive Secretary.

### **Publications**

Volume 37 of Acta Crystallographica and Volume 14 of the Journal of Applied Crystallography were published in 1981, as were Volume 45A of Structure Reports and Volume 12 of

Molecular Structures and Dimensions. In addition, Fifty Years of Electron Diffraction was published just prior to the Ottawa Congress.

### **Adhering Bodies**

The latest list of Adhering Bodies of the Union, the memberships of the National Committees for Crystallography and the names and addresses of their secretaries are included as an annex to the report of the Twelfth General Assembly and Congress.

### Work of the Commissions

### Commission on Journals

Volume 37 of Acta Crystallographica (Acta) and Volume 14 of the Journal of Applied Crystallography (JAC) were produced in 1981. The large deficit incurred by the 1980

journal accounts [see Acta Crvst. (1981). A37, 922-941 for details] and the need to avoid a similar deficit in 1981 made it necessary to reduce the number of pages published in 1981. The actual number of pages and papers published in the Union journals over the last six years is given in Table 1. The reduction in number of pages for Acta A Volume 37 compared to Volume 36 was 14%, for Acta B, Volume 37 compared to Volume 36 was 30% and for JAC Volume 14 compared to Volume 13 was 23%. The average length of full articles increased slightly in Acta A and decreased slightly in Acta B and JAC in 1981, as the highest information density per page consistent with clarity was maintained. Sixteen percent more crystal structure papers appeared in the Short Structural Paper format than as full articles in Acta B. Volume 37 compared to 5% more in Volume 36. Essentially the same number of Short Communications and other short items were published in JAC, Volume 14 as in Volume 13.

Median publication times, the average elapsed time in months between the published date of acceptance and the nominal publication date, increased sharply for each of the

Table 1. Survey of the contents of the Union journals

### Acta Crystallographica

				Full A	rticles		tructural pers	Short Communications		
Vol.	Year	Number of pages*	Number of papers	Number	Average length	Number	Average length	Number	Average length	
A32 B32	1976	1038 3360) 4398	188 823 1011	${152 \atop 535}$ 687	$\begin{array}{c} 6.0 \\ 5.0 \end{array}$ 5.2	_ 260	_ 2·5	$\frac{36}{28}$ 64	$1 \cdot 1$ $1 \cdot 1$ $1 \cdot 1$	
A33 B33	1977	1046 $3974$ 5020	$ \begin{array}{c} 201 \\ 991 \end{array} $ 1192	181 548 729	$5.6 \\ 5.2 $ 5.3	409	2·6	$\begin{vmatrix} 20 \\ 34 \end{vmatrix}$ 54	$\begin{cases} 1.1 \\ 1.5 \\ 1.4 \end{cases}$ 1.4	
A34 } †	1978	$   \begin{array}{c}     1048 \\     3848   \end{array} $ 4896	$189 \\ 1040$ 1229	$\binom{158}{510}$ 668	$\begin{array}{c} 6.0 \\ 5.0 \end{array}$ 5.2	490	2·5	$     \begin{array}{c}       31 \\       40     \end{array}     $ 71	$\begin{array}{c} 1.3 \\ 1.0 \\ 1.0 \end{array}$ 1.1	
A35 ) B35 )	1979	$1090 \\ 3130 $ 4220	$\binom{187}{898}$ 1085	${162 \atop 412}$ 574	$6.0 \\ 4.7$ 5.0	- 457	2.5	$\binom{25}{29}$ 54	$\begin{cases} 1.5 \\ 1.5 \end{cases}$ 1.5	
A36 ) B36 ) A37 ) †	1980	$1096 \ 3212 \ 4308$	$194 \\ 877 $ 1071	$\begin{vmatrix} 168 \\ 417 \end{vmatrix}$ 585	$\begin{array}{c} 6.1 \\ 5.0 \end{array}$ 5.3	438	_ 2·5	$\binom{26}{22}$ 48	$\begin{array}{c} 1.3 \\ 1.3 \end{array}$ 1.3	
B37 }	1981	$\binom{944}{2250}$ 3194	$\binom{158}{630}$ 788	$\binom{136}{286}$ 422	$6.4 \\ 4.9$ 5.4	333	_ 2·5	$\binom{22}{11}$ 33	$\begin{array}{c} 1.1 \\ 0.6 \end{array}$ 0.9	

### Journal of Applied Crystallography

	Number Number			Full Articles § Communications				Crysta	al Data		puter rams	Short Items¶		
Vol.	Year	of pages*‡	of papers	Number	Average length	Number	Average length	Number	Average length	Number	Average length	Number	Average length	
9	1976	514	136	71	6.2	19	1.6	25	1.6	3	1.7	18	0.5	
10	1977	510	134	76	5.5	14	1.8	22	1.3	6	1.6	15	0.9	
11‡	1978	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	

<sup>\*</sup> Excluding indexes.

<sup>†</sup> 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.

<sup>‡</sup> 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.

<sup>§</sup> Excluding Lead Articles and Conference papers.

<sup>¶</sup> Excluding Union Announcements, Crystallographers, and Book Reviews.

Union journals in 1981 as a consequence of the smaller number of pages published. Publication times for full articles in Acta A were about three weeks longer, in Acta B about five weeks longer and in JAC about six weeks longer than in 1980, at  $5 \cdot 8$ ,  $6 \cdot 1$  and  $6 \cdot 3$  months respectively. The delays increased as the backlog of papers accumulated toward the end of the year. These delays are regarded as entirely temporary and it is expected that normal publication times will again be achieved in 1982.

The informal grouping of structural papers as inorganic, organometallic, or organic used in the last three volumes of *Acta* has been continued in *Acta* B37 for both full articles and Short Structural Papers. A total of 72 inorganic, 66 organometallic and 148 organic full articles appeared in 1981 with 57 inorganic, 77 organometallic and 148 organic Short Structural Papers. The expanded *Index* format for *Acta* A and B used in the last three years was again used for Volume 37.

The distribution of papers and authors by country in *Acta* A, *Acta* B and *JAC* for 1980 and 1981 is given in Table 2. The three largest absolute changes in year-to-year distribution for papers published in *Acta* A were for the Federal Republic of Germany, Japan and the USA; in *Acta* B, they were for Poland, France and the Federal Republic of Germany; and in *JAC*, they were for the USA, France and Israel. However, the normal fluctuation from year to year together with the smaller issues in 1981 renders any interpretations of these changes open to ambiguity. It may be noted that two countries represented in 1979 are not included in Table 2, but that five other countries have been added.

Considerable effort is made by the editorial staff in Chester to ensure that chemical formulae and nomenclature in all papers published conform to the rules established by the International Union of Pure and Applied Chemistry, the International Union of Biochemistry and other appropriate bodies. Approximately half the papers received require at least a minor change, and about 15% require major nomenclature modification. Information concerning nomenclature has been published [Acta Cryst. (1983), A39, 179].

Plans for establishing an in-house computer-controlled typesetting system, which had reached a very advanced stage in early 1981, were abandoned when the size of the deficit in the journal accounts for 1980 was realized. A primary motivation for undertaking our own composition was the rapid increase in commercial composition rates. The Union is fortunate that current rates have ceased to climb and may even decrease in future years.

The Commission appointed an advisory committee in August 1980 (R. A. Young, Chairman; E. Prince and R. A. Sparks) to develop guidelines for the publication of Rietveld analyses and pattern decomposition studies with powder diffraction patterns. Following extensive consultation with the international community in this field the committee drew up a set of suggested guidelines now in press in JAC [J. Appl. Cryst. (1982), 15, 357–359]. Comments on these suggestions will be taken fully into account by the Commission before action is taken to adopt any as Union policy.

The Commission met in Ottawa for a series of sessions immediately before the opening of the XIIth Congress. All active members were present together with nearly all recent past members. Among the matters considered was the forthcoming subdivision of *Acta* B [see the Editorial in *Acta Cryst.* (1982), A38, 1; B38, 1] and the detailed format for

papers in Acta C [see Acta Cryst. (1983), A39, 175, 182–183]. Notes for Authors was reviewed and a new edition was planned for publication in 1982 [Acta Cryst. (1983), A39, 174–186]. Many other aspects of publishing the Union journals were given careful examination.

M. Nardelli, R Norrestam and D. H. Templeton were appointed Co-editors of *Acta* in succession to G. Allegra, S. Jagner and E. C. Lingafelter, whose resignations had been accepted. M. Schlenker was appointed Co-editor of *JAC* in succession to J. C. Joubert.

### Commission on Structure Reports

Volume 45A (Metals and Inorganic Compounds for 1979, 445 pages) was published in 1981. Volume 46A (Metals and Inorganic Compounds for 1980) is with the printer, and co-editorial work is in progress on Volume 48A (Metals and Inorganic Compounds for 1981).

Volume 44B (Organic Compounds for 1978, 1279 pages in two parts) was published in 1981. Co-editorial work is in progress on Volumes 45B (1979), 46B (1980), and 48B (1981).

G. Ferguson was appointed Chairman of the Commission and General Editor of Structure Reports in succession to J. Trotter in August 1981.

### Commission on International Tables

The third and final proof-reading of the plane-group and space-group tables was carried out by the Editor and the Union's Technical Editor in May and June of 1981.

The preparation of the text of the Introduction continued throughout the year. The Introduction was completed in late spring of 1982, comprising about 600 typewritten pages.

Tables and Introduction were exhibited during the XIIth Congress in August 1981. In addition to numerous small meetings, the Commission held its final meeting on 23 August 1981 during this Congress. It was attended by ten Commission members and six guests. Topics were the proof-reading of the Introduction, future volumes of *International Tables*, and suggestions for the Chairman and members of the new Commission. A list of candidates was subsequently submitted to the Executive Committee.

With this meeting, the Commission on International Tables completed its tenure. No new Commission was appointed during the XIIth General Assembly.

### Commission on Biological Macromolecular Crystallography

The Commission was established by the XIIth General Assembly in August 1981 at Ottawa and held its first meeting there on 21 August. It was decided that, at this time, the Commission should concern itself primarily with the quality of suitable scientific meetings and journals.

The enormous change in the representation of biological work at the Ottawa Congress as opposed to the Warsaw Congress was greatly appreciated. In order to assure a continuation of this trend, T. L. Blundell agreed to have his name proposed to the Programme Committee for the Hamburg Congress.

Table 2. Distribution of papers and authors, by country, in the Union journals for 1980 and 1981

Errata have been excluded. 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. 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.

				Acta Crys	tallographica					Journ	al of	
	Section A Section B						Appl	ied Crys		phy		
	Pap			hors	Pap			hors	Pap	•	Aut	•
Country	1980	1981	1980	1981	1980	1981	1980	1981	1980	1981	1980	1981
Algeria	_	_	_	_	1.3	_	5	-	_	-	-	_
Argentina	_	0.3	1	4	2.6	_	13	_	1.0	1.0	3	4
Australia	8.2	6.0	17	9	17.9	25.0	52	58	3.0	1.0	7	3
Austria	0⋅8	-	4	_	4.0	1.0	6	3	2.0	1.0	2	1
Bangladesh	-	-	_	_	-	1.0	-	1	1.0	- 1⋅0	1 2	- 1
Belgium	_	3.0	_	6	18.2	11·4 6·7	80 14	51 21	1·0 —	1.0	_	2
Brazil	2.0	1·0 1·3	2	I 3	4·0 48·0	28.7	111	62	3.0	2.0	- 8	6
Canada Chile	<b>-</b>	-	_	_	0.4	0.7	2	2	1.0	1.0	2	3
China, People's Rep.	_	_	_	2	-	0.5	_	ī	_	_	2	_
Costa Rica	_	_	_	_	0.6	_	3	_	_	-	_	_
Cuba	0.3	_	1	_	_	_	_	_	1.0	_	-	_
Czechoslovakia	1.0	1.0	2	5	9.0	6.3	34	19	1.0	2.0	3	3
Denmark	0.8	1.0	3	2	4.0	11.3	8	27	0.7	1.0	2	2
Egypt	1.0	_	2	_	_	-	_	_	_	_	-	_
Finland	3.3	1.3	6	3	11.6	2.0	30	4	_	_	-	-
France	14-1	13.3	34	31	141.9	89.4	352	303	25.2	21.9	70	59
German Dem. Rep.	-	1.0	-	1	1.4	1.5	6	4	1·0 8·3	2·0 7·0	3 16	3 19
Germany, Fed. Rep.	16-4	24·6 –	29 _	40 -	86·7 –	56⋅8 0⋅7	181	118 3	8.3	- -	-	-
Ghana Greece	_	_	_	1	3.0	1.0	10	3	_	_	_	_
Hong Kong	_	_	_	_	-	_	2	_	_	_	_	_
Hungary	0.7	_	2	_	5.1	2.5	19	9	0.3	_	3	_
India	15.0	11.0	30	23	15.3	21.3	41	59	4.0	7.0	13	18
Iran	_	1.0	-	1	_	-	_	_	1.0	-	1	_
Iraq	_	_	_	-	_	_	1	1	-	_	_	_
Ireland			-		3.0	2.0	9	6	_	_	_	_
Israel	0.3	3.5	1	6	12-1	7.2	22	16	3.3	2.0	6	- 15
Italy	9.7	6.0	23	13	38.7	23.4	110	76	5.0	3·8 -	13	15
Ivory Coast	21.0	- 14·5	-	- 35	1·1 61·1	4·8 43·7	5 215	16 151	- 12·0	10.0	_ 29	_ 25
Japan Korea, South	21·0 –	14.3	56 -	-	-	43.1	213	131	-	-	_	_
Malaysia	_	_	_	_	_	_	_	1	_	_	_	_
Mexico	_	_	_	_	_	0.3	_	i	_	_	_	_
Netherlands	7.9	9.0	22	14	19.8	19.2	45	48	4.0	2.8	9	7
New Guinea	_	_	_	_	0.3	_	1	_	_	_	_	_
New Zealand	1.0	_	3	-	3.0	1.0	8	4	_	-	-	-
Nigeria	_	_	-	-		0.7	_	2	_	_	-	_
Norway	_	1.0	_	2	1.7	5.3	5	9	2.0	_	4	_
Pakistan	1.0	_	6	_	-	-	150	_ 47	- 1·0	- 1·5	3	3
Poland	1.0	2·5 1·0	2	5 5	56⋅8 1⋅0	17·1 –	150 5	47 _	1.0	-	_	_
Portugal Romania	_ 1∙0	1.0	2	3	-	_	_	_		_	_	_
Saudi Arabia	1.0	_	_	_	1.0	_	1	_	_	_	_	_
South Africa	1.0	_	1	_	10.0	2.4	31	5	1.0	_	1	
Spain	_	0.3	ī	1	11.0	18.6	38	58	0.9	3.0	3	8
Sweden	_	1.0	-	5	30.9	16.0	55	34	4.3	2.3	13	7
Switzerland	9.3	4.6	16	9	20.2	6.3	43	16	1.3	1.0	3	1
Taiwan	_	_	_	-	2.0	1.0	8	1	-	_	-	_
Thailand	_	_	_	-	_	1.0	2	6	_	_	1	_
Tunisia	-	-	-	_	0.6	1.2	3	6	-	- 2	_	_
Turkey	_	-	_	_	-	_	-	_	0.3	0·3 —	1 1	1
Uruguay	- 7∙0	- 5⋅0	_ 17	- 10	_ 2·7	- 1·0	1 7	2	_	_ 1∙0	_	13
USSR			56	41	2· / 64·8	53.8	199	170	13.0	11.8	20	22
UK	24·5 31·8	21·5 19·4	60	41	132.9	118.2	378	319	27.4	30.8	74	63
USA Venezuela	0.3	19.4	1	-	132.9	-	-	-	_	1.0	_	2
Yugoslavia	0.5	_	i	_	17-4	9.0	49	32	3.0	_	11	_
1 450014114	0.5		•		•			. –				

The current problems with publication in *Acta* of material relevant to the concerns of the Commission was recognized. A lengthy proposal for changes to *Acta* policy was drawn up and subsequently sent to the Commission on Journals. The major thrust was for the appointment of a special editor with knowledge and experience of macromolecular biology to *Acta*. He should promote review articles and encourage submission of interesting manuscripts at all stages of investigations.

A meeting of the Commission was held in Erice, Sicily, in June 1982, in conjunction with the Workshop on Crystallography of Molecular Biology.

### Commission on Charge, Spin and Momentum Densities

A new Commission was elected in Ottawa upon the occasion of the XIIth Congress; several founder members of the Commission concluded their period of office and K. V. J. Kurki-Suonio was succeeded as Chairman by M. J. Cooper. During the Congress the Commission ran three microsymposia (including the Open Meeting of the Commission) and in addition F. Hirshfeld, a new member of the Commission, delivered one of the plenary Congress lectures.

The projects of the Commission made good progress. A data bank for X-ray diffraction data used in charge density studies was established by H. Burzlaff at the Universität Erlangen-Nurnberg and an advisory committee which includes three members of the Commission was set up and met at the end of the year. Experimentalists are requested to contact Professor Burzlaff with a view to lodging their data in the bank. The Commission also devised a set of guidelines for the publication of charge density diffraction studies in response to a request from the Editor of *Acta Crystallographica*.

The oxalic acid project is nearing completion and P. Coppens is preparing a project report for publication in *Acta Cryst*. Chemically significant features were observed in all the contributing studies and the quality of the data suggested that oxalic acid might be considered a good standard for the calibration of experimental and data reduction techniques in charge density determinations.

Planning for the 1982 Sagamore VII Conference continued under the chairmanship of Y. Saito; Sweden was tentatively chosen as the site for Sagamore VIII in 1985.

# Commission on Crystal Growth and Characterization of Materials

The Commission organized an international school in India, and two microsymposia at the XIIth Congress. The name of the Commission was extended to include materials research activities other than crystal growth.

The International School on Synthesis, Crystal Growth and Characterization of Materials for Energy Conversion and Storage was held 12–23 October at the National Physical Laboratory (NPL) in New Delhi, in honour of the 60th birthday of A. R. Verma, under the co-direction of E. Kaldis and Krishan Lal. The Commission acted as the programme committee, to select 18 lecturers from abroad who, together with 10 lecturers from India, gave 56 lectures to about 150 participants. The high standard of the

participants, mostly from over 110 universities and numerous research laboratories of India, resulted in excellent scientific discussions between participants and lecturers. The superb organization due to Dr Krishan Lal, Assistant Director of the NPL, and the excellent facilities of this institution contributed to the great success of the school. The generous financial and moral support of the Government of India is greatly appreciated by the Commission.

In contrast to these gratifying results, the success of the two open sessions in the XIIth Congress was rather small, although the Commission made great efforts to present two interesting programmes on Materials Science and Crystallography and on Fundamental Aspects of Crystal Growth. The rather low number of participants may be explained to some degree by interesting parallel sessions.

It is intended to hold a school on Materials Research for Energy Problems in Egypt in March 1983, with the emphasis on applied research.

### Commission on Crystallographic Apparatus

The Commission met twice during the Ottawa Congress. Members and Consultants not present have taken part in Commission activities by correspondence.

- 1. Microdensitometer Project (S. Abrahamsson, P. Kierkegaard, G. Lundgren). Phase two of the project concerning a comparison between data from the same crystal recorded on film and on a diffractometer, was presented at a microsymposium at the Congress. The final written report is in progress.
- 2. Survey of Film Characteristics (M. Elder, O. S. Mills). Various properties of X-ray films of some 30 brands have been evaluated and were discussed at a microsymposium in Ottawa. The final write-up of the paper is in progress.
- 3. X-ray Attenuation Project (D. C. Creagh). 18 sets of silicon samples have been distributed to different laboratories. Preliminary results were reported at a microsymposium in Ottawa. A paper on data presented so far has been produced.
- 4. Polarization Ratio Survey (L. D. Jennings). The surprisingly low response by the crystallographic community to provide information on measurements of the polarization ratio has delayed the project. The data received so far will, however, now be summarized.
- 5. Radiation Safety (S. Martinez Carrera). The Commission will make further attempts to approach regulatory agencies in different countries concerning X-ray safety problems.
  - 6. New Projects.
  - (a) Accurate determination of X-ray intensities on diffractometers (H. Hope). A detailed plan for a project to evaluate procedures to measure X-ray intensities accurately on a diffractometer is being worked out.
  - (b) Profile analysis project (J. Cěrmák). The aim of the project is to investigate the agreement in pure diffraction profiles obtained by conventional computing methods from measured X-ray or neutron diffraction lines on a set of defined samples in different laboratories.
- 7. Meeting. The Commission has sought Union sponsorship for an Intercongress Symposium on the Accurate Determination of X-ray Intensities and Structure Factors. The exact date of the meeting is yet uncertain.

### Commission on Crystallographic Computing

The Commission arranged two microsymposia at the XIIth Congress entitled 'From Microprocessors to Array Processors and Pipeline Machines' and 'Languages, Portability, Systems and Networks'. Both these sessions were well attended and generated lively discussions, especially in relation to array processors and to language considerations.

Preceding the Congress there was held an International Summer School on Crystallographic Computing organized superbly by D. Sayre. The Commission was pleased to play a supporting role to Dr Sayre in relation to some of the programme for that school, proceedings of which have been published [Computational Crystallography (1982), Clarendon Press, Oxford University].

At the closed meetings of the XIIth Congress the Commission members and consultants considered the following main items of business.

- S. R. Hall succeeded R. Diamond as Chairman, and one new member was elected.
- (i) Bank of Trial Structures and Standard Tests. A bank of trial structures is being prepared by G. Sheldrick and is expected to be ready for distribution in 1982. No further activity was reported on standard tests for crystallographic calculations.
- (ii) Communication of Program Information. A proposal to organize a clearing-house of crystallographic computer programs in place of the World List approach was discussed. It was decided that a clearing-house would pose special difficulties of its own and a more practical approach would be to encourage program developers to publish an abstract in the Journal of Applied Crystallography outlining new and existing software. In addition to informing crystallographers of the existence of programs it would provide a suitable reference for publication purposes. The Commission is currently discussing this proposal with the journal's editors.
- (iii) Future Computing Schools. The Commission discussed a number of venues and dates for IUCr Computing Schools in the 1981–84 triennium, and the opinions of several national delegations were sought during the course of the Congress. Japan was considered the most suitable site for the next school, and an invitation has been received to hold a school there in 1983.

### Commission on Crystallographic Data

The Commission held two closed meetings during the XIIth Congress. I. D. Brown succeeded D. G. Watson as Chairman and four new members were elected.

The Commission appointed an *ad hoc* committee on 'Crystallographic Keywords' jointly with the Commission on Journals. Its task is to collect crystallographic terms and concepts in different languages, clarify their meaning, recommend their proper use in the primary and secondary literature and recommend ways to facilitate their documentation and retrieval, especially automatic retrieval. G. Bergerhoff is the Chairman.

The Commission recommended that Pearson symbols be used to differentiate different solid-state phases. The ASTM proposal for phase designators did not find favour with the Commission.

A standardized setting for the description of crystal structures was proposed by E. Parthé. The Commission felt

the proposal had merit but that more experience was needed in its use before it was adopted as a standard.

The reduced cell used by *Crystal Data* is particularly helpful in analysis during early stages of a structure determination and the Commission encourages authors of crystallographic computer systems to incorporate an algorithm to permit its calculation.

In response to concern that many primary crystallographic data (e.g. atomic coordinates) are now being lost because journals are no longer printing them, the Commission passed a motion encouraging journal editors and database producers to enter into agreements to ensure that unpublished crystallographic data are deposited in an appropriate database.

In a joint session with the Commission on Crystallographic Computing the report of the working party on a Standard Crystallographic File Structure was received. The Commissions urged the widespread adoption of this standard and have passed it to the Commission on Journals for their approval with the intention that it should be published in Acta Crystallographica | Acta Cryst. (1983), A39, 216–224].

Members of the Commission have also been active in a number of informal discussions designed to improve the flow of data from the laboratories to the journals and thence to the databases in a way that would minimize unnecessary handling of the data and the consequent introduction of errors.

### Commission on Crystallographic Nomenclature

The Commission met in Ottawa on 15 August 1981. A draft report on the nomenclature of polytype structures was received from the ad hoc Committee on the Nomenclature of Disordered, Modulated and Polytype Structures [see Acta Cryst. (1980), A36, 1077 for membership] and an informal report from the ad hoc Committee on the Nomenclature of Symmetry [see Acta Cryst. (1981), A37, 928 for membership]. Good progress is being made by both ad hoc committees with their important tasks. The Commission declined to endorse the requested use of a particular name for a method of analyzing diffraction data. Constructive correspondence was exchanged with the IUPAC Commission on Nomenclature of Inorganic Chemistry.

# Commission on Crystallographic Studies at Controlled Pressures and Temperatures

The Commission organized a microsymposium at the XIIth Congress. It intends to devote its main effort to the organization of an open Commission meeting at the XIIIth Congress. Since X-ray synchrotron radiation has recently become an important tool for crystallographic studies at controlled pressures and temperatures, this subject is proposed as the main theme of the meeting. It seems to be especially appropriate, as DESY in Hamburg is a centre for synchrotron radiation research.

### Commission on Crystallographic Teaching

During the Ottawa Congress in August 1981, the Commission held three business meetings and organized a microsymposium on 'Teaching Crystallography for

Materials Scientists'. The session attracted a large number of participants and there was animated discussion of the presentations made by five speakers. The first ten pamphlets published by the Commission to facilitate the teaching of crystallography were displayed at the Congress and have been made available for sale through the University College Cardiff Press, Cardiff, UK. Two hundred sets of ten pamphlets each have been made available for distribution in developing countries through Unesco. C. A. Taylor, Editor of the pamphlets, reported that nearly 3000 single copies of the pamphlets had already been sold by August 1981 and he expected the sales soon to reach the break-even point of 6000 copies for making this a self-supporting project. Ten more pamphlets are in preparation and are expected to come out in 1983.

Members of the Commission contributed to the comprehensive list prepared by J. H. Robertson of crystallographic books published all over the world between 1970 and 1980. This list [J. Appl. Cryst. (1982), 15, 640–676] supersedes earlier lists brought out by the Union. J. Lima-de-Faria has prepared a Historical Atlas of Crystallography for the Commission. Since it is too large for a pamphlet, other avenues for publishing it are being explored.

The Commission has prepared a detailed proposal and programme for a Summer School in Brazil on 'Teaching Crystallography for Materials Science'. S. Caticha-Ellis and A. Authier have agreed to be co-directors of the school and it will be held in July 1983.

### Commission on Electron Diffraction

During the XIIth Congress at Ottawa in August the Commission organized a microsymposium on gas electron diffraction (organized by K. Kuchitsu) and was jointly responsible for one on low-energy electron diffraction (organized by G. A. Somorjai). It also held two closed meetings, and ad hoc meetings on the subjects of gas diffraction and space-group determination. The microsymposia attracted interest from outside as well as inside the area of electron diffraction, in spite of parallel sessions. This prompted some advance thinking towards the Hamburg meeting in 1984, with a view to obtaining suitable timing as well as content of microsymposia.

Final proofs for Fifty Years of Electron Diffraction were corrected in February, and the volume of 432 pages was on display at the Congress. Everyone concerned with its production within the Commission was very pleased with the appearance achieved by D. Reidel, the publishers, and was grateful to them for achieving a very short production time. The volume was the first to combine a gas diffraction history with a comprehensive history of electron diffraction in general, and in spite of its title, spans a period from the earliest ideas in 1924 up to the present day. Independently of this volume, the gas diffraction group have this year prepared a volume entitled Bibliography of Gas Phase Electron Diffraction 1930–1979, of particular value to workers in that field.

Continuing activities of the Commission include the following:

1. Space-Group Determination. The plan to publish an article on this subject was discussed in detail at Ottawa where some of the authorship responsibilities were allocated. The aim is to make the theory and practice of the relatively

new methods of electron diffraction accessible to crystallographers in general. The initial target of a six-section article is planned for completion in 1982.

- 2. Accurate Structure Factors. The Commission has a continuing interest in promoting accurate structure-factor methods, and is circulating new results in this field.
- 3. Gas Electron Diffraction Information Service Project (GEDIS). This project was started to provide rapid distribution of results in this field, and in this it is evidently succeeding, two further issues (the sixth and seventh) being distributed during 1981.
- 4. From the nature of these projects, contacts with other Commissions of the Union, and in particular the Commissions on *International Tables*, on Charge, Spin and Momentum Densities, and on Crystallographic Computing, continue to be an important function of this Commission.

### Commission on Neutron Diffraction

An essential part of the Commission's activity was the two-day symposium in connection with the XIIth Congress, organized at Argonne National Laboratory by H. Mueller with D. Cox as programme chairman. The meeting attracted a total of 148 participants; there were 60 contributed papers, and 20 invited talks were given. There were five main sections covering instrumentation, pulsed sources, disordered materials, magnetism and biology, showing the wide range of applications of neutron scattering. The proceedings, edited by J. Faber, will be published as an American Institute of Physics Conference Proceedings.

During the year the compilation of absorption and total neutron cross sections by W. Yelon and T. Sabine was completed, and is now available from the authors. The survey on neutron diffractometer software done by H. Dachs and M. S. Lehmann is completed and is also available from the authors.

Closed meetings of the Commission took place both at the Argonne Symposium and at the Congress when, in particular, the possible next sites for a symposium, the powder Al<sub>2</sub>O<sub>3</sub> project, and the *Newsletter* were discussed.

Finally, towards the end of the year decisions were made to transfer the Magnetic Structure Data file from Brookhaven (D. Cox) to Trombay (S. Murthy) and to transfer the Form Factor file from Oak Ridge (W. Koehler and R. Moon) to Grenoble (J.-X. Boucherle).

### 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 1981 the Executive Committee approved sponsorship of the following schools and meetings, mostly with financial support:

- 1. VII Iberoamerican Congress of Crystallography, Coimbra, Portugal, 20–26 September 1981.
- 2. Workshop on the Crystallography of Molecular Biology, Erice, Italy, 7–19 June 1982.
- 3. Sagamore VII Conference on Charge, Spin and Momentum Densities, Nikko Kanayo Hotel, Japan, 25–30 August 1982.

- 4. Seventh European Crystallographic Meeting, Jerusalem, Israel, 29 August-3 September 1982.
- 5. International School on Materials Science and Solar Energy, Cairo and Alexandria, Egypt, 18 March-1 April 1983.
- 6. International School on Teaching Crystallography for Materials Science, Brasilia, Brazil, 18–27 July 1983.
- 7. Fifth European Meeting on Ferroelectricity, Torremolinos, Spain, 26 September 1 October 1983.

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 Th. Hahn, Institut für Kristallographie, RWTH, Templergraben 55, D-5100 Aachen, Federal Republic of Germany.

### Representatives on Other Bodies

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

The Abstracting Board of the International Council of Scientific Unions met at Callaway Gardens, Georgia, USA, from 30 May to 3 June. There were three applicants for membership: Kent-Barlow Information Associates, Biosis UK, and the International Institute for Applied Systems Analysis (IIASA). The first is a consultancy formed by the former representatives of INSPEC and UKCIS; the second is an operating company formed by BIOSIS to produce Zoological Record (formerly the responsibility of the Zoological Society of London), and the third is an internationally funded organization, situated in Austria. All three were accepted after some discussion.

As noted in last year's report, the financial situation of the Board has much improved recently. The technical programme of the Board is mainly carried on by Working Groups in the fields of science covered by the Board. Among the tangible products of the Working Groups is a classification scheme in physics; this is now under revision, and a new version is expected in 1982 or 1983. Similarly, the Working Group in Geology, in collaboration with the International Union of Geological Sciences and other organizations, is preparing a multilingual thesaurus, with similar expectations of publication date. Among activities of the Technical Planning and Steering Committee are studies of user education, document delivery, scientific information at the secondary-school level, and the role of the Board in the 1980s.

The question of the role to be played by representatives of Member Countries arose in several contexts in the course of the discussions. According to the Statutes, the Adhering Body should be broadly representative of the scientific and technical interests of the country as a whole, but the reports of several representatives adopted a narrower interpretation, and resembled a member-service report, rather than a broadly based national one. The Board felt that the broad interpretation was the correct one, and Professor Cocking's presentation of the Royal Society document A Study of the Scientific Information System in the United Kingdom (British Library R&D Report No. 5626) was particularly welcomed in this connection. A proposal that the words 'Adhering Body' should be replaced by 'National Member' is under consideration.

It is intended to hold the next meeting of the Board in the REI in Amsterdam during the week beginning 24 May 1982. A seminar on the theme of information and the innovative process is planned for 24–25 May, and the Board programme will include a session on the role of ICSU and the Scientific Unions within ICSU AB.

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

This year falls between two biennial Congresses of CODATA but the Committee continues active in the publication of bulletins and newsletters. Plans are continuing for the eighth Congress in Poland in October 1982 though, because of the political situation, the location has been changed from Kozubnik to a site near Warsaw.

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

According to the reorganization of COSPAR no annual meeting took place this year (1981). The next COSPAR meeting took place in Ottawa in May 1982. There has been little progress in materials science for two years because of the continuous postponements of the Spacelab flight, and few scientific results are expected to appear until, at least, the end of 1982.

New technological developments coming after the first successful flights of the space shuttle may have an important impact on materials science in space. Using the crane of the shuttle, retrievable platforms can be constructed which will allow experiments of up to six months' duration in space. In this way the time problem, which was a severe boundary condition for the growth of perfect single crystals, seems to lose its importance.

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

The Committee met 28–29 November 1981 in Paris. Of particular interest to the Union are the programmes for (i) an international conference on Science and Technology Education and the Quality of Life in 1985 and (ii) the training of technicians in developing countries. The Committee has sought the participation of various scientific Unions in the conference and the IUCr has agreed to collaborate in organizing it. The Commissions on Crystallographic Teaching and Crystallographic Apparatus are considering the organization of a workshop for training technicians for the maintenance of crystallographic equipment in developing countries. It is proposed to collaborate with the CTS in this venture.

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

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

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

In the on-going SCOPE project, the global biogeochemical cycles of carbon, nitrogen, phosphorus and sulphur have been studied extensively and general surveys are now available. From these studies it is becoming increasingly apparent that all these fundamental cycles are closely interrelated and therefore their global interactions have also become of high interest. All SCOPE projects were reported during the General Assembly held in Ottawa on 30 May-5 June 1982.

A document Common Perceptions of Environmental Issues, which examines environmental problems which the international community should consider during the next twenty years, has been prepared by the Governing Council of the United Nations Environment Programme. The IUCr Representative sent some suggestions for minor changes of the document to the Secretary General of SCOPE.

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

The IUPAP General Assembly, held in Paris, 31 August-3 September 1981, approved the new name of the Commission 'C.10. Commission on the Structure and Dynamics of Condensed Matter'. The new chairman, secretary and members were elected. It seems that the assumed area of interests of this Commission will be closer to crystallography than it was before.

### Conference Committee of the European Physical Society

At their meeting in October 1981 the members of the Committee were informed about the decision of the EPS Executive Committee to set up two new Advisory Committees. One of these will deal with problems of scientific freedom while the other will inspect financial questions of the EPS.

Applications for EPS approval and sponsorship were discussed and it was stated that on average in the last few years the EPS had organized 10–11 meetings and sponsored about 30–40 conferences per year. The representative presented information about future physics conferences in Europe for inclusion in the Forthcoming Meetings section in the Journal of Applied Crystallography.

The Committee also discussed conflicts of political character which occurred for two conferences.

It was recommended to use the Young Physicists Fund also to support participation in divisional and sectional meetings.

The organization of EPS General Meetings in the past and in the future was discussed.

### International Organization for Crystal Growth

The main activity, only indirectly associated with IOCG, was the International Conference on Crystal Growth and Epitaxy which was for the first time combined with the American Crystal Growth Conference in San Diego (July 1981). The great scientific success of the combined conference (about 500 participants) can be explained by a general positive trend in all crystal growth activities (including the *Journal of Crystal Growth*) during recent

years. Industrial and government sponsors are slowly understanding that crystal growth technology without thermodynamic, kinetical and structural studies cannot solve complex materials problems. In this way many crystal growth studies are allowed to be performed on a wider basis of fundamental investigations. The strong interaction between theory and experiment led to the presentation of some very interesting papers at this conference.

The 7th International Conference on Crystal Growth will be held in Stuttgart in September 1983 and a summer school will be held in Davos.

### European Crystallographic Committee

The Union Representative attended the meeting of the ECC held on 20 August 1981 during the XIIth IUCr Congress. Progress reports were presented on the European Crystallographic Meeting held in Jerusalem in 1982, and those to be held in Liège in 1983 and Torino in 1985. A notice will be published in Acta Crystallographica inviting crystallographers in developing countries to join in cooperation schemes for the exchange of information and assistance in data collection by automatic diffractomers and microdensitometers [Acta Cryst. (1982), A39, 750; J. Appl. Cryst. (1982), 15, 577-578].

Dr B. Kamenar was elected President of the Committee to succeed Dr Olga Kennard, who had held this office for six years. Professor G. S. D. King was elected Vice-President and Professor P. T. Beurskens was re-elected Secretary.

### International Council of Scientific Unions

The Union was represented at the meeting of the ICSU General Committee at Dubrovnic, Yugoslavia, 24–25 September 1981, by the Immediate Past President, Professor N. Kato. The ICSU President reminded members of the main objectives of ICSU:

- (a) to encourage international scientific activity for the benefit of mankind, and to promote the cause of peace and international security throughout the world,
- (b) to facilitate and coordinate the activities of the international Scientific Unions,
- (c) to stimulate, design and coordinate international interdisciplinary scientific projects, and,
- (d) to facilitate the coordination of the international scientific activities of its National Members.

He reported on the international interdisciplinary activities of the various committees and inter-Union commissions.

The International Union of Food Science and Technology was accepted as a Scientific Associate and Upper Volta as a National Associate.

The proposal for a programme of Scientific Research Applied to World Needs was supported, and it was agreed that the representatives of the scientific unions should suggest to the Secretary General the areas of primary importance so that the subject of the first conference could be selected. Further steps seeking to resolve the problem of the adherence of the China Association for Science and Technology to ICSU were approved. There should be closer cooperation with the Federation of Arab Scientific Research Councils, especially in the creation of a biosciences network in Arab countries. Scientists were urged to do their best to demon-

strate to the governments and peoples of all countries the vital necessity of preventing nuclear warfare.

The General Committee accepted the reports of the International Scientific Unions, the Scientific Committees, the Inter-Union Commissions, etc. It reviewed relations with a wide range of intergovernmental and non-governmental organizations. Particular reference was made to input by ICSU into Unesco's Draft Medium Term Plan (1984–89), and the cooperation with WMO in the World Climate Research Programme, and with several UN bodies for the International Biosciences Networks. A suggestion for an International Geosciences Network was also considered.

Attention was drawn to two booklets published by the Committee on the Safeguard of the Pursuit of Science concerning the Florence Agreement on Importation of Educational, Scientific and Cultural Materials and Human Rights Laws, and a small booklet *ICSU*: A Brief Review prepared by the Executive Secretary in both English and French. These are available free of charge from the ICSU Secretariat.

### **Finances**

The audited accounts for the year 1981 are given at the end of this Report. For comparison, the figures for 1980 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. In previous years they have been presented in US dollars.

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 1981 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 deficit has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 180 942. This deficit has been divided amongst the ten Fund Accounts with credit balances, in direct proportion to the balances on these accounts at 31 December 1981.

The General Fund account shows a surplus of SwFr 72 235 as compared with a deficit of SwFr 2671 in 1980. The administrative expenses were SwFr 142 666 in 1981 as compared with SwFr 130 767 in 1980. Of this amount, SwFr 44 011 was charged to the publications of the Union. SwFr 32 435 was spent on supporting scientific meetings. The General Assembly and Congress expenses totalled SwFr 49 949 including SwFr 19 744 for the Executive Committee and SwFr 29 400 for travel grants. The Congress organizers kindly met the accommodation costs for the Executive Committee. The Union received SwFr 20 680 from the Unesco subvention to ICSU and a grant of a further SwFr 15 710 from ICSU. The subscriptions from Adhering Bodies totalled SwFr 89 114. The Sixth Edition of the World Directory of Crystallographers was published. Sales income yielded SwFr 21 252 whilst publication and editorial costs were SwFr 18 740.

In preparation for the establishment of the in-house computerized typesetting nearly all of the Union's investments were sold in December 1980 and early in 1981, and the proceeds were placed on deposit terms in sterling. There was a net profit of SwFr 45 211 in 1981 and a loss of SwFr 24 509 in 1980 compared with the Swiss Franc equivalent of their cost. Hence investment income fell dramatically to SwFr 3354, but bank interest rose to SwFr 82 817.

The President's Fund account received SwFr 791 in donations during 1981; travel grants of SwFr 1611 were made from the fund.

The Acta Crystallographica account for 1981 shows a deficit of SwFr 231 628 as compared with a deficit of SwFr 288 063 in 1980. The deficit resulted mainly from the decrease in the value of the Danish kroner with respect to sterling and the Swiss Franc. The publication expenses are incurred in sterling and the subscriptions received in Danish kroner. In spite of a 20% increase in the subscription rates in Danish kroner the net income in Swiss Francs was less than for 1980, because of the dramatic fall in the value of the kroner with respect to the Swiss Franc and sterling. A loss of SwFr 93 446 was sustained from cancelling the computerized typesetting facility, and the reduction in the size of the journal was not as large as planned.

The number of paid subscriptions to both sections of the journal dropped from 1418 in 1980 to 1319 in 1981, including 150 personal subscriptions in 1980 and 126 in 1981. There were also 258 paid subscriptions to Section A and 145 paid subscriptions to Section B in 1981, compared with 250 and 137 respectively in 1980. The cost of assessment of the computerized typesetting facility and the cost of the technical editing office have been divided between the Acta Crystallographica and the Journal of Applied Crystallography accounts in percentages based on the number of text pages published during the year; 87% and 13% respectively for 1981. The technical editing costs for Acta Crystallographica were SwFr 250 718 in 1981 as compared with SwFr 222 138 in 1980. The journals accounts have also been charged with administrative expenses as in previous years and as shown in the General Fund.

The Journal of Applied Crystallography account shows a deficit of SwFr 15 695 as compared with a deficit of SwFr 30 520 in 1980. The subscription rates were increased by 20% for 1981. The number of paid subscriptions decreased slightly from 1168 in 1980 to 1126 in 1981, including 102 personal subscriptions in 1980 and 96 in 1981.

The Structure Reports account shows a surplus of SwFr 3146 as compared with a deficit of SwFr 29 448 in 1980. Publishing and editorial expenses in 1981 were SwFr 19 616 and SwFr 71 363 respectively, as compared with SwFr 52 916 and SwFr 100 108 in 1980. The publication expenses of Volume 44B were held over until 1982. The net income from sales was SwFr 94 525 in 1981 as compared with SwFr 123 576 in 1980.

The *International Tables* account shows a surplus of SwFr 11 700 as compared with a surplus of SwFr 11 518 in 1980. Sales income fell from SwFr 22 921 to SwFr 12 335 as Volume I went out of print. The publisher, Kynoch Press, ceased to trade and sales have been taken over by Reidel from 1982 onwards.

SwFr 953 was received from the sale of 60 copies of Fifty Years of X-ray Diffraction. SwFr 1683 was received from

the sale of 87 copies of Symmetry Aspects of M. C. Escher's Periodic Drawings, as well as SwFr 2214 royalties for the North American and Japanese editions of this book. SwFr 1305 was received from the sale of 45 coies of Volume I and Volume II of Early Papers on Diffraction of X-rays by Crystals, reducing the deficit on this fund account to SwFr 10 159. Fifty Years of Electron Diffraction was published in 1981. Publication costs were SwFr 31 145 and net sales were SwFr 7784 from 181 copies.

The Molecular Structures and Dimensions account shows no surplus for 1981, because this account was charged with a contribution of SwFr 11 384 towards the publication costs of Volume 12, the volume published in 1981. The sales income was similar to that for 1980 with many orders outstanding at the end of the year. 225 copies of Volume 12 were sold in 1981, as compared with 275 copies of Volume 11 in 1980.

As on previous Balance Sheets, the investments have been valued according to their quotations at the end of the year. Their appreciation in value, together amounting to SwFr

720, 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 1981 the Union held investments of SwFr 18 000 in government bonds.

The total of SwFr 700 564 with the banks at the end of the year was represented by Dfl 96 211 and \$8784 with the Amsterdam-Rotterdam Bank, \$33 910 with the Bankers Trust Company, £155 327 with the National Westminster Bank and SwFr 17 217 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 and the sale of the sterling investments, due at 31 December 1981. Where appropriate, these amounts 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 180 942 resulting from fluctuations in rates of exchange, have decreased during the year, from SwFr 1 009 076 to SwFr 709 687.

# International Union of Crystallography Balance Sheet as at 31 December 1981

0	110,815	12,206 223,847 8,858	355,726 258,241 97,485			165'116	1,009,076
rancs 1980	50,770 60,045			949,052	902,612		
Swiss Francs	700,564	10,545 161,183 4,503	876,795 191,850 684,945			24,742	709,687
1981	71,600 628,964			18,270	18,990		
	CURRENT ASSETS Cash at banks Current Accounts Deposit and Savings Accounts	Cash with Union Officials Debtors Subscriptions from Adhering Bodies, due for 1979 to 1981	Deduct Creditors Net Current Assets	FIXED ASSETS Investments At market value Depreciation/(Appreciation) in value	At cost Office Equipment at cost, less depreciation	Total Fixed Assets	
1980		265,503 7,527 365,225	81,598 227,216 (51,325) 91,740	4,612 20,072 (11,464) 8,372	1 1	1,009,076	1,009,076
	Balance at 31 December 1981	274,330 5,448 108,515	53,530 187,113 (39,625) 74,517	4,520 19,469 (10,159) 6,800	(23,361)	709,687	709,687
Swiss Francs	(Excess of expenditure over income for the year)	72,235 (820) (231,628)	(15,695) 3,146 11,700	953 3,897 1,305	(23,361)	(118,447)	
S 1981	(Loss on fluctuations in rates of exchange)	(63,408) (1,259) (25,082)	(12,373) (43,249) - (17,223)	(1,045) (4,500) – (1,572)	(11,231)	(180,942)	
	As at 31 December 1980	265,503 7,527 365,225	81,598 227,216 (51,325) 91,740	4,612 20,072 (11,464) 8,372	1 i	1,009,076	
		FUND ACCOUNTS General Fund President's Fund Acta Crystallographica	Journal by Applica Crystallography Structure Reports International Tables General Publications Fifty Vores of X-roy	Diffraction Escher Drawings Early Papers Molecular Structures and Dimensions	Fifty Fears of Electron Diffraction Special Publications Fund	·	

# Report of the Auditors to the International Union of Crystallography

We have audited the financial statements on pages 492 to 499 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.

Subject to the above in our opinion, the financial statements give a true and fair view of the state of affairs of the Union at 31 December 1981 and of its excess of expenditure over income and source and application of funds for the year then ended.

Manchester, England 2 July 1982

Signed: TOUCHE Ross & Co.

Chartered Accountants

General Fund Account for the year ended 31 December 1981

08	13,680	75,924	12,015	1,541	(%000'+7)	I	251	5.5	3		140		40,655								206,158	
Francs 1980												29,412	7,632 1,411									
Swiss Francs 1981	20,680	89,114	82,817	1 2 4 4	43,211	21,252	720	1			207		44,011								323,076	
19					rs:							32,100	1,211									
	Grant received from UNESCO Subvention to ICSU Grant received from ICSU	Subscriptions from Adhering Bodies Interest on Investments	Interest on Bank Accounts	Profit on Redemption of Investments	Sale of World Directory of Crystallographers:	6th Edition Net cale of World Directors of	Crystallographers: 5th Edition	Net sale of the Proceedings of the Madrid Conference on Anomalous Scattering	Net sale of Sundry Publications	(Bibliographies, Book List, List of Computer Programs and Index of	Crystallographic Supplies) Amount charged to Journals and Publications.	Acta Crystallographica Journal of Annied Crystallography	Molecular Structures and Dimensions									
1980	1,866	919	684								130,767				15,848	23,138	8,071	666,12	I	2,671	206,158	
					2,898	8,873	1,140	2,223	3,208	2,2/3	104,714	I	1	1 1	15,848							
Swiss Francs	2,060	727	828								142,666				49,949	I	3,436	52,435	18,740	72,235	323,076	
198					2,971	9,170	1,210	2,990	3,966	077,1	119,286	19,744	29,400	615	e I							
	Subscriptions to ICSU (2½% of subscriptions received from Adhering Bodies in 1980)	Subscription to ICSU Abstracting Board	Teaching of Science	Administration Expenses: Honoraria: General Secretary Treasurer	and Secretarial Assistance	Audit and Accountancy Charges Taxation and other services	Legal Fees	Postages, Stationery, Printing and Sundries	Travelling Expenses	bank Charges  Executive Secretary's Office:	Salaries and Expenses Depreciation of Office Equipment	Twelfth General Assembly and Congress: Executive Committee	Travel Grants	Expenses of Commissions Incidental Expenses	Meeting of the Programme Committee	Meeting of the Executive Committee	travel Expenses of 1001 Nepresentatives on Other Bodies	Sponsorship of Meetings Publication and editorial expenses of World Directors of Cristallographers	6th Edition  Fixors of Income oner Frankling corried	to Balance Sheet		

President's Fund Account for the year ended 31 December 1981

836 (836) —			849,106	1,886	288,063			1,139,055
Swiss Francs 1980 791 820 1,611		897,710 30,645 13,075 209	941,639 92,533	2,218				' " "
Swiss 1981 791 791 820			832,866	1	231,628			1,064,494
19		883,309 29,031 10,401 362	923,103 90,237	1 1				
Donations received Excess of Expenditure over Income carried to Balance Sheet	Crystallographica Account for the year ended 31 December 1981	Subscription to Volume 37 (1980 Volume 36) Sale of Back Numbers and Single Copies Airfreight Charges to Subscribers Royalties and Copyright Fees	Less Publisher's Commission on Sales	Income from Advertisements  Loss Advertising Agent's Commission	Excess of Expenditure over Income carried to Balance Sheet			
	za Account fo			802,893	38,265		268,485	29,412
Swiss Francs 1,611 1,611 1,611	ographic	679,164 83,137 23,148	785,449	17,444		23,251 6,344 14,601	222,138 2,151	
	Crystalle			644,820	93,446		294,128	32,100
1981	Acta	529,976 50,868 22,871	603,715	18,599		20,171 13,708 7,789	250,718 1,742	
Travel Grant		Publication Expenses: Printing and Binding Volume 37 (1980 Volume 36) Distribution and Postage Airfreight Costs	Printing Acta Supplement to A37	Printing Index to Volume 36 (1980 Volume 35)	Cancellation of Computerised Typesetting Facility Assessment of Computerised Typesetting Facility	Editorial Expenses: Editorial Honoraria Secretarial Assistance Postages, Telephone and Office Sundries	Technical Editing: Salaries and Expenses Depreciation of Office Equipment	Administration Expenses

Journal of Applied Crystallography Account for the year ended 31 December 1981

90		149,497	863	30,520			180,880
Swiss Francs 1980	163,274 3,978 3,064 87	170,403	1,015				
Swiss 1981		145,562	009	440			162,297
19	156,792 6,625 2,469 103	165,989	706 106				
	Subscriptions to Volume 14 (1980 Volume 13) Sale of Back Numbers and Single Copies Airfreight Charges to Subscribers Royalties and Copyright Fees	Less Publisher's Commission on Sales	Income from Advertisements $Less$ Advertising Agent's Commission	Donation Excess of Expenditure over Income carried to Balance Sheet			
0861	125,907	I	5,718		39,422	9,833	180,880
Swiss Francs 19	112,819 7,659 5,429		3 557	1,539	33,193 306		
	94,733	13,964	I		42,900	10,700	162,297
1981	83,488 5,880 5,365		3.966	1,220	37,464 250		
	Publication Expenses: Printing and Binding Volume 14 (1980 Volume 13) Distribution and Postage Airfreight Costs	Cancellation of Computerised Typesetting Facility Assessment of Computerised Typesetting	Facility Editorial Expenses: Editorial Honoraria	Secretarial Assistance Postages, Telephone and Office Sundries Technical Editing:	Salaries and Expenses Depreciation of Office Equipment	Administration Expenses	

Structure Reports Account for the year ended 31 December 1981

<i>0</i> 8		123,576			123,576			22,921	I		22,921
Francs 1980	130,151 39,043	169,194 45,618						32,656 9,735			
Swiss Francs		94,525			94,525			12,335	1,170		13,505
1981	85,793 43,207	129,000 34,475						18,869 6,534			
	Sale of Copies of Volumes 44B and 45A (1980 Volumes 43B and 44A) Earlier Volumes and Indexes	Less Publisher's Commission on Sales					ernational Tables Account for the year ended 31 December 1981	Sale of Copies of Volumes I, II, III and IV Less Publisher's Commission on Sales	Copyright Fees		
98	52,916	I	100,108	(29,448)	123,576		Account	9,154	2,249	11,518	22,921
rancs 1980	47,582 5,334						ıl Tables	7,187 1,967	2,143		
Swiss Francs 981	19,616	400	71,363	3,146	94,525		rnationa	I	1,805	11,700	13,505
198	11,062 8,554						Inte	1 1	1,683		
	Publication Expenses: Printing and Binding Volume 45A (1980 Volumes 43B and 44A) Typing of Manuscripts	Depreciation Editorial Expenses: Salary and Honoraria: Editors.	Abstractors and Assistants	excess of income over expensionee carried to Balance Sheet				Publication Expenses: Binding Volume IV Artwork for Volume on Direct Space	Editorial Expenses: Secretarial Assistance and Postages Travelling	Excess of Income over Expenditure carried to Balance Sheet	

Fifty Years of X-ray Diffraction Account for the year ended 31 December 1981

1980	498	498		1,713	782	2,495		740	740
	213			2,447 734	†			1,056 316	
Swiss Francs 81	953	953		1,683	2,214	3,897		1,305	1,305
1981	1,361			2,307 624				1,864 559	
	Sale of Copies Less Publisher's Commission on Sales		Escher Drawings Account for the year ended 31 December 1981	Sale of Copies Less Publisher's Commission on Sales	Royalties		Early Papers Account for the year ended 31 December 1981	Sale of Copies of Volumes I and II Less Publisher's Commission on Sales	
Swiss Francs 1980	498	498	s Account for t	2,495		2,495	Account for the	740	740
Swiss 1981	953	953	Escher Drawing	3,897		3,897	Early Papers A	1,305	1,305
	Excess of Income over Expenditure carried to Balance Sheet			Excess of Income over Expenditure carried to Balance Sheet				Excess of Income over Expenditure carried to Balance Sheet	

## INTERNATIONAL UNION OF CRYSTALLOGRAPHY

Molecular Structures and Dimensions Account for the year ended 31 December 1981

1980	36726	CC0'/7	27,635		1 1	I	1	<b>I</b>	1	1
Swiss Francs 19	19,562 18,800 38,362	10,/2/			1 1					
	, , , , , , , , , , , , , , , , , , ,	21,134	27,734		7,784	23,361	31,145		59,821	59,821
1981	14,619 23,488 38,107	10,3/3		981	10,519 2,735					
	Sale of Copies of Volume 12 (1980 Volume 11) Earlier volumes	Less Publisher's Commission on Sales		of Electron Diffraction Account for the year ended 31 December 1981	Sale of Copies $Less$ Publisher's Commission on Sales	Excess of Expenditure over Income carried to Balance Sheet		Special Publications Fund for the year ended 31 December 1981	Donations Received	
1980	8 6 0 26,224	1,411	27,635	ffraction Acco	ı		1	== ons Fund for th	ı	ı   ı <b> </b>
Swiss Francs	14,388 1,966 523 9,870	1,211	27,734	lectron D <sub>i</sub>	145		145	= Publication	50.871	59,821
1981	1,384 755 1,384 26,523	I	7,72	ars of E	31,145		31,145	Special P	08	ξ.   ξξ.
	27 17			Fifty Years o						
	Publication Expenses: Printing and Binding Volume 12 (1980 Volume 11) Carriage and Miscellaneous Expenses Salaries	Administration Expenses Excess of Income over Expenditure for the year: University of Cambridge IUCr carried to Balance Sheet			Publication Expenses				Excess of Income over Expenditure	culted to Dudnice Steel

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### Statement of Source and Application of Funds

### Year ended 31 December 1981

	1981	1980
	SwFr	SwFr
Source of funds		
(Excess of expenditure over income) for the year	(118,447)	(334,614)
(Loss) on fluctuations in rate of exchange	(180,942)	(90,235)
	(299,389)	(424,849)
Adjustment for items not involving the movement of funds:		
Depreciation	3,891	4,237
(Profit)/loss on sale of investments	(56,016)	24,509
(Profit) on redemption of investments	_	(1,541)
Loss on fluctuations in rates of exchange on investments	_	84,394
Loss/(profit) on fluctuations in rates of exchange on office equipment	1,275	(720)
Total (absorbed) from operations	(350,239)	(313,970)
Proceeds of sale of investments	939,638	90,608
Proceeds of redemption of investments	_	25,865
Increase in creditors	_	95,408
Decrease in debtors	67,019	153,732
	656,418	51,643
Application of funds		
Decrease in creditors	(66,391)	<del>-</del>
Purchase of investments		(152,400)
Purchase of office equipment	(1,939)	(489)
Increase/(decrease) in net liquid funds	588,088	(101,246)
Net liquid funds include cash at banks and with Union officials.	=======================================	

### Notes to the Financial Statements

### 1. Accounting Policies

(a) The financial statements have been 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.

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### (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.

### 2. Rates of Exchange

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

	1981	1980
Netherland Guilders	1.36	1.22
Danish Crowns	4.03	3.45
Pounds Sterling	0.289	0.248
US Dollars	0.568	0.585
German Marks	1.25	1.12

### 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.