

## International Union of Crystallography

### Report of the Executive Committee for 1986

#### Meetings

The Union sponsored the following meetings held during 1986: Winter School on Teaching, Characterization and Properties of Epitaxial Electronic Materials, Trieste, Italy, 13-24 January 1986; Gordon Research Conference on Electron Distributions and Chemical Bonding, Plymouth, USA, 30 June-4 July 1986; First International Symposium on Shaped Crystal Growth, Budapest, Hungary, 22-25 July 1986; Symposium on Organic Crystal Chemistry, Poznań-Rydzyna, Poland, 1-4 August 1986 (satellite meeting of ECM-10); One-day Tutorial Workshop on Inorganic Molecular Crystals, Wrocław, Poland, 4 August 1986 (satellite meeting of ECM-10); Tenth European Crystallographic Meeting, Wrocław, Poland, 5-9 August 1986; Satellite Conference on Crystal Growth and Liquid Crystals, Łódź, Poland, 11-13 August 1986 (satellite meeting of ECM-10); International Summer School on Crystallographic Computing, Leipzig, German Democratic Republic, 11-20 August 1986; Research Course on Neutron Diffraction Techniques in Crystal Structure Determination, Studsvik and Uppsala, Sweden, 18-29 August 1986; Workshop on Crystallography in Molecular Biology: Structure of Biological Macromolecules, Poushchino, USSR, 4-13 September 1986; International Symposium on Molecular Structure: Chemical Reactivity and Biological Activity, Beijing, People's Republic of China, 15-19 September 1986; Symposium on Computational Methods in Chemical Design: Molecular Modelling and Computer Graphics, Schloss Elmau, Federal Republic of Germany, 19-26 October 1986; International School on Solar Cell Materials and Applications, Fayoum, Arab Republic of Egypt, 19-26 October 1986.

The Executive Committee met at Foxhill, near Chester, England, in July 1986. The most important items of business dealt with were (1) approval of the audited accounts for 1985; (2) subscription rates and other matters concerning the journals, including the appointment of Professor C. E. Bugg to succeed Dr S. C. Abrahams as Editor of *Acta Crystallographica* at the XIV General Assembly in Perth in August 1987; (3) other publications of the Union; (4) initiation of an agreement with Oxford University Press to start the IUCr/OUP Book Series; (5) establishment of a Book Series Committee to develop the IUCr/OUP Book Series; (6) the General Fund estimates and proposal for the level of the unit contribution for the next triennium; (7) sponsorship of meetings; (8) financial support for young scientists attending meetings receiving IUCr sponsorship; (9) free circulation of scientists; (10) discussion of the arrangements for the XIV General Assembly and Congress with the Congress Programme Committee; (11) level of financial support for the above Congress, including assistance for Commission Chairman, Editors and Co-editors; (12) review of the activities of the Commissions; (13) application by the JCPDS-ICDD to become a Scientific Associate of the Union; (14) nominations for Officers of the Union, and Chairman and members of the Commissions; (15) upgrad-

ing the office technology in the Union office in Chester; (16) refurbishment of these premises.

The Finance Committee met at the Chester office in January and then at Foxhill immediately prior to the Executive Committee meeting in July.

#### Publications

Volume 42 of *Acta Crystallographica* and Volume 19 of the *Journal of Applied Crystallography* were published, as were Volumes 48B and 52A of *Structure Reports*. A short-run reprint of *International Tables for Crystallography* Volume A was made, to keep this volume in print until a new edition could be published in 1987. No more volumes of *Molecular Structures and Dimensions* have been published since Volume 15, which was published in 1984.

#### 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 42 of *Acta Crystallographica* (*Acta*) and 19 of the *Journal of Applied Crystallography* (*JAC*) were produced and published in 1986. The total number of papers published in *Acta* increased 4% while those in *JAC* decreased 4% compared with 1985, see Table 2. A total of 1201 papers were submitted to *Acta* in 1986 compared with 1075 in 1985, 1138 papers being sent for publication in 1986 and 920 in 1985. Corresponding figures for *JAC* were 143 papers submitted in 1986 and 144 in 1985, with 117 papers sent for publication in 1986 and 127 in 1985. A substantial backlog in processing manuscripts developed during the year due to the resignation of the previous Technical Editor and the death of the Deputy Technical Editor, see *Acta* (1987). A43, 137-139. By year's end, considerable progress had been made toward eliminating the backlog.

The average length of all articles in *Acta* increased very slightly in 1986 to 3.4 pages from 3.3 pages in 1985, reversing the previous downward trend. The largest increase was in Section A from 5.5 pages in 1985 to 6.0 pages in 1986. The average length in *JAC* decreased from 5.1 pages in 1985 to 4.7 pages in 1986. Median publication time, the average elapsed time between the published acceptance and nominal publication dates, was 5.7 months for *Acta* A and B and 4.8 months for *Acta* C and *JAC*. Corresponding publication times in 1985 were 5.0, 5.6, 3.8 and 5.1 months. The increased time in *Acta* A was caused in part by the Ewald issue of November 1986. The remaining increases in publication time were due to the temporary understaffing in the Technical Editor's office and these are expected to return to normal in 1987.

Table 1. *Adhering Bodies*

<i>Country</i>	<i>Category*</i>	<i>Adhering Body</i>	<i>Secretary of National Committee</i>
Argentina	I	Consejo Nacional de Investigaciones Cientificas y Técnicas	M. A. R. DE BENYACAR, División Física del Solido, Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires
Australia	III	Australian Academy of Science	The Executive Secretary, Australian Academy of Science, PO Box 783, Canberra City, ACT 2601
Austria	I	Österreichische Akademie der Wissenschaften	A. PREISINGER, Institut für Mineralogie, Kristallographie und Strukturchemie der Technischen Universität Wien, Getriedemarkt 9, A-1060 Vienna
Belgium	II	Académie Royale des Sciences, des Lettres et des Beaux-Arts de Belgique	E. LEGRAND, Materials Sciences Department, Studiecentrum voor Kernenergie, B-2400 Mol
Brazil	III	Conselho Nacional de Desenvolvimento Cientifico e Tecnológico	S. CATICHA ELLIS, DESCM, Instituto de Física, Universidade Estadual de Campinas, Campinas, São Paulo 13100
Canada	III	National Research Council	J. T. SZYMANSKI, CANMET, Department of Energy, Mines and Resources, 555 Booth St, Ottawa, Ontario K1A 0G1
Chile	I	Comision Nacional de Investigacion Cientifica y Tecnologia	D. BOYS, Departamento de Fisica, Universidad de Chile, Casilla 5487, Santiago
China, People's Republic of	IV	Academia Sinica	XU XIAO-JIE, Department of Chemistry, Peking University, Beijing 100871
Czechoslovakia	I	Československá Akademie Věd	V. PETŘÍČEK, Physical Institute, Czechoslovak Academy of Sciences, 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. VAHVASELKA, Department of Physics, University of Helsinki, Siltavuorenpenger 20 D, SF-00170 Helsinki 17
France	IV	Académie des Sciences (Institut de France)	Y. EPELBOIN, Association Française de Cristallographie, Tour 26, 4 place Jussieu, 75230 Paris CEDEX 05
German Democratic Republic	I	Vereinigung für Kristallographie in der GGW de DDR	P. RUDOLPH, Humboldt-Universität-Berlin, Sektion Physik, Invalidenstrasse 110, 1040 Berlin
Germany, Federal Republic of	IV	Arbeitsgemeinschaft Kristallographie	W. PRANDL, Institut für Kristallographie der Universität Tübingen, Charlottenstrasse 33, 7400 Tübingen
Hungary	I	Magyar Tudományos Akadémia	P. GADÓ, Pogany u.4, Budapest H-1124
India	II	Indian National Science Academy	A. K. SINGH, Materials Science Division, National Aeronautical Laboratory, Kodihalli, Bangalore 560 017
Israel	I	Israel Academy of Sciences and Humanities	M. HAREL, Weizmann Institute of Science, Rehovot
Italy	III	Consiglio Nazionale delle Ricerche	G. FILIPPINI, Centro CNR, Dip. Chim. Fis. Elettrochim, Università di Milano, Via Golgi 19, 20133 Milano
Japan	IV	Science Council of Japan	J. HARADA, Department of Applied Physics, Faculty of Engineering, Nagoya University, Furo-cho, Chikusa-ku, Nagoya 464
Mexico	I	Consejo Nacional de Ciencia y Tecnologia	M. SORIANO-GARCIA, Instituto de Quimica, Circuito Exterior, UNAM, Delegacion Coyoacan, 04510 Mexico D.F.
Netherlands	II	Stichting voor Fundamenteel Onderzoek der Materie met Röntgen- en Elektronenstralen	The Executive Secretary, FOMRE, Koningin Sophiestraat 124, 2595 TM's-Gravenhage
New Zealand	I	The Royal Society of New Zealand	J. SIMPSON, Chemistry Department, University of Otago, PO Box 56, Dunedin
Norway	I	Det Norske Videnskaps-Akademi	B. F. PEDERSEN, Institute of Pharmacy, University of Oslo, PO Box 1068, Blindern, 0316 Oslo 3
Poland	I	Polska Akademia Nauk	A. PIETRASZKO, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, PO Box 937, 50-950 Wrocław 2
Portugal	I	Sociedade Portuguesa de Fisica	M. M. R. R. COSTA, Departamento de Fisica, Universidade de Coimbra, 3000 Coimbra

\* 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 Africa Council for Scientific and Industrial Research	E. P. DU PLESSIS, FRD, South African ICSU Secretariat, PO Box 395, Pretoria 0001
Spain	III	Consejo Superior de Investigaciones Cientificas	M. MARTINEZ RIPOLL, Instituto Rocasolano - CSIC, Serrano 119, 28006 Madrid
Sweden	II	Kungliga Vetenskapsakademien	P. KIERKEGAARD, Arrhenius Laboratory, University of Stockholm, S-106 91 Stockholm
Switzerland	II	Schweizerische Gesellschaft für Kristallographie	H.-B. BÜRGI, Universität Bern, Laboratorium für Chemische und Mineralogische Kristallographie, Freiestrasse 3, CH-3012 Bern
UK	V	The Royal Society	The Executive Secretary, The Royal Society, 6 Carlton House Terrace, London SW1Y 5AG
USA	V	National Academy of Sciences-National Research Council	R. F. BRYAN, Department of Chemistry, University of Virginia, Charlottesville, VA 22901
USSR	V	Akademija Nauk SSSR	V. I. SIMONOV, Institute of Crystallography, Academy of Sciences of the USSR, Leninsky prospekt 59, Moscow 117333
Yugoslavia	I	Jugoslavenska Akademija Znanosti i Umjetnosti	B. KAMENAR, Laboratory of General and Inorganic Chemistry, Faculty of Science, The University, Ulica Soc. Revolucije 8, 41000 Zagreb

\* See footnote on preceding page.

A total of 53 inorganic, 5 organometallic and 27 organic related papers appeared in Section B in 1986, compared with 38, 1 and 25 respectively in 1985. The increased number of papers is most welcome, but a larger representation from the organometallic and organic fields would be gladly received. The corresponding totals for Section C in 1986 were 80 inorganic, 201 organometallic and 449 organic crystal structure communications, compared with 95, 198 and 400 respectively in 1985. In Section B, 16 papers report two structures, 3 report three structures, 2 report four structures, 1 reports five structures, 1 reports seven structures and 1 reports eighteen different structures. In Section C, 64 papers report two structures, 15 report three structures, 3 report four structures, 1 reports five structures and 1 reports eleven different structures. The increasing tendency to report multiple structures is highly encouraged, in view of the greater impact such work makes on the branch of science associated with the materials reported.

The distribution of papers and authors by country, for all sections of *Acta* and for *JAC*, is given in Table 3. The largest single change is the increased contribution by the USA to Section C in 1986. The contribution to this Section from Canada and the Federal Republic of Germany each increased while that from Spain decreased by more than ten papers in 1986. All other changes were less than ten papers.

Publication of the *Index* to Volume 41 of *Acta* was very late for the third consecutive year: the staffing shortage and interface difficulties encountered by the printer in using our keystrokes delayed production, but both problems have now been fully overcome. The computer prepared *Index* to Volume 19 of *JAC* appeared on time, bound in with the final issue.

Michael H. Dacombe was appointed Technical Editor, Susan E. Lowe and Peter R. Strickland were appointed Assistant Technical Editors and Brian McMahon was appointed Editorial Assistant, joining Andrea Sharpe, Editorial Assistant, in the course of 1986. Fuller information on the appointments is given in *Acta* (1986). A42, 288.

André Durif was appointed Co-editor of *Acta* succeeding Jean Protas, and Bruno Morosin and Edward Prince were appointed Co-editors of *JAC*, succeeding Harry L. Yakel.

#### Commission on Structure Reports

Volume 48B (Organic Compounds for 1981, 1852 pages in two volumes) was published in 1986. Co-editorial work is at an advanced stage for Volumes 49B and 50B, and is in progress for 51B and 52B (Organic Compounds for 1982, 1983, 1984 and 1985 respectively). Preparation of the 10-year *Index* (Volume 47B) is under way. Volume 52A (Metals and Inorganic Compounds for 1985, 374 pages) was published in 1986; Volume 51A (Metals and Inorganic Compounds for 1984) was sent to the publisher and will appear in 1987. Work is nearing completion on the material necessary to finish off Volumes 49A and 50A (Metals and Inorganic Compounds for 1982 and 1983 respectively).

The Executive Committee decided, after much discussion and with regret, to discontinue the publication of the Organic Volumes of Structure Reports after the 1985 Volume 52B is published. It was decided to continue with the Metals and Inorganic Volumes but in a modified format, and to explore ways of collaborating in the production of these volumes with the Inorganic and Metals Crystallographic Data Bases.

#### Commission on International Tables

The Editors of the volumes and the members of the Commission remain as given in the report for 1984. Work continued actively throughout the year; the networks BITNET and EARN have been used to great advantage in speeding communications between the Editors and with some contributors. Network transmission of contributions has been found to be only partially successful as yet, primarily because of the great diversity of marking-up schemes and control characters.

Withdrawal of authors has posed problems for the Editors of Volumes B and C; several authors in each volume have failed to meet their promised deadlines, and it has

Table 2. *Survey of the contents of the Union Journals**Acta Crystallographica*

Vol.	Year	Full Articles		Short Structural/Short-Format Papers		Short Communications										
		Number of Pages*	Number of Papers	Number	Average Length	Number	Average Length	Number	Average length							
A38 } B38 }	1982	880 } 3176 }	4056	155 } 905 }	1060	129 } 370 }	499	6.3 } 4.9 }	5.3	—	—	26 } 17 }	43	1.5 } 0.8 }	1.2	
A39 } B39 } C39 }†		1983	950 } 770 } 1714 }	3434	146 } 121 } 645 }	912	129 } 118 } 636 }	247	6.4 } 6.4 }	6.4	—	—	17 } 3 }	29	1.0 } 0.6 }	0.8
A40 } B40 } C40 }‡	1984		728 } 616 } 2126 }	3470	123 } 99 } 811 }	1033	109 } 99 }	208	6.2 } 6.2 }	6.2	—	—	14 } — }	36	1.1 } — }	0.9
A41 } B41 } C41 }			1985	624 } 456 } 1836 }	2916	114 } 67 } 703 }	884	108 } 66 }	174	5.4 } 6.4 }	5.8	—	—	6 } 1 }	16	0.8 } 0.6 }
A42 } B42 } C42 }		1986		588 } 640 } 1892 }	3120	98 } 90 } 732 }	920	85 } 89 }	174	6.3 } 7.0 }	6.7	—	—	13 } 1 }	23	1.1 } 2.2 }

*Journal of Applied Crystallography*

Vol.	Year	Full Articles¶		Short Communications		Crystal Data		Computer Programs		Short Items**			
		Number of Pages*	Number of Papers	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length		
15§	1982	676	132	89	6.2	8	1.0	19	1.7	9	2.3	7	0.9
16	1983	661	135	86	6.8	11	1.7	21	0.6	12	2.7	5	1.0
17	1984	488	104	66	6.2	11	1.5	7	0.5	7	2.4	14	0.9
18	1985	546	108	80	5.5	9	1.8	5	0.4	7	3.3	7	0.8
19	1986	492	104	71	6.1	12	1.6	10	0.4	3	1.9	8	0.8

\* Excluding indexes.

† Volume 39 divided into three new Sections in 1983.

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

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

¶ Excluding Lead Articles

\*\* Excluding Union Announcements, Crystallographers, New Commercial Products, and Book Reviews. The 1985 statistics have been restated to exclude New Commercial Products.

not yet been possible to find willing authors for all sections. The Editors are endeavouring to find authors for the missing sections and to encourage the slow ones, but it is not proposed to continue this process indefinitely. Some sections may have to be postponed to later editions of the volumes.

*Volume A (Space-Group Symmetry)*

A fully revised second edition of Volume A was sent to the printer in January 1986. It contains corrections of all errors discovered so far, substantial revisions of several portions of text, new diagrams for the plane groups and the trigonal space groups, and two new sections dealing with normalizers of space groups. Proof reading was completed in February 1987, and it is scheduled for publication in May 1987. Preparation of a revised second edition of the Brief Teaching Edition of Volume A has begun.

*Volume B (Reciprocal Space)*

The Volume is in five Parts, each divided into chapters and sections. The current position (early 1987) is:

1. General Relationships and Techniques
  - 1.1 Reciprocal Space in Crystallography [AD]
  - 1.2 The Structure Factor [AD]
  - 1.3 Fourier Methods [0]
  - 1.4 Symmetry in Reciprocal Space [AD]
2. Reciprocal Space in Crystal-Structure Determination
  - 2.1 Statistical properties of the Weighted Reciprocal Lattice [AD]
  - 2.2 Direct Methods [C]
  - 2.3 Patterson and Molecular-Replacement Techniques [C]
  - 2.4 Isomorphous Replacement and Anomalous Dispersion [0]

Table 3. *Distribution of papers and authors, by country, in Acta and JAC for 1985 and 1986*

Country	<i>Acta Crystallographica</i>								<i>Journal of Applied Crystallography</i>							
	Section A				Section B				Section C							
	Papers		Authors		Papers		Authors		Papers		Authors		Papers		Authors	
1985	1986	1985	1986	1985	1986	1985	1986	1985	1986	1985	1986	1985	1986	1985	1986	
Algeria	—	—	—	—	—	—	—	0.3	0.5	2	1	—	—	—	—	
Argentina	—	1.0	—	5	—	0.3	—	1	1.8	4.8	6	18	1.0	—	2	—
Australia	7.5	4.5	12	8	7.3	7.2	18	19	13.5	19.7	39	50	6.0	4.0	11	8
Austria	1.0	1.0	1	1	—	—	—	—	10.7	6.5	2	12	—	—	—	—
Bangladesh	—	—	—	—	—	—	—	—	1.5	0.5	6	1	—	—	—	—
Belgium	2.1	—	5	—	4.9	1.3	20	3	11.4	14.9	4.2	50	1.3	1.0	4	3
Brazil	0.5	0.5	1	1	—	—	—	—	2.4	10.2	8	43	—	—	—	—
Cameroon	—	—	—	—	—	—	—	—	0.5	—	1	—	—	—	—	—
Canada	2.1	3.0	5	5	3.3	2.3	7	4	36.5	49.4	107	135	2.0	—	3	—
Chile	—	—	—	—	—	—	—	—	0.9	1.2	4	4	—	—	—	—
China, Peoples' Rep.	5.0	1.0	13	3	0.7	5.0	2	13	1.2	0.4	5	8	1.0	—	1	—
Czechoslovakia	0.3	2.0	2	2	—	—	—	—	8.0	8.4	24	38	1.4	3.0	5	7
Denmark	—	—	—	—	—	3.0	—	8	6.5	7.9	11	17	1.1	1.5	4	5
Egypt	—	—	—	—	—	—	—	—	—	0.7	—	3	—	—	—	1
Finland	—	—	—	1	—	—	1	—	3.0	3.0	9	7	1.0	1.0	1	3
France	6.3	8.7	18	11	8.1	10.4	39	38	75.9	67.5	262	239	11.8	13.5	35	33
German Dem. Rep.	1.7	2.0	5	4	—	—	—	—	0.8	2.0	3	8	3.6	1.5	8	2
Germany, Fed. Rep.	7.7	9.0	18	18	4.3	7.6	15	17	50.2	71.3	137	193	10.3	6.3	22	16
Greece	3.6	—	10	—	—	—	—	—	1.3	7.4	5	15	1.0	1.0	2	2
Hong Kong	—	—	—	—	—	—	—	—	—	3.1	—	9	—	—	—	—
Hungary	—	—	—	—	—	—	—	—	1.5	2.9	6	12	—	0.5	—	1
India	1.0	—	2	—	1.0	1.3	4	4	22.8	26.9	79	102	1.0	4.0	2	9
Ireland	—	—	—	—	0.4	—	2	—	0.5	—	2	—	—	—	—	—
Israel	0.8	0.5	3	1	4.0	2.0	12	9	1.0	—	3	—	1.1	—	3	—
Italy	8.3	1.0	19	2	0.1	4.3	1	13	24.6	21.8	91	64	4.0	1.0	7	2
Ivory Coast	—	—	—	—	—	—	—	—	1.8	0.3	7	2	—	—	—	—
Japan	3.3	4.0	9	8	7.1	5.0	18	16	48.1	49.7	173	181	3.0	11.3	8	35
Jordan	—	—	—	—	—	—	—	—	—	1.0	—	1	—	—	—	—
Korea, South	—	—	—	—	—	—	—	—	0.3	1.0	1	2	—	—	—	—
Libya	—	—	—	—	—	—	—	—	—	0.5	—	1	—	—	—	—
Madagascar	—	—	—	—	—	—	—	—	—	0.2	—	1	—	—	—	—
Malaysia	—	—	—	—	—	—	—	—	1.0	1.9	2	8	—	—	—	—
Mexico	—	—	—	—	—	—	—	—	6.7	9.0	26	37	—	—	—	—
Netherlands	2.6	4.0	9	7	3.0	4.5	9	14	23.0	22.2	90	79	2.0	4.8	3	8
New Zealand	—	—	—	—	1.0	—	2	—	4.0	5.0	11	18	—	—	—	—
Nigeria	—	—	—	—	—	—	—	—	—	—	1	—	—	—	—	—
Norway	1.0	2.0	1	4	—	—	3	—	3.7	1.1	9	4	—	—	—	—
Poland	2.0	0.3	4	1	—	2.0	—	6	29.7	21.3	71	64	1.5	1.2	3	5
Portugal	—	1.0	—	2	—	—	—	—	—	0.5	—	1	—	—	—	—
Puerto Rico	—	—	—	—	0.2	—	1	—	—	—	1	—	—	—	—	—
Saudi Arabia	—	—	—	—	—	—	—	—	2.0	1.0	6	3	—	—	—	—
Sierra Leone	—	—	—	—	—	—	—	—	0.3	—	1	—	—	—	—	—
South Africa	—	—	—	—	—	1.0	—	3	3.5	6.0	9	19	2.0	1.0	6	3
Spain	3.0	1.0	9	2	0.3	2.3	1	9	32.8	22.5	123	83	2.1	1.7	10	10
Sweden	—	—	—	—	1.0	1.3	1	3	5.4	5.0	12	12	1.0	0.6	3	2
Switzerland	2.3	—	5	—	2.0	2.0	3	4	9.0	10.0	26	28	1.0	—	2	—
Taiwan	—	0.5	—	1	0.8	—	3	—	7.7	9.5	31	42	—	—	—	—
Tunisia	—	—	—	—	0.4	—	2	—	—	1.3	1	3	—	—	—	—
Turkey	—	1.0	—	1	—	0.3	—	1	—	—	—	1	—	—	—	—
UK	11.8	12.3	28	20	10.5	9.9	33	22	68.5	66.2	214	215	13.9	9.3	52	18
USA	28.7	18.8	56	53	21.0	11.7	69	27	107.5	148.8	344	459	24.0	25.0	62	57
USSR	8.5	6.0	28	19	1.5	5.0	5	9	8.5	4.0	43	26	1.7	—	11	—
Venezuela	—	—	—	—	—	—	—	—	2.0	—	8	—	—	—	—	—
Yugoslavia	—	1.0	—	1	—	0.5	—	1	7.6	6.1	23	22	1.0	—	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.

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| <ul style="list-style-type: none"> <li>2.5 Electron Diffraction and Microscopy in Structure Determination [AD,C]</li> <li>3. Dual Bases in Crystallographic Computing <ul style="list-style-type: none"> <li>3.1 Distances, Angles, and their Standard Deviations [C]</li> <li>3.2 Best-Plane Calculations [PD]</li> <li>3.3 Molecular Modelling and Graphics [AD]</li> <li>3.4 Accelerated Convergence and Lattice Sums [AD]</li> </ul> </li> </ul> | <ul style="list-style-type: none"> <li>4. Diffuse Scattering and Related Topics <ul style="list-style-type: none"> <li>4.1 Thermal Diffuse Scattering of X-rays and Neutrons [C]</li> <li>4.2 Disorder Diffuse Scattering of X-rays and Neutrons [AD]</li> <li>4.3 Diffuse Scattering in Electron Diffraction [AD]</li> <li>4.4 Small Crystallite Size and Texture [0]</li> </ul> </li> </ul> |
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- 4.5 Strain [0]
- 4.6 Scattering from Mesomorphic Structures [0]
- 4.7 Small-Angle Scattering [PD]
- 5. Dynamical Theory and its Applications
  - 5.1 X-ray and Neutron Aspects of Dynamical Theory [0]
  - 5.2 Dynamical Theory of Electron Diffraction [AD]

The symbols in square brackets indicate: C = complete, D = in draft (P = preliminary, A = advanced), 0 = nothing in the hands of the Editor.

Experiments with direct photocomposition of computer-generated tables, as in Chapter 1.4, are under way.

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

Many authors have submitted final drafts, and several have provided machine-readable floppy disks or tape. Two substantial contributions and one extensive table have been successfully photocomposed from these submissions; trials with others continue.

The Volume is in ten Parts, each divided into chapters and sections. The current position (early 1987) is:

1. Crystal Geometry [0]
2. Diffraction Geometry [H]
3. Preparation and Examination of Specimens [H]
4. Production and Properties of Radiations [S]
5. Determination of Lattice Parameters [H]
6. Interpretation of Diffracted Intensities [H]
7. Measurement of Intensities [H]
8. Refinement of Structural Parameters [S]
9. Basic Structural Features [H]
10. Precautions Against Radiation Injury [C]

The symbols in square brackets are as for Volume B, plus S = some sections missing, H = in rough draft or about half complete.

In suitable cases editorial updating of the corresponding parts of the old Volumes II-IV will be used to avoid gaps where authors have withdrawn or have not been found.

#### *Commission on Biological Macromolecules*

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

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

The Commission held no formal meetings in 1986, although several members were present, and held informal discussions, at the Gordon Research Conference on Electron Distributions and Chemical Bonding organized by E. Stevens and M. Newton which was held in New Hampshire in June.

During the year proposals for representation of the activities of the Commission at the XIV IUCr Congress were forwarded to the Chairman of the Programme Committee. A microsposium on charge, spin and momentum densities organized by J. Schneider, Hahn-Meitner-Institut, Berlin, will be held at the Congress.

Plans for the IX Sagamore Conference are now well under way. It will be held at a site near to Coimbra in Portugal from 27 June to 1 July 1988 under the Chairmanship of L. M. Alte de Veiga. The theme of the conference will be charge, spin and momentum densities in transition metals.

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

The main activities of the Commission during 1986 have been the organization of two International Schools on crystal growth technology and related characterization methods and applications, with the aim, on one hand, to favour the transfer of expertise to developing countries and, on the other, to expand the relationship between crystallography and modern materials science.

The two Schools organized by the Commission were:

(1) Winter School on Technology, Characterization and Properties of Epitaxial Electronic Materials, Trieste, Italy, 13-24 January 1986. The School was directed by C. Paorici and A. Baldereschi, and the Commission acted as the International Steering and Programme Committee, selecting the 19 speakers. The attendance (90 participants) included attendees from 28 countries (20 from developing countries). The optimum selection of lecturers, which included the Nobel prize winner Leo Esaki, the high scientific standard and great interest of the participants and the superb local organization of the International Centre for Theoretical Physics, co-sponsor and host of the School, all contributed to make this School a great success.

(2) International School on Solar Cell Materials and Applications, Cairo, Egypt, 19-29 October 1986. The School, co-sponsored by the Egyptian Academy of Scientific Research and Technology (and intended as a sequel to a previous School organized by the Commission in 1983), was directed by C. Paorici. The object of the School was to extend some results of modern technology in solar energy conversion to developing countries, with special reference to the Middle-East area. The Local Organizing Committee, headed by S. Arafa, contributed to the success of the School, in particular by planning sections of the School in different Egyptian universities (Cairo, Ismailia, Alexandria).

Further to these activities, organizational work has begun for the preparation of two International Schools in the next triennium [Cuba, end 1987; India, 1988 (?)].

#### *Commission on Crystallographic Apparatus*

During 1986 the Commission's activities have been largely directed towards discharging its responsibilities with respect to the production of *International Tables for Crystallography* Volume C. Members of the Commission have been actively involved in the production of a number of sections of this volume.

Organization of a project referred to the Commission by the Commission on Journals is proceeding. This project has as its aim the examination of experimental methods for the measurement of single crystal lattice constants. The project Chairman will be S. Martinez-Carrera and G. T. De Titta has been invited to join the Commission as a Consultant to assist with the project. For future records this project will be referred to as the Single Crystal Lattice Constant Project.

The only other project being considered by the Commission is the Profile Refinement Project. This project has so far had two Chairmen, J. Čermák, who could not continue because of a change in the direction in his research work, and M. Zocchi, who regrettably has had to resign from the Commission because of ill-health. Because of its chequered background it was decided to hold this project

in abeyance until the XIV IUCr Congress, when it is hoped to find a new Chairman and to recruit a number of laboratories to participate in the project. Because of the strong emphasis on powder diffraction and profile refinement at the Congress and its associated meetings it is hoped that it will be possible, at last, to inaugurate this important project.

Finally, the organization of the Open Commission Meeting on Recent Advances in X-ray Powder Diffractometry at the XIV IUCr Congress has recently been completed.

#### *Commission on Crystallographic Computing*

The major effort of the Commission went in organizing an International Summer School on Crystallographic Computing in Leipzig (11–20 August 1986). The Programme Committee Chairman was H. Schenk, and the Local Organizing Committee Chairman was P. Paufler. The Proceedings of the School (237 pages) have been published by Karl-Marx-Universität Leipzig Press under the title *Crystallographic Computing*. P. Paufler, V. Ceist and D. Klimm were the editors. Emphasis was on graphics, powder methods and data bases. Morning lectures (26) were followed by afternoon tutorials selected according to the interest of the students. The number of participants was 107 from 17 countries, with 18 lecturers. The School was financially supported by the IUCr, Fachinformationszentrum Energie, Physik, Mathematik, GmbH Karlsruhe, and Karl-Marx-Universität, Leipzig.

By the end of 1986, work on the Open Meeting which will be held during the XIV IUCr Congress in Perth had progressed. It will be a joint meeting with the Commission on Crystallographic Teaching. Five lectures will be dedicated to Crystallographic Microcomputing.

Great effort was also put into the preparation for the Post-Congress International School on Crystallographic Computing in Adelaide (22–29 August 1987). N. W. Isaacs is the Programme Committee Chairman, M. R. Taylor is the Local Committee Chairman. The School will provide expert tuition on a range of crystallographic computing techniques of interest to both post-graduate students and practising crystallographers. The emphasis will be on instructing participants in the practical application of modern computing techniques and procedures to the solution of typical problems encountered in crystallographic studies. It is expected that approximately 27 lecturers and more than 100 students will participate.

#### *Commission on Crystallographic Data*

In 1986 the Commission prepared two reports. One of them, *The Deposition of Crystallographic Results: Current Problems and Their Causes*, has been published in *Acta Cryst.* (1986), C42, 1671–1675. The other, *Recommendations for the Standardization of Unit Cell Descriptions*, has been prepared but is still under discussion.

In July, the Chairman attended the CODATA meeting in Ottawa and presented a poster on the Union's activity in data management. Subsequently, he discussed at Foxhill with the Executive Committee and others plans to combine the preparation of *Structure Reports* and databases.

For the forthcoming XIV IUCr Congress in Perth, two Open Meetings have been organized with the Commission on Journals covering the most acute problems of Accuracy of Crystallographic Data and The Future of Crystallo-

graphic Journals and Databases. The whole data activity in crystallography will be collected in a booklet on *Crystallographic Databases* with 13 contributions by 26 authors.

#### *Commission on Crystallographic Nomenclature*

The principal accomplishments of the Commission in 1986 were those achieved through the continuing efforts of its three committees. The *ad hoc* Committee on the Nomenclature of Symmetry has further refined its definition of terms related to symmetry elements in space and point groups. These will be presented for public discussion at the XIV IUCr Congress during an Open Commission Meeting in Perth, organized by Committee Chairman P. M. de Wolff.

A second draft report was circulated within the Subcommittee on Statistical Descriptors in Crystallography late in 1986, as the result of numerous and constructive rounds of subcommittee correspondence [see *Acta Cryst.* (1987), A43, 143 for the subcommittee membership]. Aspects covered by the report in its subsequent revisions will be presented in Perth at another Open Commission Meeting, organized by Committee Chairman D. Schwarzenbach.

The Subcommittee on the Nomenclature of Inorganic Structure types met in Marburg and, later, in Geneva during 1986 thereby producing an advanced version of their extensive report. Copies of the revised report will be available for public discussion in Perth and each member will present a major section of their recommendations in the course of the third Open Commission Meeting, organized by Committee Chairman J. Lima-de-Faria.

The Commission has remained in close communication with the International Union of Pure and Applied Chemistry throughout the year. The greater part of the correspondence and contacts concerned the Interdivisional Committee on Nomenclature and Symbols of IUPAC, as reported thereunder.

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

During the last annual report, the Chairman initiated a round-robin study on ZnS to investigate the potential for providing a calibration point on the pressure scale for use at elevated temperatures. The phase transition in zinc sulfide occurs at 15 GPa at room temperature. A well characterized determination of the phase boundary as a function of pressure and temperature would provide the basis for a fixed point at elevated temperatures (<573 K), thereby satisfying a critical need in the high-pressure community.

A high-purity boule of ZnS was purchased from Eagle Picher Industries and the material was cut into small samples for distribution to various laboratories worldwide. Measurements were carried out in the National Measurement Laboratory, National Bureau of Standards, Washington, with diamond anvil cells and the ruby fluorescence method of pressure measurement to determine the effect of temperature on the transition pressure. Results of those measurements indicate that the 15 GPa phase transition in ZnS is either independent of temperature or slightly negative in its dependence (lowering the pressure of the transition with increasing temperatures in the range <573 K). However, the measurements were very difficult to make because (1) two variables,  $P$  and  $T$ , need to be carefully controlled, (2) the hydrostatic-pressure-transmitting liquid must be both chemically inert in the presence of ZnS and

chemically stable at the elevated temperatures required, (3) the transition, which is very rapid at elevated temperatures, can easily be overshoot leading to an erroneously high value for the transition pressure, and, finally, (4) the transition has a large hysteresis affecting the pressure of the reverse transition. Faced with a difficult experiment and with the many problems associated with it, few measurements have been made to date, and the results so far are inconclusive. More data need to be obtained and analysed before reporting a definitive result.

#### *Commission on Crystallographic Teaching*

##### *Open Activities in Perth*

In collaboration with the Commission on Crystallographic Computing, an Open Meeting on the use of microcomputers is being organized by both Chairmen. The Commission is also involved in other activities, such as the microcomputer lab which will be open during the whole Congress, a film show (H. von Philipsborn), and as catalyst in the book and non-commercial exhibitions. The computing lab will be equipped with some 15 computers, IBM PC's, Mac's, Amigas, C64 and possibly Atari 1040.

##### *Schools*

Madras, 1985. The proceedings of the school have been published by World Scientific, Singapore under the title: *Direct Methods, Macromolecular Crystallography and Crystallographic Statistics*, edited by H. Schenk, A. J. C. Wilson and S. Parthasarathy. It has been published through the joint efforts of the Commission and COSTED.

China, 1988. The original plans for the School in 1987 have been delayed because of the death of the local organizer, Professor Peng. A new team is being set up and it is expected that the School will now take place in September 1988. The programme is in discussion and will be circulated in or before Perth.

##### *History*

The *Historical Atlas of Crystallography* has been finalized by its editor J. Lima-de-Faria. The IUCr decided on sponsorship, but a delay has been caused by the fact that very expensive typesetting is necessary. J. Lima-de-Faria and J. H. Robertson are trying to solve the problems.

##### *Files of the Union*

H. Kamminga has reduced the files of the IUCr to a reasonable size while saving documents with historical value.

##### *Film list*

H. von Philipsborn is working on a crystallographic film list. He expects to have drafted it this summer and he will use it to compile the film shows in Perth.

##### *Booklist*

The last booklist was published by J. H. Robertson (Book-Review Editor of *Acta* and *JAC*) in *J. Appl. Cryst.* It is probable that a system will be set up to produce regular updates, which will be the responsibility of the Book-Review Editor.

##### *Pamphlets*

C. A. Taylor wishes to resign as editor of the series. The search has begun for his successor.

##### *IUCr Visiting Professors*

Similar activities are undertaken by ICSU. The idea is a financial possibility. A proposal will be presented in Perth for discussion.

##### *Closed Meeting in Perth*

There will be one or more Closed Meeting(s) in Perth.

##### *New possible activities*

Book scheme. Many crystallographers live in countries with currency problems and cannot buy scientific literature. Can we do something about this? (UNESCO may be co-sponsoring.)

Public understanding. When the general public understands a subject it is both fruitful for the public and for the subject, for instance the talk by Th. Hahn in Hamburg. It may be possible to set something up so that this type of information is spread on a wider scale.

##### *Commission on Electron Diffraction*

The Commission has been active concerning the XIV IUCr Congress and suggested topics and names of speakers for Plenary/General lectures, Symposia and an Open Commission Meeting. The Open Commission Meeting will be on Dynamical Electron Diffraction in Transmission and Reflection (THEED, MEED, LEED, RHEED), and is planned to be an integrated approach to these complementary techniques in electron diffraction covering a wide energy range. The Commission is also supporting, and has advised on, two Satellite Meetings connected with the XIV Congress: the Symposium on Validity of Structures from Electron Microscopy, and the Symposium on Accuracy in Structure Factor Measurements.

The Commission continues to advise the Editors of Volumes B and C of *International Tables for Crystallography* on sections dealing with electron diffraction and microscopy, and various members of the Commission have written articles for *International Tables*.

The Commission was delighted that one of its members, J. M. Cowley, will be awarded the first Ewald Prize of the IUCr, jointly with A. F. Moodie. The presentation will occur at the XIV IUCr Congress and is in recognition of their pioneering work in electron diffraction and microscopy leading to reliable structural information about crystals.

Finally, towards the end of 1986 news of the discovery of high-temperature ceramic superconductors began to filter out, first informally and then more formally. Members of the Commission are now actively studying the crystallography of these materials, and it is discoveries such as this that ensure a healthy future for electron diffraction and for its IUCr Commission.

##### *Commission on Neutron Diffraction*

Final arrangements were made for the Symposium on Neutron Scattering, to be held in Sydney, Australia, 8-10 August 1987. The Symposium is a satellite meeting of the XIV IUCr Congress. It has been organized by the Commission with T. J. Hicks as the Chairman of the Programme Committee.

The Commission gave assistance to G. E. Bacon in preparing the book *Fifty Years of Neutron Diffraction* (published by Adam Hilger Ltd, 1987). One of the chapters in this



book summarizes the activities of the Commission on Neutron Diffraction since its inception in 1969.

Two Newsletters were circulated in 1986 to over 850 scientists world wide. The Spring Newsletter, edited by H. G. Smith, emphasized progress in neutron diffraction in the USA. The Autumn Newsletter, edited by T. J. Hicks, concentrated on Australia and the Far East.

The Commission has offered assistance to U. Shmueli and A. J. C. Wilson in the commissioning of a number of articles for Volume B and Volume C of *International Tables*.

#### *Commission on Small Molecules*

##### *A. Meetings organized with assistance from CSM*

1. VI Symposium on Organic Crystal Chemistry, Poznan, Poland, 1-4 August 1986. The Symposium brought together senior scientists with a substantial number of young Polish crystallographers. Sixteen oral and thirty-eight poster presentations were held. Included were the following topics: substitution effects on the geometry of aromatic systems; drug structure, drug design and molecular graphics; disorder in molecular crystals; crystal chemistry of biologically active molecules; structure and properties of polymers; methods for solving crystal structures. The meeting was held in a former palace, a location which provided all participants the opportunity to interact informally, which fostered many interesting scientific discussions.

2. ECM Tutorial-Workshop on Inorganic Molecular Crystals. At the request of the CSM, F. Herbststein and J. A. K. Howard organized a one day Workshop/Tutorial in conjunction with ECM-10 (Wrocław, Poland). Topics covered included electron density deformation in organometallic complexes, transition-metal-phosphate bonds, molecular coordination complexes, and organic-transition-metal chemistry.

3. Molecular Structure: Chemical Reactivity and Biological Activity. An International Symposium on this topic was held in Beijing, China, 15-21 September 1986. The meeting was sponsored by the IUCr and organized with assistance from the CSM, the Chinese National Committee of Crystallography and the Chinese Chemical Society. The programme included sessions on structures of biological interest ranging from small peptide hormones to the 50S ribosomal subunit, chemical reactivity (*e.g.* crystal surfaces) and crystal properties (*e.g.* electron distributions and packing energies). The Meeting was attended by over 250 participants (about half from outside China), including three Nobel Laureates (Herbert Hauptman, Dorothy Hodgkin and William Lipscomb). The transactions of the meeting are being prepared for publication in the IUCr/OUP Book Series.

4. Steroid Molecular Structure. A Symposium on this topic was included in the programme of the International Congress of Steroid Hormones (Madrid, Spain, September 1986). The Symposium was organized at the suggestion of the CSM.

5. Computational Methods in Chemical Design: Molecular Modelling and Computer Graphics. An International Symposium on this topic was sponsored in part by the IUCr with the assistance of the CSM. The meeting covered a broad range of topics ranging from small-molecule to macromolecule crystallography, NMR spectroscopy, empirical and *ab initio* energy calculations, and artificial intelligence. Lectures stressed the value of combin-

ing experimental and theoretical approaches in the study of structure.

##### *B. Future meetings*

Recognizing that international meetings foster current awareness (in an interdisciplinary manner in favourable cases) and promote the advance of the role of small-molecule crystallography in chemistry, physics and biology), the CSM has prepared guidelines for colleagues interested in obtaining IUCr sponsorship and support for such meetings.

##### *C. International cooperation in intensity data collection*

The CSM has initiated a programme to establish contacts between crystallographers lacking state-of-the-art facilities for data collection and colleagues who have the capacity to collect at least one intensity data set per year to assist them. Since 1 June 1986, requests to initiate collaboration were dispatched to 26 volunteers. It is hoped that this programme will not only satisfy immediate needs but promote substantial international cooperation and collaboration.

Those wishing to apply for data collection assistance or to volunteer their services are requested to contact the CSM Secretary (Dr William L. Duax, Medical Foundation of Buffalo, 73 High Street, Buffalo, NY 14203, USA).

##### *D. Open Meetings*

An Open Meeting of the CSM was held in Wrocław at ECM-10. There was an extensive discussion of the publication policy of *Acta Crystallographica* Sections B and C. The data collection programme and possible future meetings were also discussed.

##### *E. Newsletters*

The Secretary of the CSM prepared and distributed three Newsletters during the year (March, August and October). The Commission strongly requests that people receiving the Newsletter copy it and distribute it further (to at least 5 colleagues).

##### *F. Survey*

The CSM conducted a survey for the Executive Committee of *circa* 100 colleagues from around the world concerning the structure of *Acta Crystallographica* Sections B and C. The replies were summarized and sent to the President of the Union in 1987.

#### **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 1986 the Executive Committee approved sponsorship of the following schools and meetings, mostly with financial support:

1. Conference on Electron Distribution and Chemical Bonding, Plymouth, NH, USA, 30 June-4 July 1986.
2. Symposium on Organic Crystal Chemistry, Poznan-Rydzyzna, Poland, 1-4 August 1986 (satellite of ECM-10).
3. One-day Tutorial Workshop on Inorganic Molecular Crystals, Wrocław, Poland, 4 August 1986 (satellite of ECM-10).
4. Satellite Conference on Crystal Growth and Liquid Crystals, Łódź, Poland, 11-13 August 1986 (satellite of ECM-10).

5. Research Course on Neutron Diffraction Techniques in Crystal Structure Determination, Studsvik and Uppsala, Sweden, 18–29 August 1986.
6. Workshop on Crystallography in Molecular Biology: Structure of Biological Macromolecules, Pouchchino, USSR, 4–13 September 1986.
7. International Symposium on Molecular Structure, Beijing, China, 15–19 September 1986.
8. Symposium on Computational Methods in Chemical Design: Molecular Modelling and Computer Graphics, Schloss Elmau, Federal Republic of Germany, 19–26 October 1986.
9. Symposium on the Validity of Structures from Electron Microscopy, Melbourne, Australia, 8–9 August 1987 (satellite of XIV IUCr Congress).
10. Symposium on Neutron Scattering and Applications, Sydney, Australia, 8–10 August 1987 (satellite of XIV IUCr Congress).
11. XIV General Assembly and International Congress of Crystallography, Perth, Australia, 12–20 August 1987.
12. Symposium and Workshop on X-ray Powder Diffraction, Fremantle, Australia, 20–22 August 1987 (satellite of XIV IUCr Congress).
13. Symposium on Accuracy in Structure Factor Measurements, Warburton, Australia, 23–26 August 1987 (satellite of XIV IUCr Congress).
14. International School on Crystal Growth and Characterization of Materials for Electronics, La Habana, Cuba, 30 November–11 December 1987.
15. School on Crystallography of Molecular Biology, Erice, Italy, 29 May–7 June 1988.
16. Summer School on Neutron Diffraction, Oxford, England, 18–30 September 1988.

Other meetings which received Union support have been listed earlier in this Report. Two tendencies can be noticed: (i) many more satellites in connection with larger meetings, (ii) more schools relating to material science.

The Executive Committee agreed that specific attention be paid to publication in *JAC* or *Acta* of original papers presented in any meeting sponsored by the IUCr. Therefore the organizers of all IUCr-sponsored meetings should recommend the journals of the Union as a suitable channel of publication for the original papers presented in the meeting. If they intend to publish proceedings they have to consider the Union's *Conference Proceedings* series.

Organizers of meetings wishing to seek Union sponsorship should submit applications at least six months in advance of the date of the meeting, writing to the Chairman of the Sub-Committee: Dr E. N. Maslen, Crystallography Centre, University of Western Australia, Nedlands 6009, Western Australia, Australia.

Applications for sponsorship of satellite meetings must be submitted through the Chairman of the Organizing Committee of the main meeting.

#### Representatives on Other Bodies

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

The General Assembly and associated meetings held in York, England, in May 1986 were the first to be held after the full transition from the Abstracting Board of the International Council of Scientific Unions became fully opera-

tive, and were marked by greater emphasis on technical and less on organizational matters than in recent years. This welcome trend is likely to continue.

##### *Technical meetings in York*

*Compact-disk read-only memories.* There was a discussion of the possible impact of CD ROMs (compact-disk read-only memories) on scientific and technical information. Many Class B Members had been experimenting with these, and opinions seemed about equally divided between those who found their capacity to be too small for practical use (at least until 'juke boxes' are further developed) and those who found the capacity too big to warrant the cost of the preparation of a master. Only PsycINFO (American Psychological Society) was ready to offer more than an experimental service; a two-disk pack suitable for use by research students on personal computers was on sale.

*Legal aspects of information transfer.* A survey of ICSTI members (including the IUCr) showed that copyright was the legal aspect of greatest interest, followed closely by contracts and international treaties. Copyright law differs greatly in different countries, and detailed surveys were given of the position in France and the United Kingdom; the latter included a review of the 'white paper' on proposed legislation. A major difference is that the UK (and the USA) are concerned only with financial rights, France is concerned also with 'moral' rights. No satisfactory English equivalent could be found for 'moral' and 'intangible' in this context: 'The author of an intellectual work is entitled, through the sole fact of his creation thereof, to an intangible property right to such work, which is exclusive and binding on all. Such right includes intellectual and moral essential characteristics and also pecuniary interests, which are determined under the terms of this law. The existence or conclusion of a work contract agreement or of a service agreement by the author of an intellectual work does not involve any derogation from the right thereto duly recognized under the terms of Paragraph 1 hereinabove.' It would appear that an author retains the right to prevent any change or abridgement that would alter the character of his work, even if he sells the copyright.

*The future of information flow.* A seminar on the Future of Information Flow included the topics: Factors in the Electronic Handling of Information, Primary Journals in the Future Pattern of the Scientific Information Network, The Future of Secondary Services in Information Flow, Future of Information Flow: Tertiary Information Providers, Future of Online Services, and The Future Role of Libraries in the Electronic Information Age.

##### *General Assembly*

At the General Assembly ten new Members were elected:  
Class A

The Institute of Physics

Class B

[US] Library of Congress

IBC

Class C (Associate Members)

Institut Européen pour Gestion d'Information

International Centre for Theoretical Physics

Salinfo

Taylor & Francis

## Class D (Honorary Members)

Dale Baker  
M. S. Day  
A. J. C. Wilson

IBC is a medical information service in South Africa; Salinfo is a consortium of libraries in the Netherlands; Taylor & Francis are scientific publishers (perhaps best known for the *Philosophical Magazine*). The General Assembly elected the Executive Board, to serve until 1989: President: J. Michel  
Vice-President: B. Stern  
General Secretary: L. Granick  
Treasurer: J. Coyne  
Other members: Académie Royale de Belgique

British Library  
CAS  
CODATA  
DIXIT  
FIZ Chemie  
INSPEC  
NTIS

This is the first occasion on which no Union is represented on the Executive Board, reflecting the increasing professionalism in the information community. It is also the first occasion on which honorary members have been admitted.

Other matters discussed at the General Assembly were the more efficient use of the time allotted to the annual meetings of ICSTI and the setting up of special groups on matters of cross-disciplinary interest.

*Groups.* ICSTI has decided to set up five special cross-disciplinary groups:

Economic Issues  
Electronic Publishing  
Primary/Secondary Relations  
Numeric Data  
Education and User Needs

The IUCr representative has been actively engaged with the Group on Education and User Needs (of which he is the Chairman) and the Numeric Data Group. He attends the other groups when there is no time-table conflict. In the future, the Technical Activities Coordinating Committee (TACC) will be constituted of the Chairmen of the new and the existing groups *ex-officiis*, instead of appointed individuals.

*Technical activities since York*

The Numeric Data Group began work rapidly, and held its first meeting, described as 'organizational', in connection with the CODATA conference in Canada in July 1986, and a technical meeting in Herstonceux Castle, England, later in the year. Aside from formal items, the following topics were discussed:

1. Scope of Numeric Data Group interests
2. Reports on data activities in
  - astronomy
  - crystallography
  - materials performance
  - physics
3. CODATA Referral Database
4. Data tagging
5. Projects and priorities
6. Future meetings
7. Electronic mail.

Somewhat surprisingly, it appeared that the IUCr representative was the only participant with personal experience of international electronic mail; it has been extensively used in the course of editing *International Tables for Crystallography*.

Meetings of several other groups scheduled for January 1987 had to be cancelled.

*Future programme*

The next meeting of the Council will take place in New York in May 1987, with the American Institute of Physics as host. The Numeric Data Group and the Group on Education and User Needs will meet on the two days preceding the main Council activities.

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

The CODATA General Assembly at Ottawa gave information on:

- (a) principal developments of data management: retrieval systems, online services, electronic publication,
- (b) national activities in documentation and databases, standardization of data structure and retrieval languages,
- (c) activities in different fields of science, problems of completeness, overlapping, cross-correlation, accessibility, acceptance, and quality control of databases,
- (d) problems of transfer of crystallographic results to non-crystallographers. Crystallographic databases have been mentioned in reports about biosciences, chemistry, geosciences. Organic crystal structures lead much more directly to chemical reactions. Between the knowledge of inorganic and metal structures and material properties a much broader gap exists. It ought to be filled by research. Results in one field are often the origin for ventures in another,

(e) with regard to databases in crystallography, an exemplary situation exists. A much more complicated situation exists in other fields. In biosciences 19 reports, in environment and resources 46, in materials properties 18, in thermodynamics 28 substantiate this statement.

CODATA activities are of direct importance for the IUCr with regard to the referral database, the coordination of protein sequence databases and materials database standards. Proposals for further working groups are welcome.

The Ottawa meeting was attended by 286 scientists, the General Assembly by representatives of 19 countries and 15 Unions. The IUCr was represented by a poster. D. Lide from NBS was elected as the new President.

At the next congress, many members of the Executive Committee will retire. The IUCr representative will only have more influence if his presence is more continuous. This should be taken into consideration when electing the next representative.

Next congresses: Karlsruhe (Federal Republic of Germany) 1988, Gaithersburg (USA) 1990, India 1992.

CODATA installed a mailbox system with DIALCOM for faster correspondence completing the existing electronic mail possibilities by EARN, BITNET etc. The Chairman set up an account with CDT0078.

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

No report has been received from the IUCr representative on this body.

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

There were no meetings of this Committee during 1986 and therefore there is nothing to report.

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

COSTED has been expanded to enhance its service to various parts of the world. There are now five COSTED Regional Secretariats to serve East Africa, West Africa, Asia, Latin America and the Caribbean located, respectively, in Kenya, Nigeria, India, Venezuela and the West Indies. Each Regional Secretariat has a high-level advisory board formed from regional scientists. In its report to the General Assembly of the International Council of Scientific Unions (ICSU), in Berne, 14–19 September 1986, the following information was presented by COSTED:

'Taking into consideration the strengthening of the COSTED central and regional structure, as well as the recommendations of the Study Group on ICSU's Activities Related to Developing Countries, the programmes and activities of COSTED will henceforth be organized around the following 7 categories:

1. Scientific Research Workshops and Seminars in Developing Countries
2. Research Grants to Scientists in Developing Countries
3. Visiting Lectureships and Travel Fellowships
4. Science Education and Training in Developing Countries
5. Technology Application and Training
6. Scientific Instrumentation: Repair, Maintenance and Development of Scientific Equipment
7. Science Communication and Organization

When these activities are of an inter-regional or global nature they will be coordinated by the central COSTED Secretariat; if they are strictly of a regional nature, they will be coordinated by the regional COSTED Secretariat concerned. In all cases, COSTED activities will be undertaken in close cooperation with appropriate national and international bodies.'

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

Numerous provisional nomenclature reports generated by various divisional committees and commissions of IUPAC were received during the year. A document of direct interest to many crystallographers, to which the IUCr contributed, will form the new edition of IUPAC's 'Green Book' (*Manual of Symbols and Terminology for Physicochemical Quantities and Units*). An inexpensive laminated and helpful list that refers to the symbols most frequently used by authors and others in chemistry and related disciplines, based on the 'Green Book', has recently been published for IUPAC by Blackwell entitled *Abbreviated List of Quantities, Units and Symbols in Physical Chemistry*.

IDCNS met 31 August to 1 September 1986 in Witney, England. The IUCr was represented by A. J. C. Wilson as alternate for S. C. Abrahams. The revised manuscript of the 'Green Book' was examined in detail to ensure that all nomenclature decisions presented were self-consistent. Revision of *Nomenclature of Inorganic Chemistry* ('Red

Book') was reported to be at an advanced stage as was the first part of *Nomenclature of Organic Chemistry* ('Blue Book'), with other divisions also making progress with revisions of their specialized nomenclature. Further strengthening of the ties between IUCr and IDCNS was agreed upon.

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

As explained in the previous report this Commission works by mail in a way similar to that followed by the IUCr Calender Sub-Committee. In 1986 the number of applications for meetings to be held in 1987 was ten, and five of these were approved.

The topics of the approved meetings were: Graphite Intercalation Compounds, Structure of Surfaces, Recent Progress in Many-Body Theories, Surface Physics, Thin Films.

A general unsolved problem of the IUPAP conferences is to publish and distribute the proceedings of international conferences in a way that make them easily available to the scientific community. Information on the proceedings is circulated through the IUPAP News Bulletin.

*Conference Committee of the European Physical Society*

The Annual Meeting of this Committee was held in Bad Honnef, Federal Republic of Germany, on 5 September 1986. During the meeting the preparations for the 7th (Helsinki, 1987) and 8th (Amsterdam, 1990) EPS General Conferences were discussed.

The guidelines for conferences proposed by the Plasma Physics division were considered suitable, after small modifications, as a useful instrument (not compulsory) for organizing divisional conferences, and instructions for invited speakers were distributed for discussion in a future meeting.

It was approved that one of the main duties of the Vice-Chairman of the Conference Committee will be of assisting the Chairman in improving the balance of the EPS activities in East and West Europe.

J. Heijn, delegate of the Dutch Physical Society, and D. Hommel, delegate of the Physikalische Gesellschaft der DDR, were nominated as new Chairman and Vice-Chairman, respectively.

It was decided that the next meeting of the Conference Committee will be held in Amsterdam on 15 May 1987.

In 1986, up to 22 August the Conference Committee approved: 10 EPS organized conferences, 24 sponsored conferences, 11 schools (2 EPS organized) and 4 study conferences.

The IUCr representative, M. Nardelli, attended also, as invited guest, the meeting of the Condensed Matter Division of EPS held in Pisa on 5 December 1986. During the meeting he had the opportunity of illustrating the general organization of the Union and its policy in giving sponsorship and financial support for meetings. To point out the interdisciplinary character of crystallography and the fields IUCr is interested in, the topics covered at the XIV IUCr Congress in Perth were considered.

*International Organization for Crystal Growth (IOCG)*

According to its Statutes, the main activities of the IOCG are the organization of an international school and an

international conference per triennium. Both events took place in 1986, hosted by the British Association for Crystal Growth (BACG).

The Sixth International Summer School on Crystal Growth (ISSCG-6) was held in Edinburgh, Scotland, 5–11 July 1986, and was attended by some 120 delegates.

The Eighth International Conference on Crystal Growth (ICCG-8) immediately followed in York, England, 13–18 July, and was attended by some 530 delegates. The proceedings of ICCG-8 have already been published as a single issue of *J. Cryst. Growth* (1987), Vol. 79.

During the IOCG Executive Committee Meeting and General Assembly at ICCG-8, a number of important decisions were made, among which it was agreed:

- (a) to publish an international newsletter, to be incorporated in *J. Cryst. Growth*; the editing work was taken care of by B. Cockayne, RSRE, Malvern, England;
- (b) to award two prizes for the best papers on crystal growth, to be distributed at each future ICCG;
- (c) to hold ICCG-9 and ISSCG-7 in Japan in 1989; the organization of the two events will be undertaken by the JACG (Japanese Association for Crystal Growth).

Finally, the composition of the new IOCG council, as approved in York after postal ballot, for the triennium 1986–89, is as follows: R. Kern, France, President; R. F. Sekerka, USA, Co-Vice-President; B. Cockayne, UK, Co-Vice-President; M. Schieber, Israel, Secretary; E. Kaldis, Switzerland, Treasurer; R. A. Laudise, USA, Past President, *ex-officio* member; F. Ainger, UK, Past Chairman ICCG, *ex-officio* member; K. W. Benz, FRG, member; J. Giling, The Netherlands, member; H. Komatsu, Japan, member; A. Chernov, USSR, member; D. T. J. Hurle, UK, IOCG representative to IUCr, *ex-officio* member; C. Paorici, Italy, IUCr representative to IOCG, *ex-officio* member.

#### *European Crystallographic Committee*

During the Tenth European Crystallographic Meeting in Wrocław, Poland, a meeting of the European Crystallographic Committee was held on 8 August 1986. A report on the attendance and organization of ECM-10 was given by the organizers and the organization of ECM-11 (Wien, Austria, 29 August–2 September 1988) was discussed.

The proposal to hold ECM-12 in Moscow at the beginning or the end of August 1989 has been accepted.

Three invitations for ECM-13 (1991) were received: Utrecht (The Netherlands), Cambridge (England) and Ljubljana (Yugoslavia). The place accepted was Ljubljana.

As guide lines for the elections of the ECC officers for 1987–1990, the principles that west and east Europe must be equally represented and that all three officers (President, Vice-President, Secretary) should not to be changed at the same time have been approved.

Travel facilities for European crystallographers to attend the XIV IUCr congress at Perth were widely discussed.

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

The 21st General Assembly of ICSU took place 14–19 September 1986 in Berne, Switzerland. More than 250 scientists from 55 countries participated. A new programme entitled International Geosphere–Biosphere Programme: A Study of Global Change was established. It concerns a multi-disciplinary long-range study of the environment of the Earth and the changes that are taking place in order to

make an assessment concerning the future of the Earth over the next 100 years and how the changes may affect the future of human and other life. The General Assembly formed a Scientific Committee on Biotechnology to coordinate ICSU's activities in this area in view of the rapid developments in many countries of the world. Other topics of major concern were toxic waste disposal, the free circulation of scientists and the effects of nuclear war. An extensive study of the latter topic had been carried out by ICSU's Scientific Committee on Problems of the Environment. During the Assembly an open Symposium on the Environmental Consequences of Nuclear War (ENUWAR) was held to present the results of the study. Not only were direct effects from the blast taken into consideration, but items such as climatic and biological effects, societal disruptions, food supplies, communications, long-range toxic levels and alterations in the atmosphere were also studied. The report concludes, '... as representatives of the world scientific community drawn together in this study, we conclude that many of the serious global environmental effects are sufficiently probable to require widespread concern. Because of the possibility of a tragedy of an unprecedented dimension, any disposition to minimize or ignore the widespread environmental effects of a nuclear war would be a fundamental disservice to the future of global civilization.' The General Assembly voted to disseminate the findings to a wide audience including decision makers 'to increase awareness of the catastrophic effects on humanity of a nuclear war'.

#### **Finances**

The audited accounts for the year 1986 are given at the end of this Report. For comparison, the figures for 1985 are provided in italics. The accounts are presented in Swiss Francs.

The Unesco rates of exchange, as issued by the ICSU Secretariat, have been used in the preparation of these accounts. As a consequence of the many fluctuations in exchange rates during the year, the following procedure has been adopted for the accounts. Assets and liabilities in currencies other than Swiss Francs at 31 December 1986 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 699 164. This loss has been divided amongst the Fund Accounts in direct proportion to the balances on these accounts at 31 December 1986.

It should be noted that this loss is not a real loss of money, but only a loss on paper resulting from the accounts being expressed in Swiss Francs. For example, if they had been expressed in US Dollars or in Sterling there would have been a gain.

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 7 616, 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 1986 the Union held investments of SwFr 275 000, £300 000, US \$475 000 and ECU 100 000 in bonds.

The total of SwFr 1 902 871 with the banks at the end of the year was represented by Dfl 652 101, US \$1 and ECU 38 277 with the Amsterdam-Rotterdam Bank, US \$35 530 with the National Westminster Bank USA, US \$298 268 with Merrill Lynch, £259 535 with the National Westminster Bank and SwFr 165 522 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, excluding stocks of unsold publications but including the loss of SwFr 699 164 resulting from fluctuations in rates of exchange, have increased during the year, from SwFr 3 630 368 to SwFr 3 807 899.

One new fund account, the Ewald Fund, was established in 1986, with the receipt of a bequest and a donation from the Ewald family. The fund was augmented by the transfer of SwFr 83 595 from the General Fund. Transfers of SwFr 50 000 and SwFr 100 000 were made to the Publications and Journals Development Fund from the General Fund and the *Acta Crystallographica* Fund respectively, whilst identical transfers were also made to the Research and Education Fund.

The General Fund account shows a surplus of SwFr 216 674, before the transfer of SwFr 183 595 to the fund accounts as detailed above, as compared with a surplus of SwFr 283 742 in 1985. The administrative expenses were SwFr 192 458 in 1986 as compared with SwFr 170 867 in 1985. Of this amount, SwFr 58 465 was charged to the publications of the Union. SwFr 27 032 was spent on supporting scientific meetings, and SwFr 5 921 was required for travel expenses of Union representatives on other bodies. The Executive Committee Meeting cost SwFr 19 974 and the Finance Committee SwFr 6 035. The Union received SwFr 17 333 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 130 830. Interest on bank accounts and investments was SwFr 285 076.

The President's Fund account received SwFr 504 in donations during 1986, whilst a grant of SwFr 85 was paid from the fund.

The *Acta Crystallographica* account for 1986 shows a surplus of SwFr 497 089, before the transfer of SwFr 200 000 to other accounts, as compared with a surplus of SwFr 542 521 in 1985.

The subscription rates were maintained unchanged from 1985. Although more pages were published in 1986 than in 1985, the costs per page were less, when expressed in Swiss Francs, because of falls in the value of Sterling and the US Dollar as compared with the Swiss Franc.

The number of paid subscriptions to all sections of *Acta* decreased from 1 182 in 1985 to 1 149 in 1986, including 139 personal subscriptions in 1985 and 129 in 1986. There were also 227, 131 and 123 paid subscriptions to Section A, Section B and Section C, respectively, compared with 243, 128 and 128, respectively, in 1985. The cost of the technical editing office has been divided between the *Acta Crystallographica* and the *Journal of Applied Crystallography* accounts in percentages based on the number of

text pages published during the year, namely 86 and 14% respectively for 1986. The technical editing costs for *Acta Crystallographica* were SwFr 232 098 in 1986, excluding the costs of office refurbishment, as compared with SwFr 297 177 in 1985. The journal's accounts have also been charged with administrative expenses as in previous years and as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a surplus of SwFr 110 760, as compared with a surplus of SwFr 109 355 in 1985. The number of subscriptions decreased from 1 070 in 1985 to 1 050 in 1986, including 118 personal subscriptions in 1985 and 113 in 1986.

The *Structure Reports* account shows a surplus of SwFr 22 069 as compared with a deficit of SwFr 21 842 in 1985. Sales were higher in 1986, with both a B Series and an A Series volume being published as compared with only a B Series volume in 1985. Editorial expenses were lower, but the level of these expenses does fluctuate from year to year. Publishing and editorial expenses in 1986 were SwFr 38 811 and SwFr 86 670 respectively, as compared with SwFr 34 174 and SwFr 106 527 in 1985. The net income from sales was SwFr 147 550 in 1986 as compared with SwFr 118 859 in 1985.

The *International Tables* account shows a surplus of SwFr 31 276, as compared with a surplus of SwFr 52 312 in 1985. The only publication expense incurred in 1986 was SwFr 17 791 for a short-run reprint of Volume A, to keep the volume in print until a new edition is published in 1987. Editorial expenses were SwFr 16 632. The net income from sales of SwFr 65 699 derived mostly from the sale of 295 copies of Volume A.

The Book Fund includes the sales of the remaining publications of the Union. SwFr 295 was received from the sale of 22 copies of *Fifty Years of X-ray Diffraction*. SwFr 614 was received from the sale of 40 copies of *Symmetry Aspects of M. C. Escher's Periodic Drawings*, as well as SwFr 168 royalties for the Japanese edition of this book. SwFr 263 was received from the sale of 11 copies of Volume 1 and 10 copies of Volume 11 of *Early Papers on Diffraction of X-rays by Crystals*. SwFr 481 was received from the sale of 20 copies of *Fifty Years of Electron Diffraction*. The Seventh Edition of the *World Directory of Crystallographers* was published in 1986, at a cost of SwFr 24 602 and for which SwFr 22 994 was received from sales. Sales of the sundry publications yielded SwFr 35.

As usual, the *Molecular Structures and Dimensions* account shows no surplus, because this account was charged with a contribution (SwFr 6 893) towards the publication costs of Volume 15, the volume published in 1984. No other volume has been published since and hence the sales income remains very low, SwFr 7 613 as compared with SwFr 10 022 in 1985.

The income for the Publications and Journals Development Fund account and for the Research and Education Fund account came entirely from transfers from other fund accounts. The expenses for the former account relate to the technical editing of the journals. For the latter account the main expense was for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union.



### General Fund Account for the year ended 31 December 1986

	Swiss Francs		1985		1986		1985	
	1986	1985	1986	1985	1986	1985	1986	1985
Subscriptions to ICSU and ICSU bodies		5,184		5,645			17,333	32,565
Administration expenses:							—	12,749
General Secretary and Treasurer: honorarium and secretarial assistance	8,540		9,856				130,830	130,830
Audit and accountability charges	13,919		14,729				46,761	43,999
Legal and professional fees	1,257		2,699				238,315	308,212
Postage and sundries	2,139		695					
Travelling expenses	4,713		2,916					
Bank charges	1,279		1,246					
Executive Secretary's office: Salaries and expenses	134,678		138,137					
Office refurbishment	25,477							
Depreciation of office equipment	456		589		170,867			
	43,309						38,445	
	14,436						12,815	
	720						930	
	58,465						52,190	
							491,704	580,545
							580,545	580,545
<b>Fourteenth General Assembly and Congress:</b>								
Programme Committee		12,295						
Meeting of the Executive Committee		19,974		30,956				
Finance Committee expenses		6,035		11,065				
Travel expenses of IUCr Representatives on other bodies		5,921		1,157				
Commission expenses		4,201		8,673				
Sponsorship of meetings		27,032		65,352				
Donation to COSTED		1,930		2,090				
Preparation of a history of the Union		—		998				
Transfers to other Funds: Publications and Journals								
Development Fund		50,000		—				
Research and Education Fund		50,000		—				
Ewald Fund		83,595		—				
Excess of income over expenditure carried to balance sheet		33,079		283,742				
		491,704		580,545				
		491,704		580,545				



### President's Fund Account for the year ended 31 December 1986

	Swiss Francs	
	1986	1985
Grants	85	—
Excess of income over expenditure carried to balance sheet	419	1,252
	<u>504</u>	<u>1,252</u>
	1986	1985
Donations received	504	1,252
	<u>504</u>	<u>1,252</u>

### Acta Crystallographica Account for the year ended 31 December 1986

	Swiss Francs	
	1986	1985
Publication expenses:		
Printing and binding Volume 42 (1985 Volume 41)	403,869	377,472
Distribution and postage	68,461	66,730
Airfreight costs	25,606	26,436
	<u>497,936</u>	<u>470,638</u>
Printing Index to Volume 39	—	16,162
Printing Index to Volume 40	—	18,804
Printing Index to Volume 41	11,555	—
	<u>509,491</u>	<u>505,604</u>
Editorial expenses:		
Editorial honoraria	28,769	37,612
Secretarial assistance	13,138	10,351
Postage and sundries	17,130	29,578
Technical Editing:		
Salaries and expenses	221,195	283,715
Computer expenses	10,903	13,462
Office refurbishment	65,731	—
Depreciation of office equipment	2,925	2,155
	<u>359,791</u>	<u>376,873</u>
Administration expenses	43,309	38,445
Transfers to other Funds:		
Publications and Journals Development Fund	100,000	—
Research and Education Fund	100,000	—
	<u>297,089</u>	<u>542,521</u>
Excess of income over expenditure carried to balance sheet	1,409,680	1,463,443
	<u>1,409,680</u>	<u>1,463,443</u>
	1986	1985
Subscriptions to Volume 42 (1985 Volume 41)	1,439,019	1,480,594
Sale of back numbers and single copies	33,934	46,958
Airfreight charged to subscribers	39,814	41,294
Royalties and copyright fees	—	2,179
	<u>1,512,767</u>	<u>1,571,025</u>
Less Publisher's commission on sales	103,087	107,582
	<u>1,409,680</u>	<u>1,463,443</u>





## Book Fund Account for the year ended 31 December 1986

	Swiss Francs	
	1986	1985
Publication Expenses:		
<i>World Directory of Crystallographers</i> ,		
7th Edition	21,222	
Printing and distribution	3,380	
Honorarium	24,602	—
<i>Excess of income over expenditure</i>	248	4,218
<i>carried to balance sheet</i>		
	<u>24,850</u>	<u>4,218</u>
	<u>24,850</u>	<u>4,218</u>
Sale of copies, net of		
Publisher's commission on sales		
<i>Fifty Years of X-ray Diffraction</i>	295	356
<i>Escher Drawings</i>	614	706
<i>Early Papers</i>	263	588
<i>Fifty Years of Electron Diffraction</i>	481	1,955
<i>World Directory of Crystallographers</i> ,		
6th Edition	—	181
<i>World Directory of Crystallographers</i> ,		
7th Edition	22,994	—
Sundry Publications	35	45
Royalties		
<i>Escher Drawings</i>	168	387
	<u>24,850</u>	<u>4,218</u>
	<u>24,850</u>	<u>4,218</u>

## Molecular Structures and Dimensions Account for the year ended 31 December 1986

	Swiss Francs	
	1986	1985
Publication expenses:		
Salaries	6,893	9,092
Administration expenses	720	930
<i>Excess of income over expenditure</i>	10,665	13,803
<i>for the year:</i>		
University of Cambridge	—	—
IUCr carried to balance sheet	—	—
	<u>3,052</u>	<u>3,781</u>
	<u>7,613</u>	<u>10,022</u>
	<u>7,613</u>	<u>10,022</u>
Sale of copies		
Volume 15	2,229	6,725
Earlier volumes	8,436	7,078
	<u>10,665</u>	<u>13,803</u>
<i>Less Publisher's commission</i>		
<i>on sales</i>	3,052	3,781
	<u>7,613</u>	<u>10,022</u>
	<u>7,613</u>	<u>10,022</u>



**Statement of Source and Application of Funds**  
**Year ended 31 December 1986**

	Swiss Francs	
	1986	1985
Source of funds		
Excess of income over expenditure for the year	876,695	971,558
Fluctuations in rates of exchange	-699,164	-148,057
	177,531	823,501
Adjustment for items not involving the movement of funds:		
Depreciation	3,843	3,499
Fluctuations in rates of exchange on office equipment and investments	87,812	-7,367
	269,186	819,633
Total generated from operations	269,186	819,633
Decrease in debtors and accrued income (including subscriptions)	13,925	—
Increase in creditors, accrued charges and income received in advance	27,966	9,540
	311,077	829,173
Application of funds		
Increase in debtors and accrued income (including subscriptions)	—	-103,888
Purchase of office equipment	-7,352	-1,515
Purchase of investments	-1,246,521	-191,388
	-942,796	532,382
Movement in net liquid funds	-942,796	532,382

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

### Notes to the Financial Statements

#### 1. Accounting Policies

*(a) Accounting convention*

The financial statements are prepared under the historical cost convention.

*(b) Rates of exchange*

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

Assets and liabilities held in currencies other than Swiss Francs at the balance sheet date are translated into Swiss Francs at the rates operative on that date.

In each of the income and expenditure accounts, transactions in currencies other than Swiss Francs are translated by applying the rates of exchange appropriate to the individual dates of the transactions.

Profits and losses arising from the fluctuations in rates of exchange during the year are divided between the fund accounts with credit balances in direct proportion to those balances at the closing balance sheet date.

*(c) Publication costs*

Publication, editorial and administrative expenses of publications are charged in the appropriate income and expenditure account as and when incurred.

*(d) Stocks of unsold copies of Union publications*

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

*(e) Expenditure on premises*

Expenditure on renovation and refurbishing is charged against the appropriate income and expenditure accounts in the year in which it is incurred.

*(f) Depreciation*

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

(ii) Office computer equipment is fully depreciated in the year of purchase.

#### 2. Rates of Exchange

The assets of the Union are recorded in the financial statements in Swiss Francs but are held in currencies which are considered to be appropriate to the Union's requirements. It therefore follows that the effect of fluctuations in exchange rates will normally only arise at the year end when the figures are reported in Swiss Francs.

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

	1986	1985
Netherlands Guilders	1.3393	1.3397
Danish Crowns	4.4643	4.3541
Pounds Sterling	0.4167	0.3225
US Dollars	0.5952	0.4785
European Currency Unit (ECU)	0.5730	0.5225

The total assets of the Union at 1 January 1986 (SwFr 3 630 368) would have had the value of US \$1 737 131 or £1 170 794 if expressed in those currencies. At 31 December 1986 these assets (SwFr 3 807 899) would have had the value of US \$2 266 461 or £1 586 752 respectively, being an increase of US \$529 330 or £415 958 from the previous year.

**3. Taxation**

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

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

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

**4. Investments**

	Swiss Francs				Holding at cost 31 December 1986
	Holding at cost 1 January 1986	Additions during the year	Disposals during the year	Fluctuations in rates of exchange	
Deposited for safe custody with the Union Bank of Switzerland Sw Fr 25,000 (4.5% Swiss Federal 1983-1995)	24,615	—	—	—	24,615
Sw Fr 250,000 (4.75% Swiss Confederation 1984-1994)	—	258,748	—	—	258,748
Deposited for safe custody with National Westminster Bank PLC, Manchester £100,000 (10.5% Treasury Stock 1989)	305,449	—	—	-69,050	236,399
Deposited for safe custody with Amsterdam-Rotterdam Bank NV ECU 100,000 (9 1/2% New Zealand 1985-1992)	191,388	—	—	-16,868	174,520
Held by Rothschild Asset Management Limited £200,000 (Old Court International Reserves Limited)	—	479,962	—	—	479,962
Held by Merrill Lynch (Corporate Government Securities)					
US \$120,000 TIGR.SER15-89RG	—	170,612	—	—	170,612
US \$200,000 TIGR.SER15-98RG	—	134,225	—	—	134,225
US \$55,000 TIGR.SER18-88RG	—	83,853	—	—	83,853
US \$50,000 TIGR.SER18-98RG (Certificates of Deposit)	—	33,560	—	—	33,560
US \$50,000 C.D. Goldome	—	85,561	—	—	85,561
	<u>521,452</u>	<u>1,246,521</u>	<u>—</u>	<u>-85,918</u>	<u>1,682,055</u>

Investments are noted in the balance sheet at their market value at 31 December 1986. The difference between cost and market value has been shown as an adjustment in order that the investments can be stated at cost. This prevents the fluctuations in value from influencing the General Fund.

## Book Reviews

*Works intended for notice in this column should be sent direct to the Book-Review Editor (R. O. Gould, Department of Chemistry, University of Edinburgh, West Mains Road, Edinburgh EH9 3JJ, Scotland). As far as practicable books will be reviewed in a country different from that of publication.*

*Acta Cryst.* (1988). **A44**, 104

**Phonons: theory and experiments II.** By P. BRÜESCH. Pp. xii + 278. Berlin: Springer-Verlag, 1986. Price DM 80.00.

This book deals with a variety of experimental techniques that provide information on phonon properties of solids. There are major chapters on infrared spectroscopy, Raman and Brillouin scattering, X-ray and neutron scattering methods, brief descriptions of ultrasonic techniques, inelastic electron tunneling, point contact spectroscopy, and an even briefer survey of surface phonons and their measurement. On the whole, these subjects are treated competently and reasonably completely, and the book provides a useful index to the literature, so that a newcomer to any particular subject area can find other relevant material if he wishes. (However, many references are to Part I of this series, published in 1982, rather than to the original papers directly.)

The level of treatment and the amount of technical detail provided for each subject are not very consistent; some parts of a given subject are treated very thoroughly indeed while other parts are glossed over superficially. I doubt that this book will have a strong appeal to the experts in any field, and the newcomer will certainly need to consult previously published textbooks or review articles to supplement what Brüesch (or Bühler, in the case of chapter 6) has written. I had difficulty deciding who is the intended reader of this book, a comment that could also be made of Part I. The most successful sections of the book (e.g. §§ 7.2, 7.3, 7.4) are those dealing briefly and succinctly with what the author calls 'Other Techniques'.

On a more trivial level, the number of typographical errors was disturbingly large, and the quality of the English left something to be desired. It would have been worthwhile having the proofs read carefully by a competent native English speaker. There are also a few relatively unimportant

factual errors: reference 2.80 is incorrectly cited and is in any case totally irrelevant in the context of its citation;  $\sigma_{inc}$  for H is almost *two* orders of magnitude larger than for other elements (p. 171). A certain amount of unnecessary repetition occurs because of the book's organization: thus much of chapter 4 on Brillouin spectroscopy simply repeats what has already appeared in chapter 3 (Raman scattering). These minor annoyances did little to enhance my enthusiasm for the book as a whole. This is a book that major scientific libraries should stock, but I cannot really recommend individuals to buy it.

GERALD DOLLING

*Chalk River Nuclear Laboratories  
Chalk River  
Ontario  
Canada K0J 1J0*

*Acta Cryst.* (1988). **A44**, 104

### Books Received

*The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.*

**Carrier scattering in metals and semiconductors.** By V. F. GANTMAKHER and Y. B. LEVINSON. Pp. xviii + 459. Amsterdam: North-Holland, 1987. Price Dfl 280.00.

**Atomic physics, 10** (Proceedings of the international conference held in Tokyo, August 1986). Edited by H. NARUMI and I. SHIMAMURA. Pp. xi + 463. Amsterdam: North-Holland, 1987. Price Dfl 150.00.