

## International Union of Crystallography

### Report of Executive Committee for 1970

#### Personal Notes

In 1970 Soviet crystallography lost one of its most distinguished members. On 27 April, Professor Alexey Vasilyevich Shubnikov died at the age of 83. He was best known for his work on antisymmetry and was Director of the Institute of Crystallography from its foundation up to 1962. An obituary for Professor Shubnikov was published in the *Journal of Applied Crystallography* (*J. Appl. Cryst.* (1970) 3, 551).

On 9 October 1970 Dr Helmuth J. Goldschmidt died. His many publications included his recent book, *Interstitial Alloys* and the I.U.Cr. Bibliography on *High Temperature X-ray Diffraction Techniques*. His death was reported in the *Journal of Applied Crystallography* (*J. Appl. Cryst.* (1971) 4, 90).

#### Meetings

Four meetings were held in 1970 under the sponsorship or co-sponsorship of the Union. The Union co-sponsored the Bragg Symposium 1970, 1–3 April, London, the Third Sagamore Conference on Charge, Spin and Momentum Densities, 9–12 September, Aussois, France and the Second International Symposium on Organic Solid State Chemistry, 14–18 September, Rehovoth, Israel. The Second International Conference on Small-Angle X-ray Scattering, 26–29 August, Graz, Austria, was also sponsored by the Union.

The Executive Committee met in London, 31 March – 3 April, on the occasion of the Bragg Symposium mentioned above. Much business was transacted, the most important items being: (1) the resignation of G. Boom as General Secretary of the Union, the combination of the offices of General Secretary and Treasurer and the appointment of D. W. J. Cruickshank, formerly Treasurer, to this combined office; (2) plans for the Ninth Congress of Crystallography; (3) invitation for the Tenth Congress of Crystallography; (4) the incorporation of the Union; (5) the finances of the General Fund and the unit contribution; (6) sponsorship of meetings and the work of the Sub-committee on the Union Calendar; (7) the progress of the Union's journals and, in particular, a review of their financial standing and the implementation of economy measures; (8) the employment of a full-time worker on *Structure Reports*; (9) the Pilot Issue for the new and expanded edition of *International Tables*; (10) the publication of *Molecular Structures and Dimensions*, as a joint venture between the Crystallographic Data Centre, Cambridge, U.K. and the Union; (11) the Fourth Edition of the *World Directory of Crystallographers* and incidental publications of the Union; (12) the Joint Committee on Nomenclature of the I.U.Cr. and the International Mineralogical Association.

#### Executive Committee

Dr G. Boom has resigned as General Secretary of the Union, his resignation taking effect from the close of the meeting of the Executive Committee, held in London from 31 March to 3 April. On 31 March the Executive Committee accepted his resignation with regret and, after agreeing to recombine the offices of General Secretary and

Treasurer, they unanimously agreed to appoint Prof. D. W. J. Cruickshank (formerly Treasurer) to this joint office as from 3 April 1970.

#### Substitutions and Appointments

At his request, the Executive Committee accepted the resignation of D. P. Shoemaker at the end of 1970 as Chairman of the Commission on *International Tables*, and appointed N. F. M. Henry (formerly Chairman of the Commission, 1963–69) to serve in that capacity until the next meeting of the Executive Committee in 1971. (At this meeting, Dr Henry's appointment was extended until the close of the Ninth General Assembly.)

The Executive Committee approved the appointment of Clara B. Shoemaker as a Co-editor of *Structure Reports* (the appointment of G. Ferguson and C. H. L. Kennard was approved in 1969).

With the authorization of the Executive Committee, the Sub-committee on Staff, Establishment and Salaries appointed Miss J. M. Booth (now Mrs J. M. Hunter) as an Editorial Assistant to the Technical Editor, to start early in 1970. The other Editorial Assistant (Mrs M. E. Douglas) had been working part-time and she resigned later in the year. A secretary was also appointed for the Executive Secretary.

#### Publications

In 1970, Volume 26 of *Acta Crystallographica* was published; Section A totalled 702 pages and Section B 2138 pages, excluding indexes. Volume 3 of the *Journal of Applied Crystallography* was also published and contained 552 pages, excluding indexes.

No volumes of *Structure Reports* or further reprints of volumes of *International Tables* were published in the year under review.

The first two volumes of a new publication, *Molecular Structures and Dimensions*, were issued as a joint venture between the Crystallographic Data Centre, Cambridge, U.K. and the Union. Both volumes provide comprehensive coverage of the literature from 1935 to 1968 and there are about 500 additional references to 1969 publications. Entries are arranged in chemical classes with extensive cross-references and there are formula, metal and author indexes. Volume 1 deals with general organic crystal structures and Volume 2 with complexes, organo-metals and metalloids. It is hoped to issue further volumes annually with cumulative indexes.

The final bibliography in the series prepared under the auspices of the Commission on Crystallographic Apparatus, Bibliography 4: *Diffusion des Rayons X aux Petits Angles* by A. J. Renouprez, was distributed free to all subscribers to the Union's journals.

#### 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.

Table 1. *Adhering Bodies*

<i>Country</i>	<i>Category*</i>	<i>Adhering Body</i>	<i>Secretary of National Committee</i>
Argentina	I	Consejo Nacional de Investigaciones Científicas y Técnicas	L. BECKA, Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, Calle 115 y 49 CC 67 La Plata
Australia	III	Australian Academy of Science	J. DEEBLE, Australian Academy of Science, Gordon Street, Canberra City, A.C.T.
Austria	I	Österreichische Akademie der Wissenschaften	J. ZEMANN, Mineralogisches Institut der Universität, Dr Karl Lueger-Ring 1, 1010 Vienna
Belgium	II	Académie Royale des Sciences, des Lettres et des Beaux-Arts de Belgique	R. PANKOWSKI-FERN, Institut des Matériaux, U.L.B., 87 Avenue Adolphe Buyl, Brussels 5
Brazil	I	Conselho Nacional de Pesquisas	R. R. FRANCO, Conselho Nacional de Pesquisas, Avenida Marechal Camara 350, Rio de Janeiro, G.B.
B.R.D. (German Federal Republic)	IV	Sektion für Kristallkunde of the Deutsche Mineralogische Gesellschaft	TH. HAHN, Institut für Kristallographie der Technische Hochschule, Templergraben 55, Aachen
Canada	III	National Research Council	F. R. AHMED, Division of Biochemistry, National Research Council, Ottawa 7, Ontario
Chile	I	National Committee for Crystallography	I. GARAYCOCHEA-WITTKÉ, Laboratorio de Cristalografía, Universidad de Chile, Casilla 5487, Santiago
Czechoslovakia	I	Československá Akademie Věd	A. LÍNEK, Institute of Solid State Physics, Československá Akademie Věd, Cukrovarnická 10, Prague 6
D.D.R. (German Democratic Republic)	II	Deutsche Vereinigung für Kristallographie of the Deutsche Gesellschaft für Geologische Wissenschaften	H. NEELS, Institut für Mineralogie und Petrographie der Karl-Marx-Universität, Scharnhorststrasse 20, 703 Leipzig
Denmark	I	Akademiet for de Tekniske Videnskaber	INGRID K. LARSEN, The Royal Danish School of Pharmacy, Chemical Laboratory C, DK-2100 Copenhagen
Finland	I	Suomalainen Tiedeakatemia	M. AALTONEN, Wihuri Physical Laboratory, University of Turku, Turku
France	IV	Académie des Sciences (Institut de France)	A. AUTHIER, Association Française de Cristallographie, 9 Quai Saint Bernard, Tour 26, Paris 5e
Hungary	I	Magyar Tudományos Akadémia	L. ZSOLDOS, Institute for Experimental Physics, L. Eötvös University, Múzeum krt 6-8, Budapest VIII
India	I	Indian National Science Academy	R. SRINIVASAN, Centre of Advanced Study in Physics, University of Madras, Guindy Campus, Madras 25
Israel	I	Israel Crystallographic Society	D. RABINOVICH, Department of Chemistry, The Weizmann Institute of Science, Rehovoth
Italy	III	Consiglio Nazionale delle Ricerche	S. QUARENI, Istituto di Mineralogia dell'Università di Padova, Corso Garibaldi 9, 35100 Padova
Japan	IV	Science Council of Japan	Y. SAITO, The Institute for Solid State Physics, University of Tokyo, Roppongi 7, Minato-ku, Tokyo 106
Netherlands	III	Stichting voor Fundamenteel Onderzoek der Materie met Röntgen- en Elektronenstralen	D. FEIL, Chemical Physics Laboratory, Technische Hogeschool Twente, Postbus 217, Enschede
New Zealand	I	The Royal Society of New Zealand	P. P. WILLIAMS, Chemistry Division, D.S.I.R., Private Bag, Petone
Norway	I	Det Norske Videnskaps-Akademi	CHR. RØMMING, Department of Chemistry, University of Oslo, Blindern, Oslo 3
Pakistan	I	Pakistan Council of Scientific and Industrial Research	M. M. QURASHI, Pakistan Council of Scientific and Industrial Research, Off University Road, Karachi-32
Poland	I	Polska Akademia Nauk	L. ŁUKASZEWICZ, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, Plac Katedralny 1, Wrocław
South Africa	I	South African Council for Scientific and Industrial Research	G. GAFNER, National Physical Research Laboratory, P.O. Box 395, Pretoria
Spain	III	Consejo Superior de Investigaciones Científicas	S. GARCÍA-BLANCO, Instituto de Química Física 'Rocasolano', Consejo Superior de Investigaciones Científicas, Serrano 119, Madrid 6
Sweden	II	Kungliga Vetenskapsakademien	S. ABRAHAMSSON, Crystallography Group, University of Göteborg, Medicinarg. 9, S-400 33 Göteborg 33
Switzerland	II	Schweizerische Gesellschaft für Kristallographie	J. D. DUNITZ, Laboratorium für Organische Chemie der ETH, Universitätsstrasse 6/8, CH-8006 Zürich
U.K.	V	The Royal Society	D. C. MARTIN, The Royal Society, 6 Carlton House Terrace, London S.W.1
U.S.A.	V	National Academy of Sciences - National Research Council	W. L. KEHL, Gulf Research and Development Co., P.O. Drawer 2038, Pittsburgh, Pa. 15110

Table 1 (cont.)

Country	Category*	Adhering Body	Secretary of National Committee
U.S.S.R.	V	Akademija Nauk S.S.S.R.	V. I. SIMONOV, Institute of Crystallography, Leninsky Prospekt 59, Moscow B-333
Yugoslavia	I	Jugoslavenska Akademija Znanosti i Umjetnosti	B. KAMENAR, Laboratory of General and Inorganic Chemistry, Faculty of Science, Ul. Soc. Revolucije 8, Zagreb

\* 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.

The full list of memberships of National Committees is given in the *Report of Eighth General Assembly*.

### Work of the Commissions

#### Commission on Journals

During 1970 the Commission on Journals produced Volume 26 of *Acta Crystallographica* and Volume 3 of the *Journal of Applied Crystallography*. *Acta Crystallographica* contained 2840 pages (Section A 702 pages, Section B 2138 pages) excluding indexes and the *Journal of Applied Crystallography* 552 pages excluding indexes. Volume 3 of the *Journal of Applied Crystallography* is thus slightly larger than *Acta Crystallographica* was at the same age (484 + indexes), and has fully justified its existence. Several issues of *Acta Crystallographica* appeared some weeks later than their nominal dates of publication; the delays had a number of causes (sickness in the Technical Editor's office and at the printers, and some priority being given to the *Journal of Applied Crystallography*). The Executive Committee has authorized an addition to the Technical Editor's staff, which should make the publications of the Union less vulnerable.

An analysis of the contents of *Acta Crystallographica* for

the last six years and of the *Journal of Applied Crystallography* for the last three years is given in Table 2. It will be noticed that the number of pages in *Acta Crystallographica* B is about 500 less than in 1969. This is partly explained by the considerable reduction of backlog achieved during 1969, partly by the difficulties already mentioned in connexion with delays in publication, and partly by the efforts of the Co-editors to ensure brevity of expression and compression of tables. Nevertheless, there are some indications that the number of structural papers offered to *Acta Crystallographica* is decreasing. The number received during any month is naturally subject to statistical fluctuations, and the apparent decrease in the monthly rate is still within its standard deviation. If the trend is real there are two possible explanations: the economic situation of university and other laboratories has caused a decrease in the rate of production of structures, or alternatively the proportion of papers going to other journals is increasing. Statistics provided by the Cambridge Crystallographic Data Centre indicate that the latter phenomenon exists, but again the interpretation is not unambiguous: *Acta Crystallographica* might be losing old authors, or might merely be failing to attract the same proportion of new ones.

Table 2. Survey of the contents of the Union journals

		Acta Crystallographica				Short Communications		
		Articles						
Vol.	Year	Number of pages	Number	Number of pages	Average length	Number	Number of pages	Average length
18 & 19	1965	2172	330	1943	5·89	134	161	1·20
20 & 21*	1966	2273*	287	1751	6·10	118	159	1·35
22 & 23	1967	2094	315	1843	5·85	97	126	1·30
A24	1968	714	108	688	6·37	27	34	1·25
B24		1706	251	1687	6·72	89	89	1·44
A25	1969	1027	120	733	6·11	25	31	1·24
B25		2672	355	2547	7·17	99	149	1·81
A26	1970	702	112	676	6·04	32	53	1·66
B26		2138	301	2046	6·80	86	95	1·72

  

		Journal of Applied Crystallography				Short Communications		
		Articles						
Vol.	Year	Number of pages	Number	Number of pages	Average length	Number	Number of pages	Average length
1	1968	330	54	303	5·60	7	10	1·39
2	1969	312	50	272	5·44	12	21	1·75
3	1970	552	79	479	6·06	26	46	1·77

\* Volume 21 includes 304 pages of abstracts of papers presented at the Moscow Congress.

† Plus 24 pages of joint (A + B) index.

‡ For the first time the number of plate-pages was included in the number of pages per paper.

§ Volume A25 includes 295 pages of abstracts communicated to the Stony Brook Congress and 276 pages of papers and discussion at the Cambridge Intensity Meeting, 1968.

During the year the Commission has produced a revised set of 'Notes for Referees', and its 'Notes for Authors' are under active revision. Most of the revision has been completed, but discussions of some important points of principle are still proceeding.

#### Commission on Structure Reports

1970, being the year after a General Assembly of the Union, was a bad year for *Structure Reports*. Volume 27 (1962), which is exceedingly long, is now, it is hoped, in its last lot of proofs and the index is being prepared. Volume 29 (1964) is with the printers. Volumes 28 (1963) and 30 (1965) are each being held up by one co-author with one section. Co-editors are appointed and working on Volumes 31 to 34, with the exception of the Metals Sections of Volumes 33 and 34, and Volume 35 (1970) is being actively prepared.

A proposal for printing *Structure Reports* from Volume 31 (1966) onwards by photo-offset from typed manuscripts is being advanced separately.

#### Commission on International Tables

The additional Volume IV of the present edition continued in preparation. It was decided to put as much as possible of the material for the Pilot Issue of Symmetry Tables into a unified mathematical framework, so that there will be a dual approach, theoretical and practical. As different Parts are related, this has necessitated an extension of the time involved. It is now, however, expected that all six Parts will be issued in the course of 1971 and 1972.

The Chairman (D. P. Shoemaker) was compelled to resign owing to heavy responsibilities involved in a new post to which he had recently been elected. N. F. M. Henry (former Chairman) was appointed to serve in that capacity until the next meeting of the Executive Committee, in 1971.

#### Commission on Crystal Growth

The Commission did not meet but work on its projects is going on steadily. In particular the preliminary work on the organization of the International Summer School on Crystal Growth to be held in June 1971 at Leiden, The Netherlands, was one of the main activities. A group of 14 lecturers was formed of which two are members of the Commission. The interest shown so far is satisfactory and the Summer School is being co-sponsored by the Union and the Comité International de Croissance Cristalline.

#### Commission on Crystallographic Apparatus

The main items of business during 1970 related to the current projects and to forward planning for Open Sessions at the Ninth General Assembly and International Congress of Crystallography. More specifically, these are as follows:

1. *Index of Crystallographic Supplies* (R. Rudman). A note concerning the *Index* and soliciting the names of manufacturers and agents interested in being listed was inserted in *Acta Crystallographica* and *Journal of Applied Crystallography*. Subsequently, information on the *Index* and questionnaires were sent to about 300 potential suppliers of crystallographic supplies. The extent of elaboration of the *Index* depends largely on the response to this step.
2. *Radiation Damage Survey Project* (S. C. Abrahams). This project was drawn to the attention of the crystallographic community by a notice in the December 1969 issues of the Union's journals and has received encour-

aging international support, there being currently 31 participants.

3. *Single Crystal Intensity Measurement Project, Phase II* (A. McL. Mathieson). This project has been initiated by the appearance of a notice in the Union's journals.
4. *Intercomparison of F values from Dynamical Procedures* (N. Kato). It has been decided that no formal project will be arranged but that the subject will form part (or whole) of a session at the Ninth Congress.
5. *Open Sessions at the Ninth Congress*. Preliminary plans have been made for Open Sessions on Simultaneous Measurement Techniques (U. W. Arndt) and, conjointly with the Commission on Crystallographic Computing, on Interactive Displays for Generating Atomic Models (probable organizers – F. R. Ahmed and U. W. Arndt). An Open Session on the Commission's projects is also envisaged. Preliminary discussions are under way concerning exhibitions (a) of non-commercial apparatus and (b) photographs of crystallographic interest.
6. *X-ray Film*. During the year, the possibility arose that the production of a widely-used X-ray film would cease. As this concerned the product of an individual firm, it was not appropriate for the Commission as part of an international scientific union to become involved. In fact, protests by concerned individuals and national professional bodies have persuaded the manufacturer to reconsider the decision with the result that production has been resumed. The episode has, however, made the Commission aware of the possibility of changes in production and in types of X-ray films since the 1963 report produced by R. Uyeda on behalf of the Commission (*Acta Cryst.* (1963) **16**, 1107). A preliminary rough survey of the current situation regarding X-ray film production is under way.

#### Commission on Crystallographic Computing

The Proceedings of the 1969 International Summer School on Crystallographic Computing were published by Munksgaard in August 1970 under the title *Crystallographic Computing*. The book was edited by F. R. Ahmed, S. R. Hall and C. P. Huber. Copies were distributed free of charge to all the school participants.

Work on the standard tests for crystallographic computer programs was continued by J. M. Stewart and A. C. Larson, and the results are being verified by F. R. Ahmed.

G. Bassi agreed to prepare and edit the Third Edition of the *World List of Crystallographic Computer Programs*. The instructions to the program authors are under preparation.

#### Commission on Crystallographic Data

Although no formal meetings of the Commission were held in 1970, correspondence allowed for some exchange of ideas and opinion. The Chairman attended a meeting of CODATA as a representative of the Union. Crystallography is a field in which the organization of data is comparatively well established using techniques of general interest, which were demonstrated at the Conference, as for instance, computerized on-line search systems and typesetting from magnetic tape data banks. There is an increasing interest in this area, particularly in systems using electronic data processing methods.

Recommendations for the presentation of powder data for publication, as approved by the Data Commission at the Eighth Congress at Stony Brook, will be published in 1971 (*J. Appl. Cryst.* (1971) **4**, 81). Similar recommenda-

tions for the publication of single-crystal data published in 1967 (Kennard, O., Speakman, J. C. & Donnay, J. D. H. (1967). *Acta Cryst.* **22**, 445) are now being reviewed, in co-operation with the Commission on Journals, and the revised version will be published in due course.

In co-operation with the Commissions on Crystallographic Computing, Journals and *Structure Reports*, the Data Commission is organizing Open Sessions at the Ninth Congress in 1972 on the use of computers for building data banks, the use of chemical notation to supplement systematic chemical nomenclature in data compilations, the deposition of data too bulky to print and the searching of data files using computers. With the Commission on Crystallographic Apparatus, a session on computer manipulation of atomic models and the use of small on-line computers for data collection and display is being organized.

Arrangements have been made for the publication of the third edition of Donnay's *Crystal Data* in cooperation with the Joint Committee on Powder Diffraction Standards and the U.S. National Bureau of Standards, Office of Standard Reference Data.

#### *Commission on Crystallographic Nomenclature*

The Commission has held no meetings during the year, though there has been a little correspondence resulting from the current revision of the 'Notes for Authors' of the Union journals. The Commission has continued to be represented through its Chairman on the Joint (with the International Mineralogical Association) Committee on Nomenclature.

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

No information has been received on the work of this Commission.

#### *Commission on Crystallographic Teaching*

There has been no meeting of the Commission in 1970 but a considerable amount of work has been done by correspondence. The Secretary and Chairman have dealt with routine enquiries about availability of teaching material, sources of information, addresses, etc. A list of summer schools was compiled by the Secretary. Preparation of a list of teaching films is under active consideration. The commission was invited by the Division of Science Teaching of UNESCO to give assistance in the preparation of a text book for interdisciplinary science teaching in physics, chemistry, biology, metallurgy, etc. using the concept of 'Order-Disorder' as the central theme. Unfortunately, though a considerable amount of preliminary thinking was done it proved impossible to find anyone prepared to take on the general editorship and the project has now, for the time being, lapsed.

Consideration is being given to the form of the Commission's Open Session at the Ninth Congress in 1972 and it is hoped to hold a meeting of some members during the conference on Current Research in Crystallography, Manchester, 14-16 April 1971, which is being co-sponsored by the Union.

#### *Commission on Electron Diffraction*

The Commission supported the holding of an International Summer School on the Investigation of the Surface Structure of Solids by LEED and Supplementary Methods, Smolenice, Czechoslovakia, 6-15 September 1971 and two members of the Commission, K. Molière and S. Gold-

sztäub, are involved in its planning. Consequently this Summer School received (in 1971) Union sponsorship.

The first phase of the preparation of gas electron diffraction data, the collection of bibliographic data, was completed by 1 August 1970 as planned. The arrangement of this data using special card formats and the second phase of the project, involving numerical data, are being undertaken by the Crystallographic Data Centre and by another member of the Commission, L. S. Bartell.

#### *Commission on Neutron Diffraction*

The Commission has undertaken, on a continuing basis, the extension and revision of the table of neutron scattering amplitudes of elements and isotopes. This project has been active during the past year and material is being assembled for updating the present list (*Acta Cryst.* (1969) **A25**, 391).

Detailed plans and preparations for the neutron spectrometer evaluation project have been completed. The purpose of this programme is to help individual experimenters to obtain the maximum performance from their instruments by making comparisons with physically similar installations. Standardized powder samples and gold foils for intensity measurements are now being distributed to participating laboratories.

The Commission is actively considering the establishment of an information service for the collection and dissemination of magnetic structure data obtained by neutron diffraction. Under the plan, structural and related information for a given material would be forwarded to a central repository from which, after suitable editing, retyping on standard data sheets, and classification, it would be circulated to interested individuals on a subscription basis. The mechanics of operation are currently under study and a survey is being prepared to determine the extent of interest among neutron diffractionists and other interested scientists.

#### **I.U.Cr. - IMA Joint Committee on Nomenclature**

The International Union of Crystallography and the International Mineralogical Association set up a Joint Committee on Nomenclature in 1970 to consider nomenclature problems that are common to the two disciplines. Each organization is represented on the Joint Committee by four regular members and an *ex officio* member. Solicitation of suitable problems for consideration has been made through both organizations and by the committee members. Discussion has been initiated on several topics by means of correspondence. These topics include the naming of polytypes and polymorphs and the usage of structural symbols, criteria for justification of new phases worthy of names, definition of epitaxy, syntaxy, topotaxy, homeotype, homeotect structures, solid solution types, and order-disorder types, usage of structural formulae, usage of *X*, *Y*, *Z* and *a*, *b*, *c*, and standardization of symbols for atomic positions in complex structures.

#### **Representation on other Bodies**

##### *Abstracting Board of the International Council of Scientific Unions*

A meeting of the Full Board was held in Columbus, Ohio, U.S.A., 21-24 July 1970, and a detailed report of this was circulated to the Executive Committee and to the Commissions on Journals, *Structure Reports*, and Crystallographic Data. The main decisions were to extend the work

of the Board to engineering and mission-oriented services, and to provide for national membership. These provisions require extensive alterations in the Statutes of the Board, and in particular provision for participation of the World Federation of Engineering Organizations (WFEO) on the same basis as the International Council of Scientific Unions (ICSU). The name ICSU Abstracting Board will thus be inappropriate, and will be altered to something like International Federation of Information Services (INFIS) or preferably International Board of Information Services (IBIS).

For the first time, the Proceedings of the Full Board Meeting have been published. They form a duplicated document of vi+265 pages, and include an account of recent developments in the information services of the I.U.Cr. (pp. 171–175).

The next meeting of the Board will be a General Assembly in Orleans, France, 8–12 July 1971. It is expected that the new Statutes will be ready for discussion, and will probably be adopted, at that time.

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

The Fifth Annual Meeting of CODATA was held in St. Andrews, Scotland in September 1970 and was attended by the Union representative, F. W. Matthews, who presented a report on the activities of the I.U.Cr. Items of likely interest to crystallographers are reported below. The Meeting was attended by nine representatives of National Member Countries and seven representatives of Scientific Unions. In addition, chairmen of Task Groups and representatives of Liaison Organizations increased the attendance to twenty-four, with six observers.

It was noted that CODATA had recently published an 'International Compendium of Numerical Data Projects', which was deemed to be the first world-wide survey and analysis of centres which compiled, evaluated and published numerical property data. One of the six main sections was 'Solid State', listing eleven projects in the field of Crystallographic Properties, including two on Mineralogy, seven on Electronic and Magnetic Properties and one on Superconductive Materials. CODATA has also issued two Newsletters concerning new developments in the field of data collection and publication, which in a sense updates the 'Compendium' referred to above.

The reports of the other Unions represented had no items of particular relevance to the I.U.Cr. Dr Matthews obtained the impression that data compilation was in a better state in the area of crystallography than in most other areas. This may be because of its more manageable proportions, or perhaps at an early stage of the development of the subject there were workers within the field who were concerned with data collection. This tradition has continued.

The U.K. report referred to the work under Mrs. O. Kenard at the Crystallographic Data Centre, Cambridge, the recent publication of *Molecular Structures and Dimensions* and also to the storage and retrieval of information on atomic and molecular physics under the direction of F. J. Smith at Belfast University. This system is designed to allow data to be retrieved 'interactively'. The U.S.A. report mentioned further progress on crystal data determinative tables and described work at the National Bureau of Standards on automatic typesetting and compilation of data tables. The report from the French National Committee carried an item on the publication of a new section of *Tables Internationales*

*de Constantes* on 'Wavelengths of Emission and Discontinuities in Absorption of X-rays'. Japan reported a wide variety of government and industry sponsored data collection, analysis and evaluation activities, but none specifically in the field of crystallography.

*Committee on the Teaching of Science of the International Council of Scientific Unions*

The Union's representative, C. A. Taylor, attended a meeting of the Committee held in London, 20–21 April, 1970 under the chairmanship of Dr M. Matyas. The Committee was reminded of its terms of reference as defined in its constitution, namely:

- (a) to further the teaching of science at all levels,
- (b) to co-operative with other organizations concerned with science teaching, and
- (c) to facilitate co-operation among the teaching committees of the individual scientific unions.

In the light of this several concrete proposals emerged:

1. That a major conference on science teaching should be held in September, 1972 or the Spring of 1973; the venue probably to be the University of Maryland, U.S.A. and to be planned by a sub-committee under Dr A. Baez. (It was later decided to concentrate on the Spring of 1973.) The conference would include sessions on both basic training and in-service training of science teachers and on objectives, new techniques in teaching, the place of social responsibility in educating science teachers, etc.
2. That preliminary conferences and symposia should be held to prepare material, and that the Proceedings should be published possibly as a special edition of UNESCO's *New Trends in Science Teaching*.
3. That a symposium sub-committee be set up under Prof. Raw and that another sub-committee be set up under Prof. C. A. Taylor, to advise UNESCO on publications relating particularly to interdisciplinary science teaching.

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

Several conferences having crystallographic interest were sponsored by the Commission or by IUPAP during 1970. One meeting (Sagamore III: Electron Charge, Spin and Momentum Densities, Aussois, France, 9–12 September 1970) was co-sponsored by IUPAP and I.U.Cr., and the Commission expressed the hope that both these Unions would sponsor the next Sagamore Conference. The two representatives of the Union, E. F. Bertaut and J. M. Cowley, and the Chairman of the (I.U.Cr.) Sub-committee on the Union Calendar would be pleased to receive suggestions for or information on any conferences of common interest to crystallographers and solid state physicists, with a view to possible co-sponsorship by the Union and IUPAP.

*Comité International de Croissance Cristalline*

One of the Union's representatives, R. F. Strickland-Constable, attended a meeting of this Committee in Zürich on 25 September 1970.

Three draft constitutions were submitted to the meeting. Two of these were chosen as suitable for further discussion. They will be slightly amended and circulated for further consideration at the Marseille meeting. A main point of discussion was the extent to which final decisions were to be

in the hands of the General Meeting of the International Conference on Crystal Growth (ICCG). A suggestion of co-operation between the Working Party on Crystallization of the European Federation of Chemical Engineers and the Committee was sympathetically discussed.

#### International Council of Scientific Unions

The Union was represented at the 11th and 12th ICSU Executive Committee meetings by the Immediate Past President, Prof. N. V. Belov, and at the 13th ICSU General Assembly by Prof. Belov and the Executive Secretary, Dr J. N. King. These meetings were held in Madrid, Spain on 23 and 29 September and on 24–29 September 1970, respectively. The business of the Executive Committee meetings mostly related to that of the General Assembly. Two new National Members, Madagascar and Singapore, were admitted to ICSU. It was agreed to extend the International Biological Programme until mid-1974. The establishment of a Special Committee on Problems of the Environment (SCOPE) was ratified and members will be added to SCOPE from India, South East Asia and Africa. The ICSU Executive Committee was directed to examine, as a matter of urgency, the possibility of producing a film on the activities of ICSU with the object of increasing public understanding of the role and achievements of ICSU. An *ad hoc* committee was set up to examine the role and structure of ICSU. The recommendation that the ICSU Abstracting Board should, until decided otherwise, function as a link between ICSU and UNISIST was approved. The work of the Global Atmospheric Research Programme (GARP) will continue and contributions from ICSU to this programme were approved, in principle, for 1972–76. An Inter-Union Commission for Lunar Studies will be established.

#### Finances

The audited accounts of the Union for the year 1970 are given at the end of this Report. For comparison the 1969 figures are provided in italics. Negative quantities are indicated by parentheses.

The *Acta Crystallographica* account for 1970 shows a profit of \$71,202 as compared with a deficit of \$26,461 in 1969. The profit is primarily due to the increase in subscription rates and also to the drop in the number of pages published, reasons for which are given in the section on 'Commission on Journals'. The Account is expected to show a much smaller profit in 1971, because of rising publication costs and an increase in the number of pages published. As in previous years, the total cost of the Technical Editor's office is divided between the *Acta Crystallographica* account and the *Journal of Applied Crystallography* account in percentages based on the number of text pages published during the year; 84 and 16% respectively for 1970. The journals' accounts have also been charged with administrative expenses shown in the General Fund account.

The *Journal of Applied Crystallography* account for 1970 shows a profit of \$3,155 as compared with \$7,946 in 1969. This reduction in profit is mainly due to the greatly in-

creased number of pages published and increased publication costs.

The *Structure Reports* account shows a profit of \$8,187 as compared with \$11,280 in 1969. No volumes were published in 1970.

The *International Tables* account shows a deficit of \$3,290 as compared with a profit of \$5,961 in 1969. This deficit is mainly the result of the expenses of the reprinting of Volume 1 in late 1969.

In 1970, \$344 was received from the sale of 42 copies of *Fifty Years of X-ray Diffraction*. 349 copies of *Symmetry Aspects of M. C. Escher's Periodic Drawings* were sold, resulting in a net deficit of \$27 after payment of royalties and an honorarium. \$1,648 was received from the sale of 183 copies of *Early Papers on Diffraction of X-rays by Crystals*, reducing the deficit on the fund account to \$1,130.

The first two volumes of *Molecular Structures and Dimensions* were published in late 1970, in a joint venture between the Union and the Crystallographic Data Centre, University of Cambridge, England. The publication expenses, which have been borne by the University of Cambridge, were substantially larger than the \$1,711 received from the sale of 112 copies of Volume 1 and 113 copies of Volume 2.

The General Fund account shows an excess of income over expenditure of \$9,067 as compared with \$5,802 in 1969. There were no major expenses relating to a General Assembly this year, as there were in 1969. However, \$3,000 was given to scientific meetings having Union sponsorship and the Executive Committee meeting cost \$5,356.

The subvention received from UNESCO through ICSU remained constant at \$5,250. However, ICSU made available a special grant of \$2,000 and also assisted by refunding the subscription paid by the Union in 1969. Interest from investments and bank accounts was \$10,838 as compared with \$9,983 in 1969.

In 1970, a profit of \$658 was made on redemptions of f.4,000 3% Nederland 1937, \$1,500 3% Nederland 1947, f.2,000 3½% Nederland 1956, f.4,000 4½% Nederland 1958, f.3,000 4½% Nederland 1959, f.2,000 4½% Nederland 1960 (I) and f.5,000 4½% Nederland 1964. As on previous Balance Sheets the investments have been valued according to their quotations at the end of the year. Their depreciation in value, together amounting to \$8,052, has not been charged against the General Fund but has again been included as an asset on the Balance Sheet to avoid annual fluctuations in value influencing the General Fund account.

The larger part of the money with the Banks is still placed in deposit accounts, namely at the end of 1970, f.86,372 with the Amsterdam–Rotterdam Bank N.V., \$20,743 with the First National City Bank of New York, Sw. Kr. 71,590 with the A.B. Svenska Handelsbanken and £7,295 with the National Westminster Bank Limited. The amounts shown on the Balance Sheet for Debtors and Creditors relate to sums, principally on the publishing accounts, due at 31 December 1970. Where appropriate these amounts have since been settled.

The Balance Sheet shows that the assets of the Union have increased during the year from \$236,904 to \$327,189, excluding stocks of unsold publications.





## General Fund Account for the year ended 31 December 1970

	U.S. Dollars		U.S. Dollars	
	1970	1969	1970	1969
Subscription to ICSU (2% of subscriptions received from Adhering Bodies in 1969)		295.60	5,250.00	5,250.00
Subscription to ICSU Abstracting Board	100.00	—	2,000.00	—
Subscription to ICSU Committee on the Teaching of Science	200.00	200.00	13,300.00	13,300.00
Administration Expenses:				
Honoraria: General Secretary, Treasurer and Secretarial Assistance	2,166.29	5,485.53	295.60	244.00
Audit and Accountancy Charges	660.00	660.00	13,300.00	6,669.15
Postages, Stationery, Printing and Sundries	772.12	1,723.05	7,569.92	3,313.54
Travelling Expenses	204.61	479.16	3,267.64	2,198.45
Bank Charges and Differences on Exchange	170.83	129.54	657.87	—
Legal Fees	1,509.00	1,200.00	10.63	47.33
Executive Secretary's Office: Salary and Expenses	13,979.48	10,379.06	2.25	57.37
Depreciation of Office Equipment	553.26	270.40	198.75	10.04
Meeting of Executive Committee			39.19	513.40
Eighth General Assembly and International Congress, Stony Brook, U.S.A.:				102.26
Travel Expenses and Travel Grants			4,455.00	4,573.50
Programme Committee Chairman's Expenses			1,485.00	1,524.50
Ninth General Assembly and International Congress: Programme Committee			240.00	—
Travel Expenses of I.U.Cr. Representatives on other bodies			6,180.00	6,098.00
Expenses of Commissions			4,000.00	—
Sponsorship of Meetings			1,267.63	—
<i>World Directory of Crystallographers</i> , 4th Edition. Miscellaneous Expenses	560.82	85.22	—	—
Contribution towards cost of manuscript for 'Crystallographic Computing'	4,000.00	—	—	—
Excess of Income over Expenditure carried to Balance Sheet	9,066.76	5,802.19	\$43,958.85	\$37,531.61
	<u>\$43,958.85</u>	<u>\$37,531.61</u>	<u>\$43,958.85</u>	<u>\$37,531.61</u>

Subvention received from UNESCO through ICSU

Grant from ICSU

Refund from ICSU of 1969

Subscription

Subscriptions from Adhering Bodies

Interest on Investments

Interest on Banking Accounts

Profit on Redemption of Investments

Sale of copies of *World Directory of Crystallographers*, 3rd Edition

Less Publishers' Commission

Sale of Sundry Publications (Bibliographies, *Book List* and *List of Computer Programs*)

Less Publishers' Commission

Amount charged to Journals and Publications:

*Acta Crystallographica*

*Journal of Applied Crystallography*

*Molecular Structures and Dimensions*

Subvention from UNESCO for manuscript for 'Crystallographic Computing'

Net Surplus from Summer School on Crystallographic Computing

**Acta Crystallographica Account for the year ended 31 December 1970**

	U.S. Dollars		U.S. Dollars	
	1970	1969	1970	1969
Publication Expenses:				
Printing and Binding Volumes A26 and B26 (1969 A25 and B25)	108,175.76	125,148.41	236,538.00	149,158.80
Distribution and Postage	14,414.81	16,965.61	16,622.76	20,135.17
	<u>122,590.57</u>	<u>142,114.02</u>	<u>253,160.76</u>	<u>169,293.97</u>
Printing Index to Volumes A24 and B24	—	639.25	31,645.09	21,161.75
Printing and Distributing Acta Supplement S3 to Volume A25	—	4,392.41	3,825.20	5,480.73
Reprinting Volume 4	—	3,496.25	573.77	703.92
Editorial Expenses:				
Editorial Honoraria	5,199.79	4,838.80		
Secretarial Assistance	1,706.43	1,499.09		
Postages, Telephone and Office Sundries	1,235.71	1,475.89		
Travelling Expenses	251.93	224.92		
Technical Editing:				
Salaries and Expenses	17,880.62	15,916.96		
Depreciation of Office Equipment	245.46	198.71		
Administrative Expenses	4,455.00	4,573.50		
Excess of Income over Expenditure carried to Balance Sheet	71,201.59	(26,460.77)	\$224,767.10	\$152,909.03
	<u>\$224,767.10</u>	<u>\$152,909.03</u>	<u>\$224,767.10</u>	<u>\$152,909.03</u>

**Journal of Applied Crystallography Account for the year ended 31 December 1970**

	U.S. Dollars		U.S. Dollars	
	1970	1969	1970	1969
Publication Expenses:				
Printing and Binding Volume 3 (1969 Volume 2)	20,423.99	12,485.41	32,504.00	30,712.00
Printing Index to Volume 1	—	309.85	3,412.80	2,189.60
Distribution and Postage	2,083.51	2,152.69	35,916.80	32,901.60
Printing and Distributing Acta Supplement S3 to Volume A25	—	531.79	4,489.60	4,386.77
Editorial Expenses:				
Editorial Honoraria	1,239.97	2,134.47	1,255.00	1,020.52
Secretarial Assistance	8.00	440.43	108.60	119.33
Postages, Telephone and Office Sundries	598.72	143.60		
Travelling Expenses	131.03	347.48		
Technical Editing:				
Salaries and Expenses	3,405.83	1,384.08		
Depreciation of Office Equipment	42.56	15.29		
Administration Expenses	1,485.00	1,524.50		
Excess of Income over Expenditure carried to Balance Sheet	3,154.99	7,946.43	\$32,573.60	\$29,416.02
	<u>\$32,573.60</u>	<u>\$29,416.02</u>	<u>\$32,573.60</u>	<u>\$29,416.02</u>



**Fifty Years of X-ray Diffraction Account for the year ended 31 December 1970**

	U.S. Dollars	
	1970	1969
<i>Excess of Income over Expenditure carried to Balance Sheet</i>		
	344-21	450-09
	<u>\$ 344-21</u>	<u>\$ 450-09</u>
	417-22	545-56
	<u>73-01</u>	<u>95-47</u>
	<u>\$ 344-21</u>	<u>\$ 450-09</u>

**Escher Drawings Account for the year ended 31 December 1970**

Binding additional copies	796-33	—	1,920-67	1,769-22
			336-12	309-61
			<u>815-62</u>	<u>807-99</u>
			768-93	651-62
			27-40	(651-62)
	<u>\$ 796-33</u>	<u>—</u>	<u>\$ 796-33</u>	<u>—</u>

**Early Papers Account for the year ended 31 December 1970**

Publication Expenses:				
Cost of Printing and Binding	—	7,541-56	—	3,500-00
Preparation of manuscript and Sundry Expenses	—	1,144-23	1,997-78	2,918-68
<i>Excess of Income over Expenditure carried to Balance Sheet</i>				
	1,648-17	(2,777-88)	349-61	510-77
	<u>\$ 1,648-17</u>	<u>\$ 5,907-91</u>	<u>\$ 1,648-17</u>	<u>\$ 5,907-91</u>

**Molecular Structures and Dimensions Account for the year ended 31 December 1970**

Publication Expenses:				
University of Cambridge	1,224-65	—	1,145-76	—
Carriage Charges	246-36	—	928-19	—
Administrative Expenses	—	—	<u>2,073-95</u>	—
			362-94	1,711-01
	<u>\$ 1,711-01</u>	<u>—</u>	<u>\$ 1,711-01</u>	<u>—</u>

We have examined the annexed Balance Sheet, and Income and Expenditure Accounts, and have obtained all the information and explanations which we considered necessary. In our opinion these accounts, together with the notes thereon, give a true and fair view of the state of affairs of the Union at 31 December 1970 and of the results for the year ended on that date.

Manchester, England

11 June 1971

Signed: MANN JUDD &amp; Co.

Chartered Accountants