

Table 3. (cont.)

Reflection	$\sin \theta$	$A_{\text{calc.}}$	$B_{\text{calc.}}$	$ F_{\text{calc.}} $	$F_{\text{obs.}}$	Reflection	$\sin \theta$	$A_{\text{calc.}}$	$B_{\text{calc.}}$	$ F_{\text{calc.}} $	$F_{\text{obs.}}$
1.11...2	0.675	12.49	-18.97	23	14	2.13...1	0.790	18.27	-10.45	21	20
1.11...5	0.835	-12.01	-3.79	13	17	2.13...4	0.895	-8.02	18.88	21	22
2.11...3	0.745	2.76	-12.53	13	17	3.13...2	0.845	-21.18	22.15	31	30
2.11...6	0.930	-5.35	25.80	27	22	4.13...3	0.915	2.02	-18.95	19	14
3.11...1	0.715	18.95	15.60	25	20	5.13...1	0.900	21.56	3.77	22	10
3.11...4	0.830	-8.82	5.64	10	w	6.13...2	0.960	-14.01	8.90	17	24
4.11...2	0.780	-2.23	17.00	17	20						
5.11...3	0.850	-20.82	19.74	29	22	0.14...1	0.785	12.95	1.36	13	17
6.11...1	0.835	-29.71	5.72	30	24	0.14...4	0.890	-5.94	-30.61	31	17
6.11...4	0.935	1.04	-12.33	12	32	1.14...2	0.835	0.43	-15.27	15	10
7.11...2	0.900	-10.00	14.36	17	10	1.14...5	0.970	-13.91	16.52	22	17
8.11...3	0.970	11.73	-6.37	13	w	2.14...3	0.900	-5.44	-1.16	6	10
9.11...1	0.970	-14.21	-1.95	14	10	3.14...1	0.880	30.30	23.08	38	20
						3.14...4	0.970	-9.99	-4.71	11	w
0.12...3	0.740	-0.51	4.21	4	w	4.14...2	0.935	7.98	7.37	11	10
0.12...6	0.925	-14.07	-25.69	29	14						
1.12...1	0.705	1.00	-4.15	4	w	0.15...3	0.895	-23.69	0.76	24	w
1.12...4	0.815	5.93	2.51	6	w	1.15...1	0.870	-30.22	-15.68	34	17
2.12...2	0.760	-19.12	-7.24	21	22	1.15...4	0.965	12.56	-15.67	20	30
2.12...5	0.905	25.80	7.01	27	w	2.15...2	0.920	-7.75	-10.73	13	14
3.12...3	0.830	12.34	8.63	15	w	4.15...1	0.970	-14.47	8.20	17	14
4.12...1	0.810	-35.04	-0.90	35	24						
4.12...4	0.910	25.51	-4.89	26	39	0.16...2	0.915	1.12	3.51	4	w
5.12...2	0.870	-22.10	6.16	23	w	1.16...3	0.970	-7.35	7.11	10	10
6.12...3	0.940	-19.63	2.11	20	17	2.16...1	0.955	11.04	1.45	11	14
7.12...1	0.930	10.32	13.76	17	14						
0.13...2	0.755	-22.27	22.74	32	20						
0.13...5	0.900	2.51	-0.67	3	24						
1.13...3	0.815	-18.25	-22.33	29	14						

Remark: 21.21...0 was observed as a strong reflection on a film exposed to  $\text{MoK}\alpha$  radiation.

Maximum possible value for  $F_{21,21,0} = 63$ ,  $F_{\text{calc.}} = 45$ .

## International Union of Crystallography

### Report of Executive Committee for 1949

#### Introduction

During 1949 the Union was engaged in carrying out the programme of activities initiated at the First General Assembly at Harvard University in 1948, and in making preliminary arrangements for the Second General Assembly to be held at Stockholm in 1951. The majority of these

activities were conducted under the auspices of the several Commissions and are reported in detail below. The number of Adhering Bodies increased to eleven, and four other countries gave notice of adhesion as from 1 January 1950. Details of these fifteen countries are given in Table 1.

Table 1. *Adhering Bodies*

Country	Group*	Secretary of National Committee
Australia	I	R. I. GARROD, Defence Research Laboratories, Private Bag No. 4, P.O. Ascot Vale W. 2, Victoria
Belgium	III	R. VAN TASSEL, Conservateur au Musée d'Histoire Naturelle, Brussels
Canada	IV	W. H. BARNES, Division of Physics, National Research Council, Ottawa
Czechoslovakia	I	The Secretary, Czechoslovak National Research Council, Opletalova 19, Prague II
Denmark	I	A. TOVBORG JENSEN, Den Kgl. Veterinær- og Landbohøjskoles kemiske Laboratorium, Copenhagen 5
France	VII	V. LUZZATI, Laboratoire Central des Services Chimiques de l'État, 12 quai Henri IV, Paris 4
India	I	The Secretary to the Government of India, Department of Scientific Research, North Block, Central Secretariat, New Delhi
Japan	I	T. ITO, National Committee for Crystallography, Science Council of Japan, Ueno Park, Tokyo
Netherlands	IV	E. H. WIEBENGA, Bloemsingel 10, Groningen
Norway	I	I. ORTEDAL, Mineralogisk Institutt, Blindern, Oslo
South Africa	I	The Officer-in-Charge, Liaison Division, South African Council for Scientific and Industrial Research, P.O. Box 395, Pretoria
Spain	IV	M. A. BERGER, Instituto 'Alonso de Santa Cruz', Serrano 119, Madrid
Switzerland	I	M. VUAGNAT, Muséum d'Histoire Naturelle, Geneva
United Kingdom	VIII	The Secretary of the British National Committee for Crystallography, The Royal Society, Burlington House, London W. 1
United States of America	VIII	R. W. G. WYCKOFF, Laboratory of Physical Biology, National Institute of Health, Bethesda 14, Maryland

\* See Statutes 8 and 10 (*Acta Cryst.* (1948), 1, 275).

### Work of the Commissions

#### *Commission on Acta Crystallographica*

Publication of *Acta Crystallographica* has continued throughout 1949, and Vol. 2 was completed with the appearance of Part 6 in December. An analysis of the contents of the first two volumes is given in Table 2. This table shows that the international character of the journal is well established, and that there is a steady increase in the rate at which material is submitted for publication. The same trend is shown by the material already in hand for Vol. 3.

The number of subscribers at the end of 1949 was about 850. This figure compares satisfactorily with the circulation of other comparable scientific journals of a specialized character, and there is no doubt that *Acta Crystallographica* is to be found in most libraries of standing. A detailed analysis of the subscribers reveals, however, that the number of personal subscribers is disappointingly small. The Executive Committee deliberately set the subscription price at a very moderate level with the object of making the journal widely available to individual workers, but it is unfortunately clear that relatively few private crystallographers have taken advantage of this opportunity. At present the income from subscriptions is little more than half the cost of producing the journal, the balance being met by the very generous subventions received from UNESCO and from British and American industrial firms and other organizations. It cannot be expected that such support will continue indefinitely, and the journal must soon be established on a self-supporting basis. The Executive Committee would be very reluctant to propose any increase in the subscription price, thereby confining the distribution of the journal to the larger libraries and making it less widely available. Unless, however, there is a considerable increase in the number of subscribers in the next few years a substantial increase in the subscription rate will unfortunately be unavoidable. Crystallographers will be rendering the Union a valuable service by making widely known the circumstances under which the journal is distributed at its present low price, and by taking all possible steps to increase the number of subscribers so that this price may be maintained.

#### *Commission on International Tables for X-ray Crystallography*

The preparation of *International Tables for X-ray Crystallography* has proceeded throughout the year. The new edition of these *Tables* will be a very considerable expansion of the original edition, and will contain much additional material demanded by recent advances in the

technique of crystal-structure analysis. At the same time some of the formal material in the earlier edition will be omitted, experience having proved that it was of limited value in experimental research. The exact contents of the *Tables*, which will run to three volumes, have been agreed after consultation with crystallographers throughout the world. The manuscript of Vol. 1 (*Theory of Crystallographic Groups*) is now complete, and the Executive Committee has accepted a recommendation of the Commission that publication should be entrusted to the Kynoch Press (U.K.). It is hoped that this volume will appear during 1951. Thanks to further generous support from UNESCO all interests in the *Tables* will be retained by the Union, and it is hoped that on this account it will be possible for them to be sold in Adhering Countries at a very favourable price.

#### *Commission on Structure Reports*

Work on the preparation of *Structure Reports* continued throughout the year, and the manuscript of the first volume, covering the years 1947-8, should be ready early in 1950. The Reports will generally resemble the former German *Strukturbericht*, but it is intended that they should be more constructively critical in character. This involves considerably more work for the Editors, but it is believed that it will greatly enhance the value of the final work. Preliminary consultations have been held with a number of possible publishers, but no final decision on the mechanism of publication has yet been reached. Expenses of preparing the *Reports* have been met by generous subventions from UNESCO and from British and American industrial firms and other organizations.

#### *Commission on Crystallographic Data*

The Commission met at Ithaca in June 1949; three of the four members of the Commission were present. A proposal to sponsor the organization of national committees to promote the collection of crystallographic data and to check and edit these in a form suitable for publication, possibly in *Acta Crystallographica*, was discussed. This proposal has been developed further by correspondence and is now ready for submission to the Executive Committee of the Union and to Adhering Bodies.

The *X-ray Diffraction Index*, published by the Joint Committee of the American Society for X-Ray and Electron Diffraction, the British Institute of Physics and the American Society for Testing Materials, in which three members of the Commission have taken an active part, has a second supplement listing 1300 compounds ready for publication. The original publication and first

Table 2. *Analysis of Volumes 1 and 2 of Acta Crystallographica*

	Vol. 1, 1948	Vol. 2, 1949
No. of pages	348	425
No. of articles in English	55	68
No. of articles in French	4	4
No. of articles in German	2	8
Total no. of articles	61	80
No. of Short Communications in English	13	20
No. of Short Communications in French	1	—
No. of Short Communications in German	1	—
Total no. of Short Communications	15	20
No. of Book Reviews	9	4
No. of countries from which authors are drawn	13	11

supplement have been revised and printed in a new format. This card index, now listing 4000 compounds, should be available in 1950.

#### *Commission on Crystallographic Nomenclature*

The Commission has agreed on a number of matters of procedure and has decided that it should not in general take the initiative in making nomenclature proposals; rather will it act in an advisory capacity in connexion with problems submitted to it. The Commission has, however, worked in close co-operation with the editors of the *International Tables for X-ray Crystallography* and has made recommendations on a number of matters raised by these editors. One proposal, that monoclinic crystals should be orientated with the symmetry axis in the [001] direction, was considered by the Commission to be likely to have far-reaching implications. The Commission has, therefore, sought the opinion of all members of the American Society for X-ray and Electron Diffraction and of the British X-ray Analysis Group before making recommendations on this point. Other crystallographers having views on this matter are also invited to express their opinions to the Chairman of the Commission.

#### *Commission on Crystallographic Apparatus*

Nothing to report.

#### *Joint Commission on Physics Abstracting*

The Union was represented by A. J. C. WILSON (U.K.) at an International Conference on Science Abstracting held in Paris under the auspices of UNESCO in June 1949. Subsequently he was nominated by the Executive Committee as the representative of the Union on a new Joint Commission on Physics Abstracting established by the International Council of Scientific Unions. This Joint Commission, on which other interested Unions are also represented, met in Paris in December 1949 and will report its proceedings in due course. Meanwhile, the principal recommendations have been brought to the notice of the editors of *Acta Crystallographica* and *Structure Reports*.

#### *Commission on Macromolecules of the International Union of Pure and Applied Chemistry*

This Commission, on which the International Union of Crystallography is represented, is engaged in discussions on the nomenclature of macromolecules, and met to consider this matter at Amsterdam in 1949. The outcome of these discussions will in due course be published as recommendations; meanwhile points on which agreement has already been reached have been brought informally to the notice of the editors of *Structure Reports*.

### International Council of Scientific Unions

The Union was represented at a meeting of the Executive Committee and at the General Assembly of the International Council of Scientific Unions, held in Copenhagen in September 1949, by R. C. EVANS and P. P. EWALD. At these meetings new statutes of the International Council of Scientific Unions were adopted, among the provisions of which is the classification of Unions as 'General' and 'Specialized'; the International Union of Crystallography has been classified as a Specialized Union

by the General Assembly. Among other matters discussed at the meetings was the policy to be adopted in admitting new Unions. It was decided to refer this question to a special Policy Committee, to report to the 1950 meeting of the Executive Committee, and to admit no further Unions until a general policy has been agreed. The appointment of R. FRASER as International Council of Scientific Unions Liaison Officer with UNESCO was confirmed, and it is appropriate here to record the very warm appreciation of the Union for the most valuable service which he renders in this capacity.

### Second General Assembly and International Congress

The Executive Committee has accepted a kind invitation from the Swedish National Committee for Crystallography to hold the Second General Assembly and International Congress of the Union in Stockholm from 27 June to 3 July 1951. These dates have been chosen in consultation with the Swedish National Committee and with the National Committees of all the Adhering Bodies. A local Committee has been established in Stockholm under the chairmanship of A. WESTGREN, Vice-President of the Union.

### Fair Copying Declaration

The Executive Committee has decided that the Union shall subscribe to the Royal Society's Declaration on Fair Copying, which reads as follows:

We will regard it as fair dealing for the purpose of private study or research when a non-profit-making organization, such as a library, archives office, museum or information service, owning or handling scientific or technical periodicals published by us, makes and delivers a *single* reproduction of a part of an issue thereof to a person or his agent representing in writing that he desires such reproduction in lieu of a loan or manual transcription and that he requires it solely for the purpose of private study, research, criticism or review, and that he undertakes not to sell or reproduce for publication the copy supplied, provided:

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We reserve the right to withdraw this declaration.

### Finances

The audited accounts of the Union for the year 1949 have already been published (*Acta Cryst.* (1950), 3, 323). These

accounts emphasize how very deeply the Union is indebted to UNESCO for the most generous support of its various activities, amounting to over £4900 in 1949 alone and totalling about £8900 since the foundation of the Union. The Union is also deeply indebted to British industrial firms, Research Associations and other bodies for subventions totalling over £5300 and to American industrial organizations for donations amounting to about £900. These very substantial contributions to the work of the Union have enabled its major activities to proceed free from financial embarrassment and have made it possible for the Union to retain full control of the various publications which it sponsors.

Income from Adhering Bodies in 1949 amounted to £959. Administrative expenses are very small, and the greater part of this income will be available for the general work of the Union, including the expenses of the Second General Assembly.

### Membership of Committees, Commissions and other bodies

The membership of Committees, Commissions and other bodies on 31 December 1949 was as follows:

#### *Executive Committee*

- President:* SIR LAWRENCE BRAGG (U.K.)  
*Vice Presidents:* A. WESTGREN (Sweden)  
 R. W. G. WYCKOFF (U.S.A.)  
*General Secretary:* R. C. EVANS, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England  
*Editor:* P. P. EWALD (U.S.A.)  
*Other Members:* M. J. BUEGER (U.S.A.)  
 A. L. PATTERSON (U.S.A.)  
 J. WYART (France)

#### *Acta Crystallographica Advisory Board*

- SIR LAWRENCE BRAGG (U.K.)  
 M. VON LAUE (Germany)  
 C. MAUGUIN (France)  
 P. NIGGLI (Switzerland)  
 L. PAULING (U.S.A.)  
 R. W. G. WYCKOFF (U.S.A.)

#### *Commission on Acta Crystallographica*

- Chairman:* P. P. EWALD, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.  
*Other Members:* R. C. EVANS (U.K.)  
 I. FANKUCHEN (U.S.A.)  
 J. WYART (France)

#### *Commission on Structure Reports*

- Chairman:* A. J. C. WILSON, Physics Department, University College, Cardiff, Wales  
*Other members:* C. S. BARRETT (U.S.A.)  
 J. D. BERNAL (U.K.)  
 P. P. EWALD (U.S.A.)  
 J. M. ROBERTSON (U.K.)  
 J. WYART (France)  
 R. W. G. WYCKOFF (U.S.A.)

#### *Commission on International Tables*

- Chairman:* K. LONSDALE, Chemistry Department, University College, London, W.C. 1, England  
*Other members:* M. J. BUEGER (U.S.A.)  
 N. F. M. HENRY (U.K.)  
 C. H. MACGILLAVRY (Netherlands)  
 J. S. KASPER (U.S.A.)

#### *Commission on Crystallographic Apparatus*

- Chairman:* I. FANKUCHEN, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.  
*Other members:* W. H. BARNES (Canada)  
 M. J. BUEGER (U.S.A.)  
 E. G. COX (U.K.)  
 H. P. ROOSKBY (U.K.)

#### *Commission on Crystallographic Data*

- Chairman:* F. W. MATTHEWS, Canadian Industries Ltd., McMasterville, Quebec, Canada  
*Other members:* D. HODGKIN (U.K.)  
 H. W. RINN (U.S.A.)  
 A. J. C. WILSON (U.K.)

#### *Commission on Crystallographic Nomenclature*

- Chairman:* W. L. BOND, Bell Telephone Laboratories Inc., Murray Hill Laboratory, Murray Hill, New Jersey, U.S.A.  
*Other members:* F. A. BANNISTER (U.K.)  
 H. BRASSEUR (Belgium)  
 J. D. H. DONNAY (U.S.A.)  
 W. DE KEYSER (Belgium)  
 K. LONSDALE (U.K.)  
 M. A. PEACOCK (Canada)

#### *Joint Commission on Physics Abstracting of the International Council of Scientific Unions*

- Representative:* A. J. C. WILSON, Physics Department, University College, Cardiff, Wales

#### *Commission on Macromolecules of the International Union of Pure and Applied Chemistry*

- Representative:* C. W. BUNN, I.C.I. (Plastics) Ltd., Black Fan Road, Welwyn Garden City, Herts, England