

**International Union of Crystallography**  
**Fourteenth General Assembly and International Congress of Crystallography**  
**Perth, Australia, 12-20 August 1987**

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### Introduction and Opening Ceremony

By invitation of The Society of Crystallographers in Australia and The Australian Academy of Science, the Fourteenth General Assembly and International Congress of Crystallography were held at the University of Western Australia, Perth, Australia, 12–20 August 1987.

The meetings were attended by 889 scientists from Australia and the following 48 countries: Algeria, Argentina, Austria, Bangladesh, Belgium, Brazil, Bulgaria, Canada, Chile, People's Republic of China, Czechoslovakia, Denmark, Arab Republic of Egypt, Finland, France, German Democratic Republic, Federal Republic of Germany, Greece, Hong Kong, Hungary, India, Israel, Italy, Japan, Korea, Kuwait, Malaysia, Netherlands, New Zealand, Nigeria, Norway, Pakistan, Philippines, Poland, Portugal, Puerto Rico, South Africa, Southern Africa (Transkei), Spain, Sri Lanka, Sweden, Switzerland, Taiwan, Thailand, UK, USA, USSR, Yugoslavia. In addition there were 188 accompanying persons.

The General Assembly and Congress were opened formally on the afternoon of 12 August. The Opening Ceremony was held at the Perth Concert Hall. Professor A. H. WHITE gave an organ prelude and also an interlude before the Bragg Lecture. Professor S. R. HALL chaired the ceremony and introduced the speakers. Professor R. H. T. SMITH, Vice-Chancellor of the University of Western Australia, gave the welcoming address and then Professor Th. HAHN, President of the IUCr, gave the opening address. The first Ewald Medals and Prizes were presented.

A special medal was given to Mr Arnold EWALD, who was representing the Ewald family. Then the awardees, Professor J. M. COWLEY and Dr A. F. MOODIE, received their medals and prizes. After an interlude Professor H. C. FREEMAN, Chairman of the Congress Programme Committee, introduced the Bragg Lecturer, Professor B. W. MATTHEWS, who gave his lecture entitled *Crystallography in the Life Sciences*. Dr A. M. MOORE, Secretary of the Bragg Lecture Fund Committee, made a presentation to Professor Matthews. The evening ended with a reception.

### Fourteenth International Congress

#### Scientific programme

The scientific programme included the Bragg Lecture by Professor Matthews mentioned above and 12 Main Lectures. Two Main Lectures were held in parallel on each morning of the six days of scientific sessions and were followed by between four and seven microsymbiosia, held in parallel. There were 32 such microsymbiosia. The afternoons were reserved for poster sessions and *ad hoc* sessions. There were also two evening symposia, on high-critical-temperature superconductors and on new developments in direct methods, the latter symposium in honour of Nobel Laureates Herbert Hauptman and Jerome Karle. About 700 papers were presented. The detailed plan for the scientific programme had been compiled by an international Programme Committee at a preparatory meeting in July 1986. The abstracts submitted were printed, by direct reproduction of the typescript copy, in a book of Collected Abstracts and in a Supplement to *Acta Crystallographica*, Volume A43, dated 1 August 1987.

#### Exhibitions

Exhibitions of commercial crystallographic equipment, non-commercial apparatus and books were held in the gymnasium which was also used for all the poster sessions.

#### Microcomputing and databases

A microcomputing display was organized by the Commissions on Crystallographic Computing and Crystallographic Teaching, whilst the Commission on Crystallographic Data organized a database demonstration.

#### Social events

There was a reception following the Opening Ceremony, a Congress excursion by steam train to York and a farewell party. A more extensive social programme was arranged for those accompanying the Congress participants.

### Minutes of the Fourteenth General Assembly

These Minutes have been prepared by J. N. King, Executive Secretary, under the authority of K. V. J. Kurki-Suonio, General Secretary and Treasurer of the IUCr and Secretary of the General Assembly.

#### Introduction and list of delegates

Sessions of the General Assembly were held on the evenings of Thursday 13 August, Friday 14 August and Tuesday 18 August. The following list shows the names of official delegates appointed by the Adhering Bodies and of the alternates who substituted at one or more sessions. The names are listed by the countries to which the respective Adhering Bodies belong, and the number of votes of the Adhering Body is given in parentheses after the name of the country. The names of the Chairmen of the delegations are printed in bold type; those of alternates are marked by an asterisk. The names of officially appointed delegates who were not present at any session of the Assembly are not included.

**Australia** (3): **H. C. Freeman** (absent on 18 August), S. R. Hall, T. J. Hicks, M. R. Taylor\* (present on 18 August).

**Belgium** (2): G. H. Evrard, **G. S. D. King**.

**Brazil** (3): I. L. Torriani.

**Bulgaria** (1): J. Maciček.

**Canada** (3): **G. Ferguson**, B. M. Powell, J. Trotter.

**China, People's Republic of** (4): Huang Jin-lin, **Liang Dong-cai**, Liang Jin-kui, Shao Mei-cheng\* (present on 14 and 18 August), Xu Xiao-jie\* (present on 13 August).

**Czechoslovakia** (1): J. Garaj.

**Denmark** (1): B. Jensen.

**Egypt, Arab Republic of** (1): S. A. Abdel-Hady.

**Finland** (1): P. Suortti.

**France** (4): Y. Epelboin, **M. Hospital**, M. Marezzio, M. Schlenker.

**German Democratic Republic** (1): P. Paufler.

**Germany, Federal Republic of** (4): H. Fuess, E. Koch\* (present on 14 and 18 August), C. Krüger (absent on 18 August), **W. Prandl**, E. Tillmanns (absent on 14 August).

**Hungary** (1): L. Zsoldos.

**India** (2): M. Vijayan (absent on 13 August), **M. A. Viswamitra**.

**Israel** (1): F. H. Herbstein (absent on 18 August), G. Kimmel\* (present on 18 August).

**Italy** (3): G. Filippini, C. M. Gramaccioli\* (present on 13 August), **M. Mammi** (absent on 13 August), A. Villa-Chiesi.

*Japan* (4): J. Harada, S. Hoshino (absent on 14 August), Y. Iitaka\* (present on 14 and 18 August), H. Iwasaki\* (present on 13 August), F. Marumo (absent on 13 August), M. Tanaka (absent on 18 August).

*Netherlands* (2): H. Schenk, F. Tuinstra.

*New Zealand* (1): G. J. Gainsford.

*Norway* (1): B. F. Pedersen.

*Portugal* (1): J. Lima-de-Faria.

*South Africa* (2): G. J. Kruger, L. R. Nassimbeni.

*Sweden* (2): P. Kierkegaard, I. Olovsson.

*Switzerland* (2): H. D. Flack, D. Schwarzenbach.

*UK* (5): A. M. Glazer, J. R. Helliwell, J. A. K. Howard, R. W. H. Small, M. M. Woolfson.

*USA* (5): R. F. Bryan, W. L. Duax, J. P. Glusker, W. A. Hendrickson, L. H. Jensen (absent on 14 August), I. L. Karle\* (present on 14 August).

*USSR* (5): K. S. Aleksandrov, G. B. Bokii, T. I. Malinovsky, R. P. Shibaeva (absent on 13 August), E. V. Suvorov, Yu. N. Vodopyanov\* (present on 13 August).

*Yugoslavia* (1): B. Prelesnik.

The second delegate from South Africa was admitted to the General Assembly after the application from the South African Council for Scientific and Industrial Research to increase its Category of Adherence from Category I to Category II had been accepted, at the first session of the Assembly on 13 August (see Minute 4).

The delegate from Bulgaria was admitted to the General Assembly after the application from the Bulgarian Academy of Sciences for membership of the IUCr had been accepted at the second session of the Assembly on 14 August (see Minute 22).

*Present as members of the Executive Committee:* Th. Hahn (President), V. I. Simonov (Vice-President), K. V. J. Kurki-Suonio (General Secretary and Treasurer), J. Karle (Immediate Past President), A. Authier, R. Diamond, A. Kálmán, E. N. Maslen, M. Nardelli, Y.-q. Tang (Ordinary Members). J. N. King was in attendance as Executive Secretary.

#### First Session, Thursday 13 August 1987, 7.35 p.m.

##### (1) *Introductory remarks by the President*

Professor HAHN welcomed the delegates and observers.

##### (2) *Procedural matters*

In order to verify the list of voting delegates, the President requested the General Secretary to read this list, and asked delegates to indicate their presence when their names were called. (This procedure was repeated at the beginning of each session of the General Assembly.)

Two delegates, H. Schenk (Netherlands) and J. Lima-de-Faria (Portugal) were appointed to act as tellers when votes had to be counted during the Assembly.

##### (3) *Approval of the Agenda*

The Agenda and the Appendices to the Agenda had been distributed to Secretaries of National Committees on 4 June 1987. Additional appendices, containing the triennial reports by the Chairmen of the Commission on Crystallographic Studies at Controlled Pressures and Temperatures and the Commission on Electron Diffraction and by the IUCr representative on the ICSU Committee on Space

Research (COSPAR) had been distributed in Perth prior to the start of the General Assembly.

Additional items were added to the Agenda concerning the application for membership from the Bulgarian Academy of Sciences at the session on 14 August (see Minute 22) and concerning the application of the Asian Crystallographic Association (ASCA) to become a Regional Associate at the session on 18 August (see Minute 35).

##### (4) *Change in Category of Adherence*

In March 1987 the Adhering Body for South Africa, the Council for Scientific and Industrial Research, requested a change in the Category of Adherence from Category I to Category II. The Executive Committee had considered this request at its meeting in Perth immediately prior to the General Assembly, and recommended acceptance of the change. The General Assembly accepted the change and welcomed the second delegate of the Council. The Chairman of the French delegation asked that the abstention of the French delegation be recorded in the Minutes.

##### (5) *Approval of the Minutes of the Thirteenth General Assembly*

The Minutes were approved and two copies were signed by the President and the General Secretary, in accordance with By-Law 1.13. There were no matters arising from the Minutes.

##### (6) *Report of the Executive Committee*

The Report of the Executive Committee on the activities of the IUCr since the Thirteenth General Assembly had been submitted to the National Committees and the Commissions on 4 June 1987, in accordance with Statute 6.8 and follows these Minutes as Annex I, Appendix A. The report was accepted without discussion.

##### (7) *Financial Report*

A Financial Report, covering the calendar years 1984, 1985 and 1986, had been prepared by the Treasurer and had been submitted to the National Committees and the Commissions on 4 June 1987. The Report follows these Minutes as Annex I, Appendix B.

The Treasurer illustrated the development of the IUCr's finances over recent years with the aid of several graphs. He showed the improvement in the total funds of the IUCr from the lowest point in 1981 to 1986, together with the balances in the General Fund account and the *Acta Crystallographica* account, which were the most important accounts in terms of finances. The new Fund Accounts, the Publications and Journals Development Fund Account and the Research and Education Fund Account, had no income of their own but received income by transfers from the General Fund, *Acta Crystallographica* and *Journal of Applied Crystallography* accounts. Another graph showed the difference between the income and expenditure for the various accounts over the same period, again illustrating the steady improvement in the assets of the IUCr.

The Treasurer reminded delegates that the fluctuations in exchange rates appeared to indicate a tremendous loss during the last triennium, particularly in 1986. The main currencies of the IUCr's operations were Pounds Sterling, US Dollars and Danish Kroner. Because the IUCr's accounts were expressed in Swiss Francs, the large changes in the first two of these currencies with respect to the Swiss

Franc were dramatically evident. However, this did not need to cause delegates serious concern because this loss or gain depended on the accounting currency. This was illustrated by looking at the assets of the IUCr at the end of each financial year when expressed in Pounds Sterling or US Dollars, when there would not be any loss, even for the worst case of 1986. This loss or gain was not taken into account in the graph of excess of income over expenditure but only in the graph of the total assets of the IUCr.

The Treasurer drew the attention of the delegates to three main points of interest in the development of the IUCr's finances, namely the investment policy, the development of the finances of *Acta Cryst.* and *J. Appl. Cryst.*, and the uses of the new funds.

There was a change in direction of the investment policy, made by the Executive Committee and based on discussions in the Finance Committee. Between 1984 and 1986 there had been a major effort to obtain high interest in the short term, because very high short-term interest rates were then available. By 1986 the IUCr's assets were more than adequate to give a high safety margin, so that the emphasis was changed to long-term safety. This caused a short-term reduction in interest income but it gave the IUCr long-term safety in that the value of the IUCr's investments would be maintained. This would have certain implications on the General Fund budget for the next triennium (see Minute 32 and Annex I, Appendix I) because the interest income occurred in that budget.

The second point was the financial development of the journals. The major points affecting this development were given in the written Financial Report. A fundamental revision of the financial basis was made in the emergency situation of 1982, which improved these finances dramatically, by increasing the subscription rates significantly in Danish Kroner, that being the currency in which the printing bills were paid. Since then the subscription rates had been kept almost constant and the Executive Committee had decided that these would remain unchanged for 1988 also, that is for five years since the last major increase. This was rather exceptional when compared with the price increases for other journals. It had been possible because the number of subscribers to the IUCr's journals had not decreased significantly, unlike the case for other journals. At the same time, the printing costs had reduced when expressed in Swiss Francs, because of several factors, including changes in exchange rates and reductions in the cost of printing in the UK. Furthermore, the costs were highly sensitive to changes in the number of pages published. The number of pages published had been less than predicted each year, which had been an essential factor in giving additional income for the journals. Another major cost item was the salaries of the technical-editing staff, and unexpected changes in the staff had reduced these costs. None of these factors were of a permanent nature and, in taking care of the journals' finances, it was necessary to have some safety margins. There had been extensive efforts to increase the coverage of the IUCr's journals. The results of these attempts were not yet clearly visible but they were expected to lead to increases in sizes of the journals with resultant increases in costs.

The third point was the financial aspects of the new funds. The first use of the Ewald Fund had just occurred in Perth. The fund had been planned so that the interest on this fund would be sufficient to cover the triennial awards. The uses

of the other two new funds, the Publications and Journals Development Fund and the Research and Education Fund, currently presented problems and the Treasurer asked all delegates to devote some thought to suitable uses for these funds. So far, these funds had not been used greatly, except for support to young scientists which was currently about Sw Fr 60 000 per annum. Other suggestions had been discussed by the Executive Committee and one major plan being developed by the Commission on Crystallographic Teaching was a Visiting Professorship Scheme. The Publications and Journals Development Fund would carry significant costs in the coming triennium in purchasing equipment for journals production and technical editing, including a new computer and equipment for electronic exchange of information and for checking procedures for the journals. The Executive Committee had also been considering the longer-term aspects where significant changes would occur in publishing.

The General Assembly accepted the report and relieved the Treasurer of financial responsibility, thanking him for managing the affairs of the IUCr so well since he was appointed in 1981.

#### (8) *Ewald Prize and Ewald Bequest*

The Treasurer reminded delegates that the Ewald Fund had been established with a major bequest which the IUCr had received from Professor Ewald himself, as his last wish to the IUCr, and some further money from the Ewald family. The Executive Committee had applied the principle that the IUCr should add the same amount of money from its own assets to the Ewald Fund.

The first Ewald Prize had been presented at the Opening Ceremony. The details of the Prize and the Bequest are given in Annex I, Appendix C.

#### (9) *New Fund Accounts*

The Treasurer had reported on these fund accounts in his financial report (Minute 7). The details as distributed to the National Committees and Commissions on 4 June 1987 are given in Annex I, Appendix D.

#### (10) *Reports of the Commissions*

Those reports of the Commissions on their activities since the Thirteenth General Assembly which had been submitted in time had been distributed to the National Committees and the Commissions on 4 June 1987, in accordance with Statute 8-4. The reports of the Commission on Crystallographic Studies at Controlled Pressures and Temperatures and the Commission on Electron Diffraction were received later and were circulated to delegates at the General Assembly, just prior to the first session. Consideration of these two reports was therefore deferred until the second session on 14 August. All these reports are reprinted as Annex I, Appendix E. The reports were taken as read, but the Chairman of each Commission, or his alternate, was invited to say a few words about any further developments and to answer any questions. These verbal reports are summarized in Minutes 11-16 (see also Minutes 23, 25 and 37).

The Chairmen of the Commissions on *Structure Reports*, *Charge, Spin and Momentum Densities*, *Crystal Growth and Characterization of Materials*, *Crystallographic Apparatus*, *Crystallographic Computing*, *Crystallographic Data*, *Crystallographic Nomenclature*, *Electron Diffraction*

tion, and Small Molecules had nothing to add to their written reports and were not asked any questions by the delegates. The Chairmen of the Commissions on Biological Macromolecules and on Crystallographic Studies at Controlled Pressures and Temperatures did not attend the General Assembly or appoint an alternate.

#### (11) *Commission on Journals*

The Chairman of the Commission and Editor of *Acta Crystallographica*, S. C. ABRAHAMS, estimated that 1,320 papers would be published in *Acta Cryst.* and *J. Appl. Cryst.* in 1987, which was very close to the highest number ever published. The lowest number published in recent years was 906, in 1981, when the number was restricted for financial reasons.

He reported on the most important recommendations made by the Commission to the Executive Committee as a result of the Commission meeting on 7-9 August. It was considered that (1) *J. Appl. Cryst.* and the three sections of *Acta Cryst.* should be retained broadly in their present form, (2) the use of colour and high-quality half-tones should be encouraged, (3) a rapid communications section should be introduced to attract papers on new subjects like quasi-crystals and high-temperature superconductors, (4) a machine-readable section in *Acta Cryst.* Section C should be introduced, which would require some investigations on an experimental basis initially, (5) a special Ewald Prize issue of either journal, and occasional special issues on selected topics, should be published, (6) a cumulative author index should be included in the final annual issue of *Acta Cryst.*, (7) the Crystal Data section of *J. Appl. Cryst.* should be terminated, a recommendation supported by the journal *Powder Diffraction*, (8) a cumulative volume index for *J. Appl. Cryst.* should be compiled, and (9) a new book list should be issued.

M. M. WOOLFSON (UK) reported that the British delegation was extremely concerned that it appeared that the publishers of the IUCr's journals were being prevented from fulfilling their obligations to the IUCr, which was a member of the International Council of Scientific Unions (ICSU), because of a law which did not allow them to follow the ICSU rules. He requested that this matter be considered by the General Assembly at a convenient time determined by the President. The President noted his request (see Minute 34).

The delegates expressed their appreciation to Dr Abrahams on the occasion of his retirement as Editor of *Acta Cryst.*, an office he had held for more than nine years.

#### (12) *Commission on International Tables*

The Chairman of the Commission, A. J. C. WILSON, reported that the Commission had met twice in Perth. He drew attention to two points in the written report, (1) withdrawal of authors had posed problems for the Editors of Volumes B and C; several authors in each volume had failed to meet their promised deadlines, and it had not yet been possible to find willing authors for all sections, and (2) in suitable cases editorial updating of the corresponding parts of the old Volumes II-IV would be used to avoid gaps where authors had withdrawn or had not been found. The Editors and the Commission felt that it was unwise to hold up the publication of the volumes until they were complete, as originally planned, partly because some of the

sections already written would then be out of date. It was proposed that for Volume B (*Reciprocal Space*) the closing date should be early 1988, and any contributions not received by the Editor by then should be held over for a second edition. A precedent had been set by a second edition of Volume A being published four years after the first edition. Volume C (*Mathematical, Physical and Chemical Tables*) was less complete at present and therefore a cut-off date of late 1988 was proposed for this volume. Such actions would require the approval of the Executive Committee.

The Commission had also considered the need for further volumes. For many years there had been a proposal for a Volume D (*Physical Properties of Crystals*), which would be largely a volume on tensors. A member of the Commission had expressed a willingness to edit such a volume. Recently there had also been a proposal for a volume on group-theoretical matters but the Commission considered that such a volume would have very limited sales and it therefore recommended that the IUCr proceed with the volume on physical properties. The Commission also recommended that the next edition of Volume A should include frieze, rod and layer groups, and that implicit and derived symmetry elements should be included in an amplified and correct but usable fashion.

The Commission had also considered a possible Volume E on *Crystallographic Computing*, to be produced in cooperation with the Commission on Crystallographic Computing. Such an idea would have to be discussed with the new members of that Commission and the Commission on Crystallographic Teaching.

It had also been suggested that the numerical tables in *International Tables* should be made available in machine-readable form. Professor WILSON considered that the only way to protect the IUCr's financial investment in the tables would be to lease such data under contract.

Finally, the Commission wished to propose some changes in its membership by including the Editor of Volume A, Professor Hahn (who had been a member of the Commission and all other Commissions during the last triennium in his capacity as President), and the Chairman of the Commission on Crystallographic Data.

M. SCHLENKER (France) asked whether there were any plans for teaching editions of Volumes B and C. Professor WILSON responded that there were no such plans but the Editors would consider the idea.

#### (13) *Commission on Biological Macromolecules*

The President explained that no report had been received from the Commission Chairman, C.-I. Brändén, and Dr Brändén was not present at the General Assembly. However, a Commission member, W. A. HENDRICKSON, had kindly agreed to answer any questions. M. GLAZER (UK) wondered whether if a Commission failed to submit a report it should be dissolved. W. L. DUAX (USA) suggested that, whilst the Chairman might be criticized for failing to present a report, the more important question was whether the Commission had accomplished something in the last triennium when delegates were considering whether a Commission should be dissolved. The President assured delegates that the Executive Committee was giving serious consideration to this point.

Two members of the Commission compiled a report during the period of the General Assembly. This report was

distributed to delegates and considered later (see Minute 23).

(14) *Commission on Crystallographic Studies at Controlled Pressures and Temperatures*

The President explained that the Chairman was not attending the General Assembly and had not appointed an alternate (see also Minute 25).

(15) *Commission on Crystallographic Teaching*

G. FERGUSON (Canada) asked for some information about the *Historical Atlas of Crystallography*. The Chairman of the Commission, H. SCHENK, explained that it described in several chapters part of the history of crystallography, and it included time charts showing the years of the most important achievements, together with pictures of many famous crystallographers.

(16) *Commission on Neutron Diffraction*

The Chairman of the Commission, B. T. M. WILLIS, reported that he had had discussions about the need for a Commission on Synchrotron Radiation. However, it was felt that the Commission on Neutron Diffraction might be expanded to include synchrotron radiation. The President noted that the Executive Committee was considering the best way to cover synchrotron radiation within the existing Commissions of the IUCr.

F. H. HERBSTEIN (Israel) asked whether the compilation of temperature factors of cubic elements mentioned in the written report would be published in a more widely accessible form. Dr WILLIS replied that it had been rejected for publication in *Acta Cryst.* so he did not know what the next steps would be.

(17) *Acceptance of the written reports of the Commissions*

The written reports of all the Commissions were accepted, with the exception of the Commission on Biological Macromolecules, for which there was no report, and the Commissions on Crystallographic Studies at Controlled Pressures and Temperatures and on Electron Diffraction, for which the reports could only be circulated at the start of the General Assembly and were therefore to be considered at the second session.

(18) *Reports of the Representatives on Scientific and Regional Associates*

In accordance with Statute 8.5 the reports of the representatives on Scientific and Regional Associates had been circulated with the Agenda papers in June 1987. These reports are printed as Annex I, Appendix F to these Minutes. The reports were taken as read. Neither representative had anything further to add nor were there any questions by the delegates. The reports were accepted.

(19) *Application by the JCPDS International Centre for Diffraction Data to become a Scientific Associate*

The General Secretary reminded delegates that the JCPDS-ICDD had been accepted *ad interim* as a Scientific Associate by the Executive Committee in 1986 until the present General Assembly. The General Assembly now accepted this body as a Scientific Associate.

(20) *Reports of the Representatives on bodies not belonging to the Union*

In accordance with Statute 8.5 the reports of the representatives on bodies not belonging to the IUCr had been submitted to the National Committees and Commissions in June. The only exception was the report on the ICSU Committee on Space Research (COSPAR), which was only received in July and had been distributed to delegates just prior to the start of the General Assembly. Furthermore, the representative on this body, E. Kaldis, was not present at the General Assembly. All these reports are printed as Annex I, Appendix G to these Minutes. None of the representatives wished to add anything to the written reports, which were taken as read, nor did the delegates ask any questions.

At the President's suggestion, consideration of the report on COSPAR was deferred to the next session, to give all delegates a chance to read it (see Minute 24). All the other reports were accepted.

(21) *Sponsorship of meetings: Sub-committee on the Union Calendar*

The President reminded delegates that this was a Sub-committee of the Executive Committee and, therefore, the General Assembly was not required to approve the report which is given in Annex I, Appendix H.

M. NARDELLI, Chairman of the Sub-committee, informed delegates that four more meetings had received IUCr sponsorship at the meeting of the Executive Committee immediately prior to the General Assembly.

M. M. WOOLFSON (UK) sought assurance that, when a country exercised a policy of not issuing visas to intending participants from one or more countries, no further meetings would be sponsored by the IUCr in that country. Professor NARDELLI confirmed that this was the case.

Professor NARDELLI expressed his pleasure at the IUCr's policy of giving financial support to enable young scientists to attend scientific meetings. R. F. BRYAN (USA) applauded this funding and asked what steps had been taken to publicize the availability of these funds for the Perth Congress. E. N. MASLEN, Chairman of the Congress Organizing Committee, replied that it had been announced in the Congress Second Circular. He considered the five months' period between the date of distribution of this circular and the submission date for abstracts was sufficient. Certainly he had received many more requests than could be accommodated.

The President adjourned the session at 9.45 p.m.

**Second Session, Friday 14 August 1987, 7.30 p.m.**

(22) *Application for membership*

The President explained that an application to join the IUCr had been received very recently from the Bulgarian Academy of Sciences. In order to consider this application it was first necessary for the General Assembly to agree to add this item to the Agenda. This was agreed unanimously.

The application was for the Academy to adhere in Category I. A National Committee for Crystallography had been formed with the following membership: I. Kostov (Chairman), J. Maciček (Secretary), I. Bonev, V. Kretev, M. Maleev, S. Peneva, K. Petrov. Dr Maciček had been

nominated as the delegate to the General Assembly, if the request for membership was accepted.

The General Assembly noted that the Executive Committee considered the request to be in good order and recommended acceptance of the Bulgarian Academy of Sciences as an Adhering Body in Category I. The General Assembly unanimously accepted the Academy in Category I and welcomed Dr Maciček with applause.

(23) *Reports of the Commissions (continued)*

Since the delegates had now had time to read the remaining Commission reports, the President invited discussion concerning the Commission on Biological Macromolecules and the Commission on Electron Diffraction. He deferred discussion of the remaining report, on the Commission on Crystallographic Studies at Controlled Pressures and Temperatures, until later (see Minutes 25 and 37). In the absence of any report by the Chairman of the Commission on Biological Macromolecules, two members of the Commission had kindly compiled a report. This report and the report by the Chairman of the Commission on Electron Diffraction are included in Annex I, Appendix E. There was no discussion and the reports were accepted.

(24) *Reports of the Representatives on bodies not belonging to the Union (continued)*

Since the delegates had now had time to read the remaining report, on the ICSU Committee on Space Research (COSPAR), the President asked that it be considered. Since the IUCr representative was not present in Perth, the President offered to answer any questions but there were none. The report, which is included in Annex I, Appendix G, was accepted.

(25) *Commission on Crystallographic Studies at Controlled Pressures and Temperatures*

The President reported that the Executive Committee had unanimously decided to recommend to the General Assembly that this Commission be dissolved. The Executive Committee considered that the fields which had been the responsibility of this Commission should still be covered by other Commissions.

One of the main reasons for proposing this action was that, since this Commission was established in 1969, the level of its activities had not warranted a separate Commission. Three years ago the Executive Committee had been ready to recommend the termination of the Commission, but it was finally decided to give the Commission one more chance. The reason for this inactivity could be that the field was too small to merit a full Commission, even though scientifically it was a very important area.

The Executive Committee had ideas on how this field might be covered and was at present consulting the appropriate Commissions. The President explained therefore that he did not wish to go into further detail at this stage other than to mention that these plans would also allow for coverage of synchrotron radiation.

The President explained that it was necessary to determine the fate of the present Commission now, as the next item of business was the determination of the number of elected members of each Commission.

M. M. WOLFSON (UK) suggested that there should be regular reviews of the status of the Commissions and that at regular intervals, perhaps every nine years, there should

be a positive recommendation to continue a Commission. The President replied that the Executive Committee was already carrying out internal reviews of all Commissions.

In response to the request for more details of how the field would be covered, the President said that discussions were being held with the Commission on Crystallographic Apparatus (see also Minute 37).

The General Assembly unanimously agreed to terminate the Commission. The General Assembly also agreed to accept the report of the Commission.

(26) *Determination of the number of elected members of each Commission*

In accordance with Statute 5-10(d), the Assembly had to determine the number of persons to be elected on the Commissions until the Fifteenth General Assembly; these numbers did not include Chairmen, Co-editors, or *ex officio* members.

The Executive Committee did not recommend any changes in these numbers at this time but there had been discussions on possibilities of reducing the size of the larger Commissions in three years' time. One way would be for Commissions to make more use of consultants.

The numbers of elected members approved by the General Assembly (Chairmen not included) are set out below.

1. Commission on Journals	0
2. Commission on <i>Structure Reports</i>	0
3. Commission on <i>International Tables</i>	0
4. Commission on Biological Macromolecules	8
5. Commission on Charge, Spin and Momentum Densities	11
6. Commission on Crystal Growth and Characterization of Materials	8
7. Commission on Crystallographic Apparatus	7
8. Commission on Crystallographic Computing	7
9. Commission on Crystallographic Data	8
10. Commission on Crystallographic Nomenclature	0
11. Commission on Crystallographic Teaching	9
12. Commission on Electron Diffraction	10
13. Commission on Neutron Diffraction	9
14. Commission on Small Molecules	10

(27) *Proposal to establish a Commission on Powder Diffraction*

The proposal to establish the Commission, together with the proposed terms of reference, was circulated with the Agenda papers. Slightly amended terms of reference, as proposed by the Executive Committee, together with the proposed size of the Commission, had been circulated to the delegates at Perth.

In answer to a question, R. A. YOUNG (USA), who was nominated by the Executive Committee for the chairmanship of the Commission, observed that one of the terms of reference required the Commission to cooperate with other IUCr Commissions on matters concerning powder diffraction.

It was agreed to establish a Commission on Powder Diffraction with the following terms of reference:

- To advise the IUCr in organizing or sponsoring meetings, schools and Congress sessions on powder diffraction and related subjects.

- ii. To promote and coordinate scientific exchange between countries in the field of powder diffraction.
- iii. To cooperate with other IUCr Commissions on matters concerning powder diffraction.
- iv. To cooperate with other international bodies interested in powder diffraction and allied subjects.
- v. To promote useful interactions of the IUCr with the large world-wide body of X-ray and neutron powder diffractionists.
- vi. To promote the scientific growth and development of the field of powder diffraction.

The size of the Commission approved by the Assembly was a Chairman, six elected members and an *ex officio* member representing the Joint Committee for Powder Diffraction Standards (JCPDS).

(28) *Commission on Modulated Structures, Polytypes and Quasi-crystals*

In October 1986 a suggestion was received by the President for a Commission on Modulated Structures, Polytypes and Quasi-crystals. The President reported that Professor Janner had consulted people in the field and had made suggestions for members of such a Commission. However, to date, no-one was willing to be nominated as Chairman. Discussions were continuing and the President hoped that the Executive Committee would be able to present a full and complete written proposal by the time of the third session of the General Assembly for establishment of a Commission on an *ad interim* basis for the next three years (see Minute 36). In the meantime he invited comments and suggestions from delegates.

M. M. WOOLFSON (UK) wondered how many people worked in this field because, when he was a Co-editor of *Acta Cryst.*, he found it difficult to find suitable referees. The President thought that one of the reasons for suggesting the Commission was the lack of papers in this field in *Acta Cryst.*

(29) *Commission on Crystallographic Information*

Without implying any criticism of the present Commissions, H. C. FREEMAN (Australia) wished to focus the attention of the IUCr, in a formal way, on the fact that there now existed means of accumulating, checking, transmitting and storing information which did not exist before. The Australian delegation therefore proposed that the General Assembly ask the Executive Committee to report to the XV General Assembly concerning the desirability of creating a Commission on Crystallographic Information to replace the present Commissions on Journals, *Structure Reports* and Crystallographic Data.

Y. EPELBOIN (France) was concerned that such a Commission would have too many members. Whilst the proposed size of the Commission would be for the Executive Committee to decide, Professor FREEMAN thought that it should not be a large Commission with many *ex officio* members, but rather a small group of thinkers and scholars capable of thinking collectively about journals, reports and databases as information.

H. D. FLACK (Switzerland) asked why *International Tables* were not included in the proposal. Professor FREEMAN thought that *International Tables* were a different way of storing information, in that they represented information which had already been digested and processed through an additional stage, but if that philosophy

was incorrect then perhaps *International Tables* should also be included.

W. A. HENDRICKSON (USA) liked the idea of a Commission of impartial people overseeing the Commission on Journals.

F. H. HERBSTEIN (Israel) felt that there was some confusion in the proposal. The Commissions of the IUCr were operational units which worked in their respective fields. He thought that the idea raised was most important but would be better tackled by setting up some form of *ad hoc* body, rather than another Commission, to consider the future of dealing with information in crystallography.

In response to other speakers, Professor FREEMAN emphasized that his idea was that the Executive Committee should consider whether it still made sense to divide crystallographic information into three subsets as at present. The motion should encourage the Executive Committee to explore other avenues of dealing with this information.

R. F. BRYAN (USA) endorsed Professor Herbstein's remarks and suggested that an *ad hoc* committee should be set up by the Executive Committee as a working party to consider the relationships between the existing Commissions and should report to the Executive Committee on the best way to achieve the result.

The motion as originally proposed by Professor Freeman was approved.

(30) *Determination of the general policy and the timetable for the period to the Fifteenth General Assembly*

The General Secretary explained that he had nothing to report under this Agenda item since the Executive Committee's proposals for activities during this period would be mentioned under other Agenda items. The President asked if there were any further comments. There were none.

(31) *Preliminary consideration of activities for the period 1990-1993*

The General Secretary had nothing to report and there were no further comments.

(32) *Budget estimates for the period to the Fifteenth General Assembly: determination of the unit contribution*

The Treasurer referred to the budget estimates distributed with the Agenda papers and printed as Annex I, Appendix I to these Minutes. He drew attention to the comparison between the General Fund budget for the triennium 1984-1986 which was considered at the previous session and the General Fund estimates for the triennium 1987-1989, and he showed a transparency giving the comparison. These estimates had been compiled in early 1987 at the time of preparation of the Agenda papers.

The subscription income had been prepared on the basis of the proposal to continue the unit contribution unchanged at Sw Fr 890.

The other main income was the yield from investments and bank accounts. In his presentation of the Financial Report (Minute 7) he had explained the change in policy from short-range high-interest investments to long-range safety with a resultant reduction in the interest rates. In addition there was the allocation of interest to the Ewald Fund. Both these factors reduced the total estimated yield from investments compared with that received in the General Fund in the previous triennium.

For the expenditure there was an increase in administration costs, which included salaries. The payments to ICSU and ICSU bodies were small but reasonably predictable. The expenses for scientific meetings included the sponsorship of such meetings and showed an increase of about Sw Fr 100 000 over the previous triennium. This estimate included the financial support of the present Congress but it did not include support to young scientists, which was charged to the Research and Education Fund and which was estimated to be Sw Fr 160 000. The transfers to other accounts represented the transfers from the General Fund to the new funds which could be made to balance the General Fund.

The General Assembly accepted the budget estimates and approved the continuation of the unit contribution at Sw Fr 890 for the years 1988, 1989 and 1990.

(33) *Confirmation of the date and place of the Fifteenth General Assembly*

M. HOSPITAL (France) confirmed that the Association Française de Cristallographie and the Académie des Sciences were pleased to invite the IUCr to hold the Fifteenth General Assembly and Congress in Bordeaux, 19–28 July 1990. He would be Chairman of the Congress Organizing Committee and Professor A. Authier would be Chairman of the Congress Programme Committee. He explained that the meeting would be held in late July to enable university accommodation to be used. A. AUTHIER (France) reported that several satellite meetings and schools were planned, including the traditional school on crystallographic computing, and meetings on the application of synchrotron and neutron radiation to the diffraction analysis of nuclear and magnetic structures and on local order by X-ray and neutron diffuse scattering and spectroscopy.

The invitation, which had been preliminarily accepted in 1984, was formally accepted unanimously.

The President then adjourned the session at 9.30 p.m.

**Third Session, Tuesday 18 August 1987, 7.40 p.m.**

(34) *Restrictions on the distribution of the IUCr's journals*

In response to an earlier request from the UK delegation (see Minute 11), the President reported that a new law had been introduced in Denmark forbidding trade by Danish companies with certain countries. This specifically affected the IUCr because it prevented Munksgaard, the publisher of the IUCr's journals, from accepting orders for journals from these countries. The problem had been under constant study by the IUCr's Finance Committee and Executive Committee.

Negotiations were currently in progress between ICSU and the Danish government, involving the Danish Academy of Sciences, and the IUCr was obtaining legal advice as to whether the collection of subscriptions to and the distribution of our journals to these countries actually constituted commercial trade, because the Danish law applied to commercial trade, or whether the IUCr, as a non-commercial organization, and Munksgaard, acting as an agent for the IUCr, could be exempt from this law.

The General Secretary reported that, after a visit to Munksgaard when he learned of this law, he asked the Danish Academy to negotiate on behalf of the IUCr to rectify this violation of ICSU's policy of non-discrimination. He indicated to the Academy that, if a satisfactory

solution could not be reached, it would be necessary for the IUCr to seek a publisher elsewhere. The reply from the Academy sounded somewhat reluctant, in that it stated that the situation called for patience and did not require action from the Academy at present. Therefore in March 1987 the President and the General Secretary wrote to ICSU, as the highest scientific authority, to take action to rectify the situation. ICSU promised to help.

M. M. WOOLFSON (UK) suggested that, in considering this question, delegates should not consider the specific problem or the specific countries affected, but rather consider the more general problem.

Professor WOOLFSON proposed the following motion: "The General Assembly notes with concern the circumstances which may prevent Munksgaard, the Union's publishers, from serving the crystallographic community in a way which fully upholds ICSU policy on the Free Circulation of Scientists and related matters.

The General Assembly urges the Executive Committee to continue monitoring the situation as it develops and to take all necessary steps to ensure that there is neither discrimination against any members of the IUCr nor handicap to the pursuance of their activity as scientists."

He requested delegates to consider this as a general motion, even though in this case Munksgaard was mentioned, and to support the Executive Committee in their attempts to obtain a solution. The motion was approved almost unanimously, by 63 votes to 3 with 1 abstention.

(35) *Application of the Asian Crystallographic Association (ASCA) to become a Regional Associate*

The President informed delegates that a new association, the Asian Crystallographic Association, had been formed on 17 August 1987, and that the Association had requested acceptance by the IUCr as a Regional Associate. He asked the General Assembly to agree to this request being added to the Agenda. The Assembly agreed.

The newly elected President of the Association, S. R. HALL (Australia) summarized the background leading to its formation. After some discussion on the region covered by the Association, the Assembly accepted it as a Regional Associate of the Union.

(36) *Ad interim Commission on Modulated Structures, Polytypes and Quasi-crystals*

The President reported that the group meeting at Perth had been able to suggest a membership for this proposed Commission, consisting of a Chairman and eight members. The Executive Committee had now set up an *ad interim* Commission with this membership. The membership was reported later in the session as D. Gratias (France) (Chairman), M. Farkas-Jahnke (Hungary), H. Jagodzinski (Federal Republic of Germany), A. Janner (Netherlands), P. Krishna (India), D. Kucharczyk (Poland), K.-h. Kuo (People's Republic of China), S. Nakashima (Japan), M. L. Senechal (USA).

(37) *Incorporation of the fields of crystallographic studies at controlled pressures and temperatures within the Commission on Crystallographic Apparatus*

The President reported on the discussions previously referred to (Minute 25) on which there was now full agreement on how to incorporate these fields in the Commission on Crystallographic Apparatus, by the formation of a

sub-committee within the latter Commission, whose Chairman, D. C. Creagh, would submit a full report on the proposals for consideration by the Executive Committee.

(38) *Incorporation of the field of synchrotron radiation within the Commission on Crystallographic Apparatus and the Commission on Neutron Diffraction*

The President reported that he had discussed this idea with the Chairmen of both Commissions, who had compiled a joint report for consideration by the Executive Committee.

(39) *IUCr/Oxford University Press Book Series*

The General Secretary reported that there had been negotiations with Oxford University Press for several years on a book series which would have two subseries, one for crystallographic symposia and one for monographs on crystallography. The background to this book series was given in the General Assembly papers and is included as Annex I, Appendix J. Acceptable terms had been determined for an agreement which had now been approved by the Executive Committee. In 1986 the Executive Committee initiated a Book Series Committee with J. H. Robertson as Chairman. The General Secretary explained that, since the Committee had been established by the Executive Committee, there was no requirement for the General Assembly to approve it, but he invited Dr Robertson to speak since he thought the General Assembly would be interested.

Dr ROBERTSON reported that the membership of the Committee would be A. M. Glazer (UK), J. P. Glusker (USA), K. Kuchitsu (Japan), V. I. Simonov (USSR), with H. Stanbury as an *ex officio* representative of the Oxford University Press, and the President and the General Secretary of the IUCr as *ex officio* members.

The work of the Committee would be divided into two: the acceptance for publication of the lectures given at IUCr-sponsored schools or symposia, and the pursuance of fresh ideas to be published in the form of monographs or textbooks. Suggestions for about four such monographs had been received already at the present Congress.

S. R. HALL (Australia) spoke against the publication of refereed papers of symposia because, when such papers were published, they were thereafter quoted in the literature. He therefore proposed that conference proceedings should be published in the IUCr/OUP Crystallographic Symposia Series only in cases where the individual contributions had been subjected to refereeing at the same standards as applied to contributions to the IUCr's journals. During the ensuing debate it was requested that such refereeing should be done in such a way as to minimize any delay in publication and the fact that contributions had been refereed should be clearly stated in the publication. The motion was approved.

(40) *Preliminary consideration of the date and place of the Sixteenth General Assembly*

In accordance with By-Law 1.3, the General Assembly could give preliminary consideration to the place of the next but one General Assembly, namely the Sixteenth General Assembly to be held in 1993. Two invitations had been received, from the Chinese National Committee for Crystallography and the China Association for Science and Technology, to hold the General Assembly and Congress in Beijing, People's Republic of China, 20-28 August 1993, and from the National Academy of Sciences in the United

States, through the US National Committee for Crystallography, to hold the General Assembly and Congress in Washington, DC, USA, during the first two weeks of August 1993. Detailed invitations had been distributed to delegates at the General Assembly.

The Executive Committee had met representatives of both prospective hosts and had discussed the invitations with them, including the details of the arrangements as known at present and the question of the free circulation of scientists. The Executive Committee found both invitations to be in order and acceptable for consideration by the General Assembly.

The President invited a spokesman from each delegation to present the invitation and to answer questions, after which a secret ballot was held in which the General Assembly gave preliminary acceptance to the invitation to meet in Beijing.

(41) *Confirmation of the appointments of the Editors of the publications of the IUCr*

In accordance with Statute 7.1, the initial appointments and reappointments of the Editors of the publications of the IUCr were made by the Executive Committee and were subject to confirmation by the General Assembly. The General Secretary explained that, in addition to the appointment and reappointments given in the Agenda papers, the Executive Committee had reappointed Th. Hahn as Editor of *International Tables* Volume A for work on future editions of that volume.

The Assembly unanimously confirmed the following appointment and reappointments for the period of three years:

- Editor of *Acta Crystallographica*: C. E. Bugg (USA)
- Editor of *Journal of Applied Crystallography*:  
M. Schlenker (France)
- Editor of *Structure Reports*: G. Ferguson (Canada)
- Editor of *International Tables* and Editor of Volume C:  
A. J. C. Wilson (UK)
- Editor of Volume A:  
Th. Hahn (Federal Republic of Germany)
- Editor of Volume B: U. Shmueli (Israel)

(42) *Election of Chairmen and members of Commissions*

The nominations made by the Executive Committee for the Chairmen and elected members of Commissions had been notified to delegates.

The General Secretary reminded delegates that this list included nominations for all elected members of Commissions but not for any *ex officio* members. The General Secretary drew the attention of delegates to the addition of the Chairman of the Commission on Crystallographic Data as an *ex officio* member of the Commission on *International Tables*, an addition which had been requested by the Chairman of the latter Commission and had been endorsed by the Executive Committee. Thus the membership of the Commission on *International Tables* would consist of the Editors listed in Minute 41 above together with the Chairmen of the Commissions on Charge, Spin and Momentum Densities, Crystallographic Apparatus, Crystallographic Computing, Crystallographic Data, Crystallographic Teaching, Electron Diffraction and Neutron Diffraction as *ex officio* members.

Since there were no other nominations for any of the Commissions, the persons nominated by the Executive

Committee were considered elected. The full memberships of the Commissions, including the *ex officio* members, together with the addresses of the Chairmen, are given in Annex III. These names include the membership of the *ad interim* Commission on Modulated Structures, Polytypes and Quasi-crystals, which were read out by the President (see Minute 36).

(43) *Election of Representatives on bodies not belonging to the Union and on Regional and Scientific Associates*

The nominations made by the Executive Committee for those representatives to be elected by the General Assembly had been notified to delegates. As no other nominations had been made these persons were considered elected.

The names and addresses of the representatives of the IUCr, including those appointed *ex officio*, are given in Annex III.

(44) *Election of Officers of the Union*

In accordance with By-Laws 2·2 and 7·1, the nominations made by the Executive Committee for Officers of the Union had been notified to delegates. These nominations had been included in the Agenda papers.

As no other nominations had been made the Officers nominated were considered elected, as follows:

President:

M. Nardelli (Italy)

Vice-President:

Y.-q. Tang (People's Republic of China)

General Secretary and Treasurer:

A. I. Hordvik (Norway)

Ordinary Members (six years):

P. Coppens (USA)

R. Diamond (UK)

S. A. Semiletov (USSR)

Professor KURKI-SUONIO expressed his great gratitude to all members of the Finance Committee, especially to the two Conveners during his six years as General Secretary and Treasurer, Professor Woolfson and Dr Diamond, to the Executive Secretary, Dr King, to the Technical Editors, first Dr Penfold and then Mr Dacombe, and to Mrs Cawley, all of whom he asked to be thanked with applause. He then

introduced his successor, Professor Hordvik, to the General Assembly.

The President greeted all members of the new Executive Committee and thanked all members of the retiring Executive Committee, particularly those members who had tonight retired, Dr Karle, Professor Simonov and Professor Kurki-Suonio, for their constant and spirited cooperation in the past triennium. This was accepted with applause by the General Assembly.

There being no other business, and therefore no need for the final session of the General Assembly which had been scheduled for the morning of 20 August, the President declared the Fourteenth General Assembly concluded at 9.40 p.m.

**Closing Ceremony, Thursday 20 August 1987, 9.00 a.m.**

Professor S. R. Hall took the chair.

V. I. SIMONOV, the retiring Vice-President, spoke on the role of the IUCr.

E. N. MASLEN, the Chairman of the Congress Organizing Committee, reported on the Congress and expressed his ideas for future Congresses.

Th. HAHN, the retiring President, thanked the members of the Congress Programme Committee and those Australians who had helped with the preparation of the excellent programme and the handling and publishing of the Congress abstracts, the University of Western Australia and its Vice-Chancellor, Professor R. H. T. Smith, and the local committee and its team of helpers who had ensured that everything ran so smoothly. He then introduced the new members of the Executive Committee and thanked the retiring members, J. Karle, K. V. J. Kurki-Suonio and V. I. Simonov, and the Chester office staff.

M. NARDELLI, the new President, thanked Professor Hahn for his friendly but firm leadership of the IUCr over the last three years. He reminded those present that crystallography was now an important section of modern science, even if this was not as well recognized as it should be. It was the duty of all crystallographers to make our science well known, particularly to the man in the street.

Professor Nardelli then declared the Fourteenth General Assembly and Congress officially closed.

## ANNEX I

## Appendices to the Agenda of the Fourteenth General Assembly

## Appendix A: Report of the Executive Committee

*Executive Committee and Finance Committee Meetings*

The Executive Committee met in Hamburg in August 1984 before and during the XIII General Assembly, in Rowton, near Chester, England, in July 1985 and in Frodsham, near Chester, England, in July 1986. The Finance Committee met twice a year, the second time being prior to the Executive Committee meeting, to prepare its advice and recommendations on finances, establishment and staff matters.

The most important items of business treated by the Executive Committee in the triennium in these meetings and in postal ballots between the meetings were:

- (1) Editorial policy, pricing policy and subscription rates, approval of appointments of Co-editors and other matters concerning the IUCr's journals.
- (2) Future of *Structure Reports* and their cooperation with data bases, including relations between the IUCr and the Cambridge Crystallographic Data Centre.
- (3) Publication and pricing of new Volumes and Editions and approval of section authors for *International Tables*.
- (4) *World Directory of Crystallographers*.
- (5) Arrangements with the publishers.
- (6) Initiation of an agreement with the Oxford University Press to start an IUCr/OUP Book Series.
- (7) Establishment of a Book Series Committee to develop the IUCr/OUP Book Series.
- (8) Future development of electronically assisted publication.
- (9) Approval of the audited accounts for the previous year.
- (10) The General Fund estimates and the level of the unit contribution.
- (11) Investment policy.
- (12) Application for US Tax-exempt Status.
- (13) Establishment of the Publications and Journals Development Fund and the Research and Education Fund, and uses of these new Fund Accounts.
- (14) Establishment of the Ewald Prize and Ewald Fund.
- (15) Appointment of the Selection Committee for the first Ewald Prize.
- (16) Sponsorship of meetings and possible financial support for meetings.
- (17) Young scientists' support to meetings.
- (18) Criteria for sponsorship.
- (19) Free circulation of scientists.
- (20) Approval of the membership of the Programme Committee for the XIV Congress.
- (21) Discussion of the arrangements for the XIV General Assembly and Congress with the Programme Committee.
- (22) Level of financial support for the Congress and its satellite meetings, including a separate fund for young scientists.
- (23) Travel support to Commission Chairmen, Editors and Co-editors for XIV Congress and General Assembly.
- (24) Review of the activities of the Commissions.
- (25) Establishment of an *ad interim* Commission on Powder Diffraction.
- (26) Review of the IUCr's representation on the Scientific and Regional Associates of the IUCr and on other bodies.
- (27) Relations between the IUCr and the JCPDS, and the application of the JCPDS-ICDD to become a Scientific Associate of the IUCr.
- (28) Nominations for Officers of the IUCr and for Chairmen and members of Commissions, and proposals from the National Committees and Commissions for these positions.
- (29) Appointment of the Editors of the IUCr's publications.
- (30) Appointment of new staff in the IUCr office in Chester. Salaries and pensions.
- (31) Upgrading of office technology in the IUCr office in Chester.
- (32) Refurbishment of the IUCr office premises.

*Publications*

The subscription prices (in Danish Kroner) of *Acta Crystallographica* and the *Journal of Applied Crystallography* have been kept constant through the whole triennium (and even up to 1987), except that *Acta Cryst.* Volumes B and C have been made available separately since 1986.

The total annual number of pages published reached a minimum in 1985. The numbers of pages in 1984, 1985 and 1986 were:

	1984	1985	1986
<i>Acta Cryst.</i> Section A	728	624	588
<i>Acta Cryst.</i> Section B	616	456	640
<i>Acta Cryst.</i> Section C	2126	1836	1892
<i>J. Appl. Cryst.</i>	488	546	492
Total	3958	3462	3612

At the same time the total number of subscriptions showed a slight decrease being 5,086, 5,115 and 4,978 in 1984, 1985 and 1986 respectively. More details are given in the Report of the Commission on Journals (see Appendix E).

The editorial policy and the development of editorial procedures were discussed at length and in detail at all Executive Committee meetings during the triennium. For this purpose the Executive Committee invited the Chairman of the Commission on Journals to each of its meetings and the Editor of *J. Appl. Cryst.* to the meeting in 1986 to report and to discuss these questions, with the view of making this a permanent practice.

Great emphasis was given to widening the coverage of the IUCr's journals, with the aim that the journals would

reflect the state of the whole of modern crystallography as it is covered in the IUCr Congresses and in the work of the IUCr Commissions.

To that effect, publication of the proceedings of selected meetings was encouraged. Several Commissions were approached to identify their publication needs. It was further agreed to ask National Committees, Commissions and conference organizers to encourage publication in the IUCr's journals. The Editors and the Commission on Journals were encouraged to develop the policies and editorial practices towards wider coverage and more flexible rules. They were invited to consider whether changes in the basic structure of the IUCr's journals would be necessary.

Volumes 52A, 46B and 48B of *Structure Reports* and Volume 15 of *Molecular Structures and Dimensions* were published in the triennium. The decreasing sales numbers reached the point where serious consideration of the future and the financial and scientific feasibility of *Structure Reports* became necessary. The Chairman of the Commission on *Structure Reports* was invited to the Executive Committee meetings, to report and to discuss the perspectives, together with the Chairman of the Commission on Crystallographic Data and Dr O. Kennard from the Cambridge Crystallographic Data Centre (CCDC). It was agreed to establish cooperation with the Inorganic Crystal Structure Data Base (Federal Republic of Germany) and the Metals Data File (Canada) for computerized production of Section A (Metals and Inorganic Compounds).

Because of the rapidly increasing accumulation rate of organic structures and the decreasing sales, the production of *Structure Reports* Section B in its present form was no longer feasible and had to be terminated. Computerized production in a simplified format, in cooperation with the CCDC, and possible combination with *Molecular Structures and Dimensions*, have been considered but no realistic solution has yet been found (see Appendix E).

For *International Tables* a Brief Teaching Edition of Volume A was published. Volume A, as well as the old Volumes II and III, were reprinted and another short reprint of Volume A was made while the revised second edition of Volume A was prepared. The editorial work for the new Volumes B and C has continued throughout the triennium (see Appendix E).

The Seventh Edition of the *World Directory of Crystallographers*, edited by Dr A. L. Bednowitz, and the second set of *Teaching Pamphlets on Crystallography*, edited by Professor C. A. Taylor with the support of the Commission on Crystallographic Teaching, were published in the triennium.

It was agreed to establish, in cooperation with the Oxford University Press, an IUCr/OUP *Crystallographic Book Series* with two subseries (Appendix J). The first subseries, *IUCr Crystallographic Symposia*, would be a continuation and extension of the series of proceedings of the computing schools organized by the Commission on Crystallographic Computing. Two of these proceedings were published in the triennium, one edited by Hall & Ashida and the other by Sheldrick *et al.* The second subseries would be *Monographs on Crystallography*.

A Book Series Committee was established to develop the Book Series, to select suitable conferences, to identify topics and authors and to evaluate proposals and manuscripts. It would submit proposals for the monograph series to the Executive Committee for approval. Dr J. H. Robertson was

appointed to serve as Chairman. The organizers of meetings and schools sponsored by the IUCr are informed of the symposia series as a possible channel for publication of their proceedings. The National Committees and the IUCr Commissions are invited to submit proposals for these series.

#### *Sponsorship of meetings*

The Executive Committee has a Sub-committee on the Union Calendar to consider and to advise the Executive Committee on questions concerning the sponsorship of meetings. The Chairman of the Committee has been Professor Nardelli in this triennium.

Because of its improved financial status, the IUCr could be more generous than earlier in providing financial support for meetings. A list of IUCr-sponsored meetings is given in the report of this sub-committee (Appendix H). Special funds were given to the meetings' organizers to support the travel and attendance of young scientists. The latter support was offered to all meetings sponsored, irrespective of the rules restricting the general financial support to regularly occurring meetings. However, no sponsorship was given to meetings held at too close a time interval to the IUCr Congress.

It was agreed that applications for sponsorship and financial support would normally only be considered if they were submitted at least six months in advance of the date of the meeting. Requests from satellite meetings should be submitted, and possible financial support should be requested, through the organizing committee of the main meeting.

In the context of problems concerning visa issuance to participants at some of the IUCr-sponsored meetings, the Executive Committee confirmed once again that the IUCr subscribes to ICSU's policy of non-discrimination and adheres to its decisions and procedures concerning Free Circulation of Scientists. In accordance with the decisions of the ICSU General Assembly in 1985, it was agreed that it was deplorable that *bona fide* scientists should be required to sign a repudiation document in order to obtain a visa for entry into a country to attend an international meeting. Consequently, it was decided that the IUCr would not sponsor a meeting in any country which required such a repudiation document to be signed.

It is up to ICSU to negotiate with the authorities of the relevant countries and to find a mutually acceptable solution to these problems.

#### *Commissions of the IUCr*

Each Commission Chairman is required to provide a written triennial report to the General Assembly. These reports are given as Appendix E.

Professor R. A. Young agreed to convene an *ad hoc* committee, with the aim of preparing firm proposals for the establishment of a Commission on Powder Diffraction.

In view of the high travel costs, a fund of US \$15 000 was made available between the non-publishing Commissions to enable the Chairmen to attend the General Assembly for the presentation and discussion of their reports.

Funds totalling US \$20 000 were similarly made available to the publishing Commissions, particularly to enable a full meeting of the Commission on Journals for discussion of IUCr journals policies.

*Relations between the IUCr and other bodies*

The reports of the representatives of the Union on other bodies are given as Appendix G.

The development of relations between the IUCr and the JCPDS became necessary when the JCPDS initiated its journal *Powder Diffraction*. It was mutually agreed that a member of the Commission on Journals will represent the IUCr on the Editorial Board. It is further intended that the JCPDS will have its representative on the proposed IUCr Commission on Powder Diffraction.

The discussions led to an application from the JCPDS to become a Scientific Associate of the Union.

*International Council of Scientific Unions (ICSU)*

Dr J. Karle represented the IUCr at the meetings of the General Committee and at the General Assemblies of ICSU held in 1984, 1985 and 1986 in Ottawa, Munich and Berne, respectively. Professor K. V. J. Kurki-Suonio attended a meeting of the Treasurers of the Unions in June 1985 in Paris.

ICSU is an international scientific organization composed of 20 international scientific Unions, 71 National Members, Associates and Observers and 21 Scientific Associates. ICSU's primary objective is to 'encourage international scientific activity for the benefit of mankind'. It does this by organizing international interdisciplinary research programmes, acting as an agent for the exchange of ideas and scientific information and the establishment of standards, nomenclature and units, sponsoring very numerous (hundreds per year) congresses, conferences, symposia, schools and meetings, and publishing a large variety of scientific information in the form of a journal, proceedings of meetings, newsletters and handbooks. Some of the major concerns in the past three years have been the establishment of a new programme entitled 'International Geosphere-Biosphere: A Study of Global Change', which concerns a long-range multidisciplinary study of changes on the earth and their implications for the future, an in-depth examination of the 'Environmental Consequences of Nuclear War' that resulted in an excellent text on the subject that is being given wide circulation, toxic waste disposal, advances in biotechnology, and a continuing dedication to the free circulation of scientists. A major enhancement of the organization of the Committee on Science and Technology in Developing Countries (COSTED) has been made with Regional Secretariats being established in five different areas of the world in order to strengthen ICSU's activities in developing countries.

*IUCr staff*

There have been several changes in the IUCr staff in the triennium. The Deputy Technical Editor, Dr J. E. Derry, died on 2 September 1985. The Technical Editor, Dr D. W. Penfold, resigned as from 31 December 1985. There have also been changes in the secretarial staff, including Mrs J. I. Heywood, who left in 1986 after working for the IUCr since 1968.

The present staff in the IUCr office in Chester is: Dr J. N. King (Executive Secretary), Mrs A. Cawley (Administrative Assistant to the Executive Secretary), Mrs K. S. Skelling (Part-time Secretary), Mr M. H. Dacombe (Technical Editor), Miss S. E. Lowe (Assistant Technical Editor), Mr P. R. Strickland (Assistant Technical Editor), Miss A. J. Sharpe (Editorial Assistant), Mr B. McMahon (Editorial

Assistant), Miss J. A. Glendenning (Secretary), Ms L. Allsop (Part-time Secretary).

The working facilities in the office have been improved by purchasing new equipment, by upgrading the IUCr computer and developing its editorial uses and by a major refurbishment of the IUCr premises. Among the purchases are: word processors for the secretarial staff, a modem to connect the computer with data bases for journal checking procedures and a facsimile machine, particularly for communications with the printers and Co-editors.

*Acknowledgements*

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the Society of Crystallographers in Australia and the Australian Academy of Science for the invitation to hold the Fourteenth General Assembly and International Congress of Crystallography in Perth. It particularly wishes to thank the Chairman of the Programme Committee, Professor H. C. Freeman, and the Chairman of the Organizing Committee, Dr E. N. Maslen.

The continuing support shown by Unesco in the form of its annual subvention received by the IUCr through ICSU, and the support of ICSU itself, is gratefully acknowledged.

Finally, the Executive Committee wishes to thank all crystallographers who have assisted in the work of the IUCr in so many ways. This cooperation between crystallographers of different nationalities constitutes a most valuable aspect of the IUCr's activities.

**Appendix B: Financial Report***The funds' structure*

The accounts of the IUCr for the calendar years 1984 and 1985 have already been published [*Acta Cryst.* (1986), A42, 58-79 and (1987), A43, 137-155]. The accounts for 1986 have been audited and will be published in *Acta Crystallographica* Section A in due course [*Acta Cryst.* (1988), A44, 81-103]. The accounts for the three years 1984, 1985 and 1986 are summarized in Tables 1-14, in which all the amounts are expressed in Swiss Francs. (In this report the notations of the international standard ISO 4217 confirmed by the International Standard Organization in 1978 are used for the currencies: CHF = Swiss Franc, GBP = Pound Sterling, USD = US Dollar, NLG = Netherlands Guilder, DKK = Danish Krone, JPY = Japanese Yen, ITL = Italian Lire.)

Table 1 shows a comparison of the fund accounts at the beginning and the end of the triennium. In 1984 two new funds, the Publications and Journals Development Fund (PJDF) and the Research and Education Fund (REF), were established, the Special Publications Fund (SPF) and the General Publications Fund (GPF) were dissolved, and the separate small book funds were amalgamated into one, the Book Fund (BF).

The SPF had been established for the special funding and costs of the office computer. It had fulfilled its purpose and was at zero balance. The resources of the GPF were shared, on the basis of their historical origin, between the *International Tables* Fund (ITF) and the PJDF.

The Ewald Fund account (EF) was opened in 1986 to carry the capital, income and expenditure of the Ewald Prize.

Table 1. *Balance Sheet, Fund Accounts*

	31 December 1983	Fluctuations in rates of exchange	31 December 1986
<i>Acta Crystallographica</i>	864 961	-297 210	1 577 901
<i>Journal of Applied Crystallography</i>	239 292	-62 514	329 591
<i>Structure Reports</i>	137 079	-17 726	110 460
<i>International Tables</i>	32 603	-32 780	176 461
<i>Fifty Years of X-ray Diffraction*</i>	5 127	—	—
<i>Escher Drawings*</i>	21 095	—	—
<i>Early Papers*</i>	-9 827	—	—
<i>Fifty Years of Electron Diffraction*</i>	-10 515	—	—
Book Fund†	—	-2 144	11 440
<i>Molecular Structures and Dimensions</i>	6 846	-985	5 861
Publications and Journals Development Fund‡	—	-63 548	366 651
Research and Education Fund†	—	-50 292	292 000
General Publications Fund*	75 023	—	—
Total of publication accounts	1 361 684	-527 199	2 870 365
General Fund	538 944	-149 807	801 077
President's Fund	16 589	-2 687	15 573
Ewald Fund‡	—	-22 195	120 884
Total accumulated balance	CHF 1 917 217	CHF -701 888	CHF 3 807 899

\* Fund closed in 1984.

† Fund established in 1984.

‡ Fund established in 1986.

*General financial development*

As seen from Table 1, a loss of CHF 701 888 has arisen in the triennium as a consequence of fluctuations in rates of exchange. This consists of a gain of CHF 145 333 in 1984 and losses of CHF 148 057 and CHF 699 164 in 1985 and 1986, respectively. The annual gains or losses have been divided between the fund accounts with credit balances, in direct proportion to these balances.

The loss is mainly due to the depreciation in value of the GBP and the USD in relation to the CHF. These are the two main currencies of operation of the IUCr, and most of the IUCr's holdings have been kept in these currencies over the triennium. The exchange rates operational at 1 January 1984 were CHF 1 = NLG 1.3899 = DKK 4.4953 = GBP 0.3142 = USD 0.4587, and at 31 December 1986 CHF 1 = NLG 1.3393 = DKK 4.4643 = GBP 0.4167 = USD 0.5952 = ECU 0.5730 (ECU = European currency unit).

In spite of the large loss from fluctuations in rates of exchange, the total assets of the IUCr have increased by a factor of 2.0 over the triennium. The loss depends on the accounting currency. In terms of GBP or USD it would have been small, if any. Expressed in these currencies the total assets went from GBP 602 390 or USD 879 427 to GBP 1 586 752 or USD 2 266 461, both corresponding to an increase by a factor of 2.6. The growth comes from two sources, the interest income and the profit from the IUCr's journals and, to a lesser extent, *International Tables*, which have both been much larger than could possibly be anticipated in 1984 at the XIII General Assembly.

*The assets*

Table 2 shows the distribution of assets. The value of the stocks of unsold copies of the journals and other publications is not included in the assets. The amount CHF 333 626 for debtors at 31 December 1986 includes the IUCr's fund-

Table 2. *Balance Sheet, Assets*

	31 December 1983	31 December 1986
<i>Current assets</i>		
Cash at banks		
Current Accounts	134 498	225 193
Deposit and Savings Accounts	1 120 197	1 677 678
	1 254 695	1 902 871
Cash with Union officials	8 321	4 075
Debtors	413 694	333 626
Subscriptions due	24 723	16 020
	1 701 433	2 256 592
<i>Deduct Creditors and accrued charges</i>	121 401	139 585
<i>Net current assets</i>	1 580 032	2 117 007
<i>Investments</i>		
At market value	333 086	1 689 671
Change in value	-1 031	-7 616
	332 055	1 682 055
<i>Fixed assets</i>		
Office equipment at cost, less depreciation	5 130	8 837
<i>Total assets</i>	CHF 1 917 217	CHF 3 807 899

ing of the XIV General Assembly and Congress paid in advance. The largest part, however, relates to amounts due at that date in respect of the publishing operations during 1986, from Munksgaard for the journals and from Reidel

for *International Tables*, *Structure Reports* and other publications. These amounts, due in 1987, and the great majority of the other amounts under debtors and creditors, have since been settled.

The nature of the assets was changed considerably during the triennium. At the end of the previous triennium about 80% of the holdings were high-yield, short-term deposits or bank accounts (under the heading 'Cash at banks' in Table 2) and the remaining 20% were medium-term government bonds (under the heading 'Investments'). Almost all, about 95%, were held in the main operational currencies, USD and GBP, in the ratio 1:1.05. Through most of the triennium the monies were kept mainly on short-term deposits, which enjoyed high interest rates, while the distribution of currencies was slowly widened. In 1986 the emphasis was changed from high-rate short-term gain to long-term protection of IUCr's assets. This was achieved by seeking medium- to long-term investments with lower interest rates but with high capital growth, while keeping the interest income at a level required by the IUCr's annual operations.

By 31 March 1987 this change had been largely accomplished. At that date 64% of the total were in investments, while Table 2 shows only 44% at 31 December 1986. They included different kinds of government bonds with maturing dates varying from 1988 to 1998, CHF 490 000 were invested through the Union Bank of Switzerland (UBS) in Geneva, GBP 204 000 or CHF 480 000 through the National Westminster Bank (NWB) in Manchester, ECU 105 000 or CHF 175 000 through the Amsterdam-Rotterdam Bank NV (AMRO) in Groningen, USD 450 000 or CHF 680 000 through Merrill Lynch Capital Markets Agency in New York. Further, GBP 300 000 or CHF 715 000 were invested through N. M. Rothschild & Sons Asset Management (C.I.) Limited in Guernsey in a Sterling investment scheme where the monies are reinvested in various currencies (at 31 March 1987 GBP, ITL and JPY were involved in the ratio 1:1:2).

The IUCr's bank accounts and short-term deposits are held with the UBS, the NWB in New York, Manchester and Chester, the AMRO and Merrill Lynch, involving the currencies GBP, NLG, CHF, USD and ECU.

In total, at the end of March 1987, the IUCr's assets were distributed among different currencies in the following percentages, 32.4% in GBP, 23.7% in USD, 12.3% in CHF, 12.1% in NLG, 9.0% in ITL, 6.0% in ECU and 4.5% in JPY.

As an association incorporated in Switzerland, the IUCr 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 UK 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. In October 1985 a recognition of tax-exempt status in the USA was received from the Internal Revenue Service, Department of the US Treasury, after a long-pending application.

#### General Fund

Table 3 summarizes the accounts for the General Fund (GF) and Table 4 compares the GF accounts for the triennium

with the budget approved by the XIII General Assembly. This fund carries the income and expenditure related to the IUCr's administration and regular scientific activities other than publications. The income has two main sources, the subscriptions and the interest income.

The subscriptions from Adhering Bodies are based on the unit contribution, which has been CHF 890 for all three years as decided by the XII and XIII General Assemblies. The total number of membership units was 149 for 1984 and 147 for 1985 and 1986, while the budget was based on 146 units.

The yield from investments exceeds the budgeted amount by CHF 497 961. This huge positive difference is due to a combination of several factors. The interest rates of the short-term deposits were much higher than assumed in the budget, which was based on cautious predictions of developments in the international money market. The unexpectedly high profit from the IUCr's publications has further contributed to the growth of the assets collecting interest. On the other hand, the expansion of the IUCr's scientific activities, the support to meetings *etc.* has not been as fast as projected.

The grants from Unesco and ICSU include, in addition to the budgeted regular grants, the support obtained for some IUCr-sponsored schools. Such support appears correspondingly as part of the expenditure on Sponsorship of Meetings.

The amounts charged to the journals are estimated as 30% of the administration costs due to the work of the Executive Secretary and his office and of the General Secretary and Treasurer.

The main item under sundry publications, appearing on both sides of the budget, concerns the Seventh Edition of the *World Directory of Crystallographers*, now included in the Book Fund accounts (Table 10).

The Executive Committee has met annually. The Finance Committee has held two meetings each year. The costs of these meetings vary, as seen from Table 3, depending on the site and circumstances. They are included in the expenses of administrative meetings, together with the costs of the IUCr representatives on other bodies. The printing expenses of the Report of the XIII General Assembly, budgeted as CHF 17 000 under these expenses, did not occur in the triennium. They will be included in the 1987 accounts.

The expenses of scientific meetings in Table 4 include the travel grants for the XIII Congress, the costs of the meeting of the Programme Committee for the XIV General Assembly and Congress held in 1986, the expenses of the non-publishing Commissions and IUCr support to meetings and schools. On the basis of a proposal made at the General Assembly in Hamburg, special grants have been offered to support the attendance of young scientists at IUCr-sponsored meetings. For 1985 this is included in the sum given in the GF account, while in 1986 the young scientists' support of CHF 50 093 is recorded separately in the REF account. With this taken into account, the support to scientific meetings in 1986 approached the projected level, but for the whole triennium it was still clearly lower than budgeted.

An essential part of the excess income in the GF account has been transferred to the three new fund accounts, the PJDF, the REF and the EF. In this way the favourable variant from the budget is reduced to CHF 261 513.

Table 3. *General Fund*

	1984	1985	1986
<i>Income</i>			
Subscriptions from Adhering Bodies	132 610	130 830	130 830
Yield from investments and bank accounts	210 674	352 211	285 076
Grant from Unesco to ICSU	37 905	32 565	17 333
ICSU grant	—	12 749	—
Commission expenses refund	4 528	—	—
Amount charged to:			
<i>Acta Crystallographica</i>	31 647	38 445	43 309
<i>Journal of Applied Crystallography</i>	10 549	12 815	14 436
<i>Molecular Structures and Dimensions</i>	908	930	720
	428 821	580 545	491 704
<i>Expenditure</i>			
Administration	140 652	170 867	192 458
Subscriptions to ICSU/ICSU bodies	5 381	5 645	5 184
Executive Committee	—	30 956	19 974
Finance Committee	14 419	11 065	6 035
XIII General Assembly and Congress:			
Travel grants	43 602	—	—
Executive Committee	47 243	—	—
XIV General Assembly and Congress:			
Programme Committee	—	—	12 295
IUCr Representatives on other bodies	7 034	1 157	5 921
Expenses of Commissions	420	8 673	4 201
Sponsorship of meetings	24 951	65 352	27 032
Donation to COSTED	—	2 090	1 930
Preparation of a History of the IUCr	—	998	—
Transfers to other Funds:			
Publications and Journals Development Fund	25 000	—	50 000
Research and Education Fund	25 000	—	50 000
Ewald Fund	—	—	83 595
	333 702	296 803	458 625
<i>Excess of income over expenditure</i>	CHF 95 119	CHF 283 742	CHF 33 079
<i>Fluctuations in rates of exchange</i>	+34 623	-37 345	-147 085
<i>Accumulated balance at the end of the year</i>	CHF 668 686	CHF 915 083	CHF 801 077

Table 4. *General Fund. Comparison of budget and accounts for the years 1984-1986 inclusive*

	Budget	Accounts	Difference
<i>Income</i>			
Subscriptions from Adhering Bodies	389 820	394 270	+4 450
Yield from investments and bank accounts	350 000	847 961	+497 961
Subventions from Unesco and ICSU	75 000	100 552	+25 552
Sale of sundry publications	22 000	—	-22 000
	836 820	1 342 783	+505 963
<i>Expenditure</i>			
Administration	351 400	351 216	-184
Subscriptions to ICSU/ICSU bodies	12 000	20 230	+8 230
Scientific meetings	306 800	181 998	-124 802
Administrative meetings	144 000	143 804	-196
Sundry publications	22 000	—	-22 000
Transfers to other funds	—	233 595	+233 595
<i>Fluctuations in rates of exchange</i>	—	149 807	+149 807
	836 200	1 080 650	+244 450
<i>Favourable variant from budget</i>			CHF 261 513
<i>Estimated profit</i>			620
<i>Excess of income over expenditure</i>			CHF 262 133

Table 5. *President's Fund*

	1984	1985	1986
<i>Income</i>			
Donations	—	1 252	504
<i>Expenditure</i>			
Grants	—	—	85
<i>Excess of income over expenditure</i>	nil	CHF 1 252	CHF 419
<i>Fluctuations in rates of exchange</i>	+906	-734	-2 859
<i>Accumulated balance at the end of the year</i>	CHF 17 495	CHF 18 013	CHF 15 573

*President's Fund*

Table 5 gives the accounts for the President's Fund, which was established in 1977 in memory of past Presidents. It is intended for use in emergencies and under special or difficult circumstances, to help crystallographers to take part in the activities of the IUCr.

*The Journals Funds*

Tables 6 and 7 give the accounts for *Acta Crystallographica* (ACF) and the *Journal of Applied Crystallography* (JACF). The most striking feature of these accounts is the high level of annual profit which has made possible a total transfer of CHF 650 000 to the PJDF and the REF. If these transfers and the losses due to fluctuations in the rates of exchange are not taken into account, the annual excesses for both journals combined would be CHF 553 238 in 1984, CHF 651 876 in 1985 and CHF 607 849 in 1986.

A basic revision of the financial principles of the production of the journals had been made in early 1982 in an emergency situation, with some further safety measures later in that triennium, as reported to the XIII General Assembly. The impact of this revision has continued. This has been fortunate because it has enabled the IUCr to build up resources beyond the estimated safety margins. However, the journals are not intended to be a source of continuous large profits. Therefore the reasons and circumstances which have made possible such a development must be considered carefully.

The annual income has stayed rather stable through the triennium. The subscription prices (Table A) have been held essentially constant. As from 1986 subscribers have been able to take Section B and Section C of *Acta* separately, and the only combined subscription is to all three Sections of the journal. An aesthetic revision of the individual prices in 1985 brought them closer to the same percentage of the regular price.

Table A. *Regular (individual) subscription prices in DKK*

	1984		1985		1986	
Acta A	1275	(330)	1275	(350)	1275	(350)
B	—	—	—	—	1275	(350)
C	—	—	—	—	3000	(850)
B+C	4200	(1150)	4200	(1200)	—	—
A+B+C	5250	(1380)	5250	(1450)	5250	(1450)
JAC	1275	(400)	1275	(400)	1275	(400)

The numbers of subscriptions have declined during the triennium only slightly (figures are given in Appendix A, *Publications*). In particular, the decoupling of the subscriptions to *Acta* Sections B and C did not cause any significant loss of the combined A+B+C subscriptions, as was predicted beforehand. These numbers, together with the small variations in the DKK-CHF exchange rate, explain fully the income side.

The general trend of the expenditure is clear. The production or operating costs (Table B) have gone down through the triennium.

Table B. *Annual operating costs in CHF*

	1984	1985	1986
Acta	944 690	920 922	912 591
JAC	203 228	179 047	165 989
Total	1 147 918	1 099 969	1 078 580

In making transfers to the PJDF and the REF the guideline has been to maintain reserves of 1.2 times the annual operating expenses in each of the publication accounts. In 1985 the Executive Committee decided to include the transfers in the 1984 accounts. In 1986 it was agreed that transfers to the PJDF and the REF, determined on the basis of accounts for a given year, should be made on 1 January of the next financial year. Hence, no transfers were made in the 1985 accounts.

The details of the expenditure are more complicated. The costs of printing and binding have gone down. This is partly due to the number of pages (Table C) being low, with a minimum in 1985.

Table C. *Numbers of pages published*

	1984	1985	1986
Acta A	728	624	588
B	616	456	640
C	2126	1836	1892
A+B+C	3470	2916	3120
JAC	488	546	492
Total	3958	3462	3612

One reason is the condensation of information through editorial measures. Further, the understaffing and changes in the editorial staff in late 1985 and in 1986 (see Appendix E) caused a backlog of manuscripts which slightly reduced the expected journals' sizes, mainly in 1986. On the other hand, the number of manuscripts received has been low, which has been a subject of serious concern in the Executive Committee discussions of editorial policies.

In addition, the circumstances in the printing industry in the UK have been favourable to the IUCr making it possible to keep the costs of printing on a low level.

The editorial expenses total CHF 393 998 in 1984, CHF 446 036 in 1985 and CHF 420 670 in 1986. Salaries and expenses of the Technical Editor's office costs form the major part of them, being about 76% in 1984 and 1985, and are divided between the *Acta* and *JAC* accounts in percentages based on the number of text pages published during the year. For *JAC* this was 12% in 1984, 16% in 1985 and 14% in 1986. Owing to changes in the staff there was in 1985 a considerable increase in the salary bill, and in 1986 a still larger reduction, which was enhanced in the accounts by the fall of the GBP in relation to the CHF.

Table 6. *Acta Crystallographica*

	1984		1985		1986	
<i>Income</i>						
Subscriptions	1 396 516		1 480 594		1 439 019	
Sale of back numbers and single copies	38 716		46 958		33 934	
Airfreight charges to subscribers	30 307		41 294		39 814	
Royalties, copyright fees	157		2 179		—	
	<u>1 465 696</u>		<u>1 571 025</u>		<u>1 512 767</u>	
Less Publisher's commission	100 466	1 365 230	107 582	1 463 443	103 087	1 409 680
<i>Expenditure</i>						
Printing and binding	416 158		377 472		403 869	
Distribution and postage	70 696		66 730		68 461	
Airfreight costs	29 552		26 436		25 606	
Indexes	21 746		34 966		11 555	
Congress Supplement	28 365		—		—	
Editorial expenses	346 526		376 873		359 791	
Administration expenses	31 647		38 445		43 309	
Transfers to other Funds:						
Publications and Journals Development Fund	125 000		—		100 000	
Research and Education Fund	125 000	1 194 690	—	920 922	100 000	1 112 591
	<u>1 465 696</u>	<u>1 365 230</u>	<u>1 571 025</u>	<u>1 463 443</u>	<u>1 512 767</u>	<u>1 409 680</u>
<i>Excess of income over expenditure</i>		CHF 170 540		CHF 542 521		CHF 297 089
<i>Fluctuations in rates of exchange</i>		+56 543		-64 036		-289 717
<i>Accumulated balance at the end of the year</i>		<u>CHF 1 092 044</u>		<u>CHF 1 570 529</u>		<u>CHF 1 577 901</u>

Table 7. *Journal of Applied Crystallography*

	1984		1985		1986	
<i>Income</i>						
Subscriptions	273 091		291 141		283 067	
Sale of back numbers and single copies	8 811		8 987		7 953	
Airfreight charges to subscribers	6 289		6 334		6 099	
Royalties, copyright fees	166		2 596		—	
	<u>288 357</u>		<u>309 058</u>		<u>297 119</u>	
Less Publisher's commission	19 733	268 624	21 009	288 049	20 370	276 749
Yield from advertisements		—		353		—
		<u>268 624</u>		<u>288 402</u>		<u>276 749</u>
<i>Expenditure</i>						
Printing and binding	66 035		82 947		77 797	
Distribution and postage	7 840		9 513		8 911	
Airfreight costs	4 030		4 609		3 963	
Editorial expenses	47 472		69 163		60 882	
Administration expenses	10 549		12 815		14 436	
Transfers to other Funds:						
Publications and Journals Development Fund	100 000		—		—	
Research and Education Fund	100 000	335 926	—	179 047	—	165 989
	<u>288 357</u>	<u>268 624</u>	<u>309 058</u>	<u>288 049</u>	<u>297 119</u>	<u>276 749</u>
<i>Excess of income over expenditure</i>		CHF 67 302		CHF 109 355		CHF 110 760
<i>Fluctuations in rates of exchange</i>		+9 392		-11 390		-60 516
<i>Accumulated balance at the end of the year</i>		<u>CHF 181 382</u>		<u>CHF 279 347</u>		<u>CHF 329 591</u>

Table 8. *Structure Reports*

	1984		1985		1986	
<i>Income</i>						
Sale of copies	180 503		161 258		200 017	
Less Publisher's commission	47 396	133 107	42 399	118 859	52 467	147 550
<i>Expenditure</i>						
Printing and binding new volumes	40 039		27 231		31 606	
Typing of manuscripts	16 622		6 943		7 205	
Editorial expenses	85 566	142 227	106 527	140 701	86 670	125 481
<i>Excess of income over expenditure</i>	CHF -9 120		CHF -21 842		CHF 22 069	
<i>Fluctuations in rates of exchange</i>	+6 987		-4 431		-20 282	
<i>Accumulated balance at the end of the year</i>	CHF 134 946		CHF 108 673		CHF 110 460	

The main part of the remaining 24% (in 1984 and 1985) of the editorial expenses is related to the work of the Editors and the Co-editors. These costs vary considerably from year to year, depending on the local circumstances of the individuals. Most of them are defined in USD and the fall in the value of the USD in 1986 caused a significant reduction from the level of 1985.

These two reductions in 1986 were largely counterbalanced by the costs (CHF 65 731) of a major refurbishment of the IUCr's office premises in Chester.

The administration expenses are those occurring on the income side of the GF accounts. They are divided between *Acta Crystallographica* and the *Journal of Applied Crystallography* in the ratio 3:1. Their variations reflect to a large extent changes in the salary bill of the Executive Secretary's office.

From these considerations it is clear that the large profit has resulted from the coincidence of several temporary factors which cannot be expected to prevail much longer. The finances of the journals are extremely sensitive to the number of subscriptions and to the sizes of the journals. The present trend indicates increases in size in the near future. There are also conscious attempts to increase the subject coverage of the IUCr's journals, to make them serve better the crystallographic community. This will definitely lead to an expansion of the journals and to the need for additional editorial staff. Hopefully, in the long run, it will also bring new subscribers, but the necessary increases in prices will work against this possibility.

The IUCr has also profited considerably from the failure of the relevant salary scales to keep in step with inflation in the UK through the last two triennia. An essential revision of these scales was made from 1 December 1986, with a further increase to follow on 1 March 1988. It is thus easy to predict that a substantial reduction of the excess income from the journals will occur in 1987.

#### *Structure Reports*

The *Structure Reports* accounts are shown in Table 8. The printing and binding costs, as well as the major part of the sales income in a particular year are for the volumes published in that year, i.e. for Volumes 48A and 45B in 1984, for 46B in 1985 and for 52A and 48B in 1986. The other expenses of a year always include editorial work for several volumes yet to be published.

The decreasing sales of *Structure Reports* caused serious concern at the time of the XIII General Assembly. The first year's sales of the B volumes (Organic Compounds) published in the triennium have been stable at 400 copies, reaching a total sales of 430-440 copies in about five years. The present B Volumes consist of two thick books each, with a total of 1542, 1452 and 1852 pages for Volumes 45B, 46B and 48B, respectively. With their prices of NLG 500, 600 and 600, the sales income is no longer sufficient to cover fully the production costs. However, higher prices have not been considered feasible.

The two volumes on Metals and Inorganic Compounds published in the triennium, 48A and 52A, are thinner, being 420 and 384 pages respectively, and have been priced at NLG 200 and 170. The total sales of Volume 48A in the triennium were 483 copies, while 429 copies of Volume 52A were sold in the first five months. The sales of the A volumes are about 500 copies in total. This will probably lead to recovery of the costs.

With the changes already decided (see Appendices A and E), the editorial costs will decline rapidly in the near future. Therefore the balance of the account will remain positive, even if all the remaining B volumes are under priced.

#### *International Tables*

The *International Tables* accounts are shown in Table 9. The sales numbers of the existing volumes are given in the Report of the Commission on *International Tables* (Appendix E).

On the dissolution of the General Publications Fund (GPF) in 1984 a part of its resources was transferred to the *International Tables* Fund. In 1964 the total sum of subventions received for *International Tables* was transferred to the GPF, because the sales had covered the costs and were producing good profit. The transfer back, 20 years later, was based on the percentage of the 1964 transfer of the balance in the GPF at that time.

Volume A continues to sell well and is producing the largest income. All its production costs, even the early costs related to the computerized production of diagrams, were recovered from the sales by early 1985. In July 1986 a price reduction from NLG 385 to NLG 340 was made with the personal price rounded down to 50% of this, or from NLG 215 to NLG 170. These lower prices have been kept for the

Table 9. *International Tables*

	1984		1985		1986	
<i>Income</i>						
Sales:						
Volume A	113 567		99 365		58 588	
Teaching Edition of Volume A	—		9 517		9 560	
Volumes II, III and IV	27 677		41 443		24 745	
	<u>141 244</u>		<u>150 325</u>		<u>92 893</u>	
Less Publisher's commission	41 090	100 154	43 842	106 483	27 194	65 699
Transfer from General Publications Fund		41 208		—		—
		<u>141 362</u>		<u>106 483</u>		<u>65 699</u>
<i>Expenditure</i>						
Printing/Reprinting Volume A	34 076		—		17 791	
Printing Teaching Edition of Volume A	—		11 894		—	
Reprinting Volumes II and III	—		34 837		—	
Editorial expenses	14 236	48 312	7 440	54 171	16 632	34 423
	<u>14 236</u>	<u>48 312</u>	<u>7 440</u>	<u>54 171</u>	<u>16 632</u>	<u>34 423</u>
Excess of income over expenditure		CHF 93 050		CHF 52 312		CHF 31 276
Fluctuations in rates of exchange		+6 861		-7 241		-32 400
Accumulated balance at the end of the year		<u>CHF 132 514</u>		<u>CHF 177 585</u>		<u>CHF 176 461</u>

Table 10. *Book Fund*

	1984		1985		1986	
<i>Income</i>						
Sale of copies (net):						
Fifty Years of X-ray Diffraction	335		356		295	
Escher Drawings	357		706		614	
Early Papers	99		588		263	
Fifty Years of Electron Diffraction	1 956		1 955		481	
World Directory of Crystallographers						
6th Edition	185		181		—	
7th Edition	—		—		22 994	
Sundry Publications	103		45		35	
Royalties: Escher Drawings	203	3 238	387	4 218	168	24 850
	<u>203</u>	<u>3 238</u>	<u>387</u>	<u>4 218</u>	<u>168</u>	<u>24 850</u>
Opening balance at 1 January 1984 from a combination of other funds*		5 880		—		—
		<u>9 118</u>		<u>4 218</u>		<u>24 850</u>
<i>Expenditure</i>						
World Directory of Crystallographers 7th Edition. Printing, distribution and honorarium	—		—		24 602	
	<u>—</u>	<u>—</u>	<u>—</u>	<u>—</u>	<u>24 602</u>	<u>—</u>
Excess of income over expenditure		CHF 9 118		CHF 4 218		CHF 248
Fluctuations in rates of exchange		+498		-542		-2 100
Accumulated balance at the end of the year		<u>CHF 9 616</u>		<u>CHF 13 292</u>		<u>CHF 11 440</u>

\* The balances on the following fund accounts were combined on 1 January 1984 to form a new fund – the 'Book Fund'

Fifty Years of X-ray Diffraction	5 127
Escher Drawings	21 095
Early Papers	-9 827
Fifty Years of Electron Diffraction	-10 515
	<u>CHF 5 880</u>

Table 11. *Molecular Structures and Dimensions*

	1984		1985		1986	
<i>Income</i>						
Sale of copies	50 077		13 803		10 665	
Less Publisher's commission	13 292	36 785	3 781	10 022	3 052	7 613
<i>Expenditure</i>						
Printing and binding	24 513		—		—	
Miscellaneous expenses	3 191		—		—	
Salaries	8 173		9 092		6 893	
Administration expenses	908	36 785	930	10 022	720	7 613
<i>Excess of income over expenditure</i>		nil		nil		nil
<i>Fluctuations in rates of exchange</i>		+374		-283		-1 076
<i>Accumulated balance at the end of the year</i>		CHF 7 220		CHF 6 937		CHF 5 861

Table 12. *Publications and Journals Development Fund*

	1984		1985		1986	
<i>Income</i>						
Transfers from other funds:						
General Fund	25 000		—		50 000	
Acta Crystallographica	125 000		—		100 000	
Journal of Applied Crystallography	100 000		—		—	
General Publications Fund	33 815	283 815	—	—	—	150 000
<i>Expenditure</i>						
Compuscripts	—		—		2 007	
Communication with data bases	—	—	—	—	1 609	3 616
<i>Excess of income over expenditure</i>		CHF 283 815		nil		CHF 146 384
<i>Fluctuations in rates of exchange</i>		+15 498		-11 726		-67 320
<i>Accumulated balance at the end of the year</i>		CHF 299 313		CHF 287 587		CHF 366 651

revised second edition as well. Also the Teaching Edition of Volume A, with its low price NLG 27·50, has now covered its production costs. The old volumes are all priced at NLG 155 and continue their steady sales.

Most of the editorial expenses during the triennium are related to the work on the two new volumes, which will be published in the ongoing triennium at close intervals. The *International Tables* Fund is well prepared to meet their production costs.

#### *The Book Fund*

Table 10 gives the accounts of the new Book Fund. In addition to the small sales income and royalties from books published several years ago it carries the expenditure and income of the *World Directory of Crystallographers* (and sundry publications), which were earlier included in the GF accounts. The initial sales of the Seventh Edition of the *Directory*, published in August 1986, almost covered the production costs, as intended. The new triennium will bring more substance to this account, once the IUCr's Book Series with the Oxford University Press gets started.

#### *Molecular Structures and Dimensions*

The *Molecular Structures and Dimensions* accounts are shown in Table 11. The last volume published was Volume

15, in 1984. There are no immediate plans to publish any more volumes. The net sales income was used to reimburse the University of Cambridge for the publication costs and as much as possible of the editing costs incurred by the Cambridge Crystallographic Data Centre. Under the terms of the agreement between the Data Centre and the IUCr, the IUCr is not required to stand any financial losses which might arise. This is why the income and expenditure shown in the accounts balance exactly.

#### *The New Funds*

Tables 12 and 13 show the accounts of the Publications and Journals Development Fund and the Research and Education Fund, both established in 1984.

Both funds have an operating and a reserve capacity. The initial funds to these accounts were obtained by transfers from the GF, the ACF and the JACF. In addition, the PJDF received a share from the resources of the GPF when it was dissolved in 1984. Other transfers to the new funds were made in 1986.

There are two items of expenditure in the PJDF accounts. One is for preliminary work by the editorial staff on the possibility of the printers accepting contributions from authors in compuscript form. In 1986 this was related to the new volumes of *International Tables*. The other item is

Table 13. *Research and Education Fund*

	1984	1985	1986
<i>Income</i>			
Transfers from other funds:			
General Fund	25 000	—	50 000
<i>Acta Crystallographica</i>	125 000	—	100 000
<i>Journal of Applied Crystallography</i>	100 000	—	—
	250 000	—	150 000
<i>Expenditure</i>			
History of the IUCr	—	—	7 615
Young scientists' support	—	—	50 093
	—	—	57 708
<i>Excess of income over expenditure</i>	CHF 250 000	nil	CHF 92 292
<i>Fluctuations in rates of exchange</i>	+13 651	-10 329	-53 614
<i>Accumulated balance at the end of the year</i>	CHF 263 651	CHF 253 322	CHF 292 000

Table 14. *Ewald Fund*

	1986
<i>Income</i>	
Bequest and donation	56 400
Interest	9 788
Transfer from General Fund	83 595
	149 783
<i>Expenditure</i>	
Administration expenses	6 704
<i>Excess of income over expenditure</i>	CHF 143 079
<i>Fluctuations in rates of exchange</i>	-22 195
<i>Accumulated balance at the end of the year</i>	CHF 120 884

the purchase of a modem, to connect the office computer with the data bases for development of the journals checking procedures.

In the REF accounts there are similarly two items of expenditure in 1986. One is a project taken up by Dr Harmke Kamminga, Cambridge, to make a study of the IUCr's early history from the old files in the Chester office. The costs are related to the critical survey and rearrangement of the files. The other item is the support given to young scientists, to assist their attendance at IUCr-sponsored meetings and schools. This support was given for the first time in 1985, but in that year was included in the GF accounts under 'Sponsorship of meetings'.

The accounts of the Ewald Fund are given in Table 14. The capital in this fund will consist of the bequest of USD 40 000 from Professor Ewald, the first half of which was received in 1986, and a donation of USD 10 000 from the Ewald family, together with an equal amount from the IUCr, of which USD 40 000 was transferred from the GF on 1 January 1986.

The interest on the capital is intended to cover the costs of the Prize. It is defined as 8% per annum and will be taken from the annual interest income, which otherwise is credited to the GF. The first Prize, however, will be funded separately.

### Appendix C: Ewald Prize and Ewald Bequest

The establishment of the Ewald Prize, for outstanding contributions to the science of crystallography, was announced in February 1986 and was given wide publicity. The name of the Prize was chosen, with the kind consent of the late Paul Peter Ewald, to recognize Professor Ewald's significant contributions to the foundations of crystallography and to the founding of the International Union of Crystallography, especially his services as the President of the Provisional International Crystallographic Committee from 1946 to 1948, as the first Editor of the IUCr's publication *Acta Crystallographica* from 1948 to 1959, and as the President of the IUCr from 1960 to 1963.

The Prize consists of a medal, a certificate and an award of USD 20 000. It will be presented once every three years during the triennial International Congresses of Crystallography. The first Prize will be presented during the XIV Congress in Perth. 1987 will be the seventy-fifth anniversary of the discovery of X-ray diffraction in 1912.

Shortly after the death of Professor Ewald, his family informed the President that Professor Ewald had wished to make a bequest to the IUCr. After consulting Mrs Ewald, this generous bequest, together with a donation from the Ewald family and a further donation from the IUCr, has been used as capital for the Ewald Prize. The interest from this capital will be used to finance the Prize.

In April 1987 it was announced that the first Ewald Prize for outstanding contributions to the science of crystallography had been awarded jointly to Professor J. M. Cowley and Dr A. F. Moodie for their outstanding achievements in electron diffraction and microscopy, especially for their fundamental contributions to the theory and technique of direct imaging of crystal structures and structure defects by high-resolution electron microscopy.

Their pioneering work on the dynamical scattering of electrons was reported in a series of papers in *Acta Crystallographica* and other journals from 1957 onwards. A theory of Fourier images led them to the multislice formulation of the scattering of an electron wave in its passage through a crystal. This formulation is able to take into account many hundreds of scattered beams, and has become the basis of widely used computer programs. The theory allows the electron micrographs, obtained with modern high-

resolution instruments, to be reliably and quantitatively interpreted, and used for the determination of the structures of both perfect crystals and crystals containing defects. Professor Cowley and Dr Moodie, together and separately, have made many further contributions to theory, methods and results in electron diffraction and microscopy. Their work has often stressed a unified approach to diffraction and microscopy through physical optics. An overview of the whole field may be found in Professor Cowley's book *Diffraction Physics* [(1981). Amsterdam: North-Holland].

John Maxwell Cowley, born in Australia in 1923 and a graduate of Adelaide University, was formerly a Chief Research Scientist at the Division of Chemical Physics, CSIRO, Melbourne, Australia. Later he was Professor of Physics at the University of Melbourne, and since 1970 has been the Galvin Professor of Physics at Arizona State University, Tempe, AZ, USA.

Alexander Forbes Moodie, born in Scotland in 1923, graduated from St Andrews University in 1948. Since then he has been a member of CSIRO in Australia where he is a Chief Research Scientist at the Division of Chemical Physics. This Division was incorporated into the Division of Materials Science and Technology at the end of 1986.

The presentation of the Ewald Prize will take place at the Opening Ceremony of the XIV Congress on 12 August. Professor Cowley and Dr Moodie will each receive a medal and a certificate and will share the award of USD 20 000. At the same ceremony an honorary medal will be presented to a member of the Ewald family, on behalf of the worldwide community of crystallographers.

#### Appendix D: New Fund Accounts

The Publications and Journals Development Fund Account (PJDF) and the Research and Education Fund Account (REF) were established in 1984, in view of the improved financial situation of the IUCr, to carry the financial reserves for new developments of the IUCr's activities and for future projects which would require special funding. In May 1985 a request for suggestions for possible projects to be supported from these funds was sent to the IUCr's Commissions and National Committees. The XIII General Assembly was also informed of this request. The various suggestions received were considered by the Executive Committee at their 1985 meeting. The situation was reviewed in 1986. Several proposals were approved in principle as possible uses depending on potential detailed proposals, a few have been started or realized, and some are subject to further planning.

In their discussions of future activities the XIII General Assembly approved the motion: "The General Assembly requests the Executive Committee, when planning the budget for the General Fund, to give high priority to the provision of scholarships to enable talented young people to attend Congresses of the Union." USD 15 000 has been provided for such scholarships for the Perth Congress and associated meetings. Special support for young scientists has been granted since 1985 to meeting and schools sponsored by the IUCr. Since 1986 it has been charged to the REF.

A project on the history of the IUCr was financed from the REF in 1986 and is continuing. Creation of a pool of crystallographic films for education purposes is a related project in preparation.

Establishment of visiting fellowships, particularly for teaching in developing countries, has been proposed. The Commission on Crystallographic Teaching is developing the idea and is trying to find schemes within the financial possibilities of the IUCr.

Scientific projects conducted by the Commissions of the IUCr can be supported from the REF. Some preliminary enquiries have been received but nothing along this line has materialized yet.

Several proposals concerning support for different kinds of publications were received. They will be largely covered by the IUCr Book Series with the Oxford University Press (Appendix J), which is expected to be mainly self-supporting. However, publication of some books of special crystallographic interest but with high production costs may require a subsidy from the REF.

The proposal to provide free copies of the IUCr's publications to developing countries was considered appropriate in principle. In earlier attempts to implement this idea it was surprisingly difficult to find interested persons or institutes and to create channels for the distribution of the publications at a reasonable price. Therefore, realization of the idea requires interested enquiries from developing countries and the use of some existing distribution channels.

Costs incurred in any projects relating to computerization of the editorial work, communications with data bases or implementation of new techniques in the IUCr's publication activities would be charged to the PJDF.

A proposal to create an IUCr Award led to the establishment of the Ewald Prize and the Ewald Fund (see Appendices C and B, respectively).

Any new proposals, whether or not in the above categories, should be sent to the General Secretary for consideration in the Finance and Executive Committees.

#### Appendix E: Reports of the Commissions of the Union

##### *Commission on Journals*

*Acta Crystallographica* and the *Journal of Applied Crystallography* have been published on or close to schedule throughout the triennium despite major changes in the office of the Technical Editor, see below. Two new categories of papers were introduced in *Acta Cryst.* and two in *J. Appl. Cryst.* Lead Articles, generally by invitation but subject to normal review, on topics of high current interest will appear occasionally in *Acta Cryst.* Sections A and B: several invitations have been issued and accepted and two Lead Articles have now reached an advanced stage. Short-Format Papers provide a means of publishing basic structural results without the need for including an Introduction or Discussion section: the format appears to be popular, with 8 appearing in 1985, 75 in 1986 and 150 estimated in 1987.

Lead Articles in *J. Appl. Cryst.* are now being published more frequently. A new category of paper entitled Computer Program Abstracts allows information to be provided on new crystallographic computer programs, but without the detail required under Computer Programs. The Commission on Crystallographic Computing was instrumental in proposing the category and continues to be involved in its present operation. New Commercial Products announce prices and manufacturer, giving brief technical details of new products likely to be of general interest. Crystal Data papers, as cooperatively planned, are increasingly being published in *Powder Diffraction* rather than in *J. Appl. Cryst.*

Each Section of *Acta Cryst.* and *J. Appl. Cryst.* contained Checklists for the convenience of authors in preparing their papers, drawn from *Notes for Authors*, in the first issues of this triennium. The ease with which a paper may be found in the *Table of Contents* of Section C has been improved, as the number of structural papers continues to increase, by dividing them into three formal categories [*Acta Cryst.* (1986), C42, 1892]. In addition, a monthly alphabetical list of authors contributing to that issue will be included commencing with the May 1987 issue.

The total number of papers in *Acta Cryst.* in this triennium was 2.8% more, at 2837, than in the previous triennium, while that in *J. Appl. Cryst.* was 17.9% fewer, at 316. Non-refereed *J. Appl. Cryst.* papers, of course, are excluded from these numbers. The small increase in *Acta Cryst.* reversed the decline in the previous triennium, but the decrease in *J. Appl. Cryst.* remained about the same as reported in the last triennial report [*Acta Cryst.* (1987), A43, 452-453]. Papers from 55 different countries have been published in the present triennium. Mean times between published acceptance and nominal publication dates, which increased in 1986 to 5.7 months for Sections A and B and to 4.8 months for Section C and *JAC*, are expected to be reduced by the end of 1987. Publication of the Ewald memorial issue in November 1986 contributed to the delay with papers in Section A, with further delays in all Sections being caused by temporary understaffing in the Technical Editor's office.

Both regular and individual subscription rates remained constant throughout the triennium (in Danish Kroner), resulting in an institutional cost of 3.3 US cents per 1000 characters for *Acta Cryst.* in 1985 and 4.5 US cents per 1000 characters for *J. Appl. Cryst.* A review of the cost of comparable journals in the December issue of *Physics Today* (1986), pages 34-36, reveals a range in 1985 from 3.4 US cents to 35 US cents per 1000 characters in journals without page charges, indicating that regular-price subscribers receive highly competitive value. The total number of subscribers decreased in the triennium by 5.3% for *Acta Cryst.* and 2.1% for *J. Appl. Cryst.* Similar or larger decreases have been reported by other scientific journal publishers.

The IUCr minicomputer has been used to maintain journal production records, checking reports for duplicate structure determination and producing the annual indexes. Interface problems encountered by the printer in using our machine-readable index information caused regrettable delays in publishing the indexes for 1984 and 1985, but that for 1986 is expected to be published on time.

F. R. Ahmed, T. A. Hamor, J. A. Ibers, J. Protas, Y. Saito, H. Schulz and G. A. Sim retired during the triennium, while N. W. Alcock, F. H. Allen, T. Ashida, C. E. Bugg, H. Burzlaff, J. Drenth, A. Durif, H. Hope, M. B. Hursthouse, H. Steinfink and J. Trotter were appointed Co-editors of *Acta Cryst.* M. Hart retired as Editor and was succeeded by M. Schlenker, while H. L. Yakel and D. Watanabe retired as Co-editors and A. M. Glazer, H. Iwasaki, B. Morosin, E. Prince and G. Will were appointed Co-editors of *J. Appl. Cryst.* The Commission is greatly indebted to the unstinting and often sacrificial efforts of all its members, and particularly those who have completed their service with such distinction. It records with deep sorrow the death of J. E. Derry, Deputy Technical Editor, on 2 September 1985. Further change was occasioned by the resignation of D. W. Penfold as Technical Editor, effective 31 December 1985.

M. H. Dacombe was appointed Technical Editor, S. E. Lowe and P. R. Strickland were appointed Assistant Technical Editors, and B. McMahon joined A. Sharpe as Editorial Assistants, with J. A. Glendenning, J. I. Heywood (now retired) and L. Allsop as Secretaries. The Commission records its high appreciation for the devoted work of all members of the Technical Editor's staff.

29 April 1987

S. C. ABRAHAMS, Chairman  
M. SCHLENKER, Co-Chairman

#### *Commission on Structure Reports*

Volume 48A (Metals and Inorganic Compounds for 1981, 420 pages) and Volume 52A (Metals and Inorganic Compounds for 1985, 374 pages) have been published. 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 Volumes 49A and 50A (Metals and Inorganic Compounds for 1982 and 1983, respectively). Volume 45B (Organic Compounds for 1979, 1542 pages in two volumes), Volume 46B (Organic Compounds for 1980, 1482 pages in two volumes), Volume 48B (Organic Compounds for 1981, 1852 pages in two volumes) have been published. 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.

The Executive Committee decided, after much discussion and with great 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.

30 April 1987

G. FERGUSON, Chairman

#### *Commission on International Tables*

Since the appointment of the Editors of Volumes B and C in 1982 until the XIII General Assembly in Hamburg in 1984, the Commission had consisted of the Editors and the President and the General Secretary of the IUCr (the latter two officers being *ex officio* members of every Commission). The Editors had received great help from certain Commissions of the IUCr, and at the Hamburg General Assembly the Chairmen of these Commissions (Apparatus; Charge, Spin and Momentum Densities; Computing; Electron Diffraction; Neutron Diffraction; Teaching) were added, *ex officio*. The Commission held an Open Meeting during the Congress associated with the XIII General Assembly. Each Editor presented his plans for his volume, and profited from the discussion. In addition, many formal and informal meetings between the Editors and Commissions took place, and the Editors were able to discuss many individual contributions with their authors, and to invite many new authors. Work continued actively throughout the triennium, chiefly by correspondence, though the Editors and a few others were able to meet occasionally at conferences and otherwise. 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

Table 1. *Sales and stocks of volumes of International Tables published to date*

Volume	II	III	IV	A	Brief A (Teaching)
Dates of publication and reprinting	1959 1967 1972 1985	1962 1968 1983 1985	1974 — — —	1983 1984 1986 1987*	1985 — — —
Number of copies sold					
Before 1 January					
1984	8497	7555	3319	1107	—
In 1984	84	129	84	504	—
In 1985	134	150	160	481	619
In 1986	110	96	100	295	647
Up to 31 December					
1986	8825	8130	3663	2387	1266
Stock at 31 December					
1986	307	752	308	116	607

\* Second revised edition scheduled May 1987.

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 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. Reports on the individual volumes follow; the sales and stock position of Volumes II-IV of the old edition and of the two versions of Volume A are given in Table 1.

Volume I, the predecessor of the new Volume A, was published originally in 1952. It was sold out in 1980, after total sales of 9501 copies.

*Volume A (Space-Group Symmetry*; Editor Th. Hahn)

The first edition of Volume A appeared in November 1983 and sold out quickly. A reprint with corrections was published in the spring of 1984; *errata* were also published [*Acta Cryst.* (1984), **A40**, 485]. Another short reprint was made in 1986 to keep the volume available while a new edition was prepared.

A second revised edition of Volume A was sent to the printer in January 1986. It contains corrections of all errors discovered, 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 continued throughout 1986, and the volume is scheduled for publication in May 1987.

A *Brief Teaching Edition of Volume A of International Tables for Crystallography* was published in June 1985. It has 128 pages, including the full entries for twenty-four selected space groups and Sections 1, 2, 3 and 5 of the explanatory text of the full edition. The price has been kept intentionally low in order to make this edition affordable by students. Preparations for a second revised edition are under way.

*Volume B (Reciprocal Space*; Editor U. Shmueli)

Much of the planning of the volume as a whole, as well as the algorithms underlying the Editor's own contributions

to Chapter 1.4: *Symmetry in Reciprocal Space*, were accomplished during the few months that preceded the XIII Congress. The plans were presented in an Open Meeting during the Congress and were communicated by the Editor to the Executive Committee. The 1984 IUCr Congress was a unique opportunity for the Editor to meet the majority of the invited authors, and complete the planning of some parts which had not yet been decided upon. The authors were informed in writing of the Editor's intention to complete the editing of the volume by the end of 1985.

There was much activity during the year following the Hamburg Congress, but certainly not enough to enable one to regard the 'end 1985' deadline seriously. It should have been realized by the Editor that even prestigious but essentially didactic contributions are likely to be assigned by the authors a lower priority than that of usual research activities. In spite of this, however, most authors kept their promises during the years 1985 and 1986.

Work on the Editor's own contributions to Volume B [Chapters 1.1 (*Reciprocal Space in Crystallography*); 1.4 (*Symmetry in Reciprocal Space*); 2.1 (*Statistical Properties of the Weighted Reciprocal Lattice*) (jointly with the Editor of Volume C)] are essentially complete; some small linking sections remain. Tests of typesetting the computer-generated tables in Chapter 1.4 directly from computer-readable material are in progress.

Volume B is in five parts, each divided into chapters and sections. The current position (early 1987) is listed below. The symbols in square brackets indicate: C = complete, D = in draft (P = preliminary, A = advanced), 0 = nothing in the hands of the Editor.

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 [C]
  - 2.2 Direct Methods [C]
  - 2.3 Patterson and Molecular-Replacement Techniques [C]
  - 2.4 Isomorphous Replacement and Anomalous Dispersion [0]
  - 2.5 Electron Diffraction and Microscopy in Structure Determination [AD, C]
3. Dual Bases in Crystallographic Computing
  - 3.1 Distances, Angles, and their Standard Deviations [C]
  - 3.2 Best-Plane Calculations [PD]
  - 3.3 Molecular Modelling and Graphics [AD]
  - 3.4 Accelerated Convergence and Lattice Sums [AD]
4. Diffuse Scattering and Related Topics
  - 4.1 Thermal Diffuse Scattering of X-rays and Neutrons [C]
  - 4.2 Disorder Diffuse Scattering of X-rays and Neutrons [AD]
  - 4.3 Diffuse Scattering in Electron Diffraction [AD]
  - 4.4 Small Crystallite Size and Texture [0]
  - 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]

*Volume C (Mathematical, Physical and Chemical Tables;*  
 Editor A. J. C. Wilson)

Volume C has presented problems rather different from those of Volume B. Volume C was originally planned as an editorial condensation of the existing Volumes II, III and IV, with obsolete or readily available material eliminated, and tables for which a pocket calculator would be an acceptable substitute reduced to a skeleton tabulation. Consultation with the Chairmen of relevant Commissions, however, convinced the Editor that much fundamental re-writing would be necessary if Volume C were to be a worthy companion to Volumes A and B. The material is widely disparate, and it was therefore necessary to invite a large number of authors to contribute, some of them responsible for only a couple of pages, others for substantial chapters. Work has therefore proceeded much as for Volume B. The current status of the ten parts that make up the Volume is listed below. The symbols in square brackets are as for Volume B, plus S = some sections missing, H = in rough draft or about half complete.

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

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.

7 May 1987

A. J. C. WILSON, Chairman

#### *Commission on Biological Macromolecules*

No report was received from the Commission Chairman, C.-I. Brändén, but a report was compiled at the time of the General Assembly by two members of the Commission, G. Dodson and W. A. Hendrickson. This report was distributed to delegates and is given below.

The Commission met during the XIII Congress in Hamburg and it is meeting again during the XIV Congress in Perth. Three main areas are recognized by the Commission as its responsibility: (1) to ensure that the programme of scientific meetings in this field is sufficiently frequent and that these cover both methods and results, (2) to ensure that outlets of high scientific and technical standards exist for the publication of methodological advances and structural results in macromolecular crystallography, and (3) to provide a forum for the discussion of policy issues affecting the discipline and to offer authoritative policy recommendations to the scientific community.

The Commission observes that the field is in excellent health. Clearly, macromolecular crystallography is in a most active and successful phase. There is a diverse menu of relevant conferences and schools, the best journals are

receptive for contributions from the field, and there is an expansion in openings for the employment of macromolecular crystallographers. Nevertheless, there are problems that arise, some produced by the expansion of the field, and these are concerns of the Commission.

The specific activities of the Commission include its role in organizing several of the scientific sessions at the XIV Congress, sponsorship of a Workshop on Crystallography in Molecular Biology in Poushchino, USSR, endorsement of the Protein Data Bank at Brookhaven as the recognized repository for structural data and results from the field, and consideration of the growing trend toward commercialization of macromolecular software. We are at present discussing several policy issues. These include inducements for the timely deposition of results from publicly supported research, encouragement of eventual public release of results from proprietary research, consideration of growing duplications of effort in the field, and changes suitable for the field in editorial policy for *Acta Crystallographica*.

14 August 1987

G. DODSON

W. A. HENDRICKSON

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

The Commission continues to encourage and promote work related to many aspects of electron density distributions.

#### *Sagamore VIII Conference*

The most important activity of the Commission during the triennium was the VIII Sagamore Conference on Charge, Spin and Momentum Densities. This conference was held at the Sanga-Säby conference centre in Sweden under the chairmanship of I. Olovsson. The special theme of the conference was electron distributions and the chemical bond. As in the past the conference brought together experimental and theoretical physicists and chemists for fruitful discussions of problems within the three subject areas of the Commission. The conference contained eleven invited lectures with other contributions in the form of posters or short oral presentations. Ample time was allowed for discussions, which proved lively. The proceedings of the conference, which includes the full text of the invited papers and abstracts of the contributed papers, has been published in *Chemica Scripta* (1986), **26**, 389-503.

During the conference the Commission met to discuss its projects and the future of the Sagamore conferences. It was generally agreed that these conferences serve a useful purpose and should be continued. It was decided to hold the IX Sagamore Conference in Portugal in 1988.

#### *Projects*

(a) *Vanadium*. A lively discussion of the results of the vanadium project took place during the IUCr Congress in Hamburg. These discussions highlighted the difficulties involved in matching theoretical band calculations with momentum density measurements.

(b) *Data bank*. Following the decision of the Executive Committee not to give financial assistance to this project, it has been shelved until a solution can be found to the problem of obtaining electron density data from experimenters in a computer-readable form.

(c) *Correlated form factors*. The Commission hopes to initiate a project to make data available from which

correlated form factors for use in electron density studies can be calculated.

Discussions of a new project, similar to but with wider scope than the vanadium project, took place at the Sanga-Säby meeting. Detailed suggestions for the organization of this project, which will be concerned with simple metals and insulators, should be brought to the Perth meeting of the Commission.

#### *Perth Congress*

The Commission is directly involved in planning a micro-symposium on charge, spin and momentum densities at the XIV Congress.

26 March 1987

P. J. BROWN, Chairman

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

The main activities of the Commission in the triennium have been the organization of two international schools on crystal-growth technology and related assessment methods, with the aim, on the one hand, to favour the transfer of knowledge and expertise to developing countries (particularly in the field of energy conversion) and, on the other hand, to expand (and underline) the ever stricter links between crystallography and modern (mainly electronic) materials science.

In more detail, 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) covered attendees from 28 countries (20 from developing countries). The optimum selection of lecturers, which included the Nobel Prize winner, Leo Esaki, the high 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 the 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 help transfer some results of modern technology for 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). There were 15 lecturers, from 8 countries, and 72 attendees.

Further to these activities, the Commission organized an Open Meeting on Physical Properties, Structural Assessment and Applications of Advanced Materials during the IX European Crystallographic Meeting held in Torino, Italy, 2–6 September 1985. An Open Meeting is being organized on Crystal Growth and Epitaxy of Advanced Materials at the XIV Congress in Perth.

10 March 1987

C. PAORICI, Chairman

#### *Commission on Crystallographic Apparatus*

During the triennium two long-standing projects of the Commission have reached a satisfactory conclusion.

(a) *The X-ray Attenuation Project* (D. C. Creagh) has completed its experimental phase and the results for silicon have been published [*Acta Cryst.* (1987), **A43**, 102–112]. The major conclusions have been incorporated into Section 4.2.3 of the forthcoming *International Tables for Crystallography* Volume C. Data for copper and graphite being analysed and the ensuing results will be submitted for publication in *Acta Crystallographica* Section A in the near future.

(b) *The Radiation Safety Project* (S. Martinez-Carrera) has had its major findings summarized in Chapter 10: Radiation Safety (D. C. Creagh and S. Martinez-Carrera) of the forthcoming *International Tables for Crystallography* Volume C. In its final form the recommendations include the most recent changes in the British and Australian Ordinances relating to radiation protection.

(c) *The Profile Refinement Project* has not made much progress. It has had two chairmen: J. Čermák, who had to withdraw because organization of the project conflicted with his employers' research interests, and M. Zocchi, who resigned from the Commission because of ill health. Because there will be a strong emphasis on powder diffraction and profile refinement at the XIV Congress in Perth, it has been decided to postpone the decision concerning the future of this project until then.

(d) A new project suggested by the Commission on Journals has commenced under the chairmanship of S. Martinez-Carrera. This project, which will examine the experimental methods for the measurement of single-crystal lattice constants, will be referred to as The Accuracy in Lattice Parameter Measurement Project. G. T. De Titta has been invited to act as a consultant to the Commission on this project.

(e) *Open Commission Meeting* (D. C. Creagh). The Open Commission Meeting at the XIV Congress in Perth will be on Recent Advances in X-ray Powder Diffraction.

6 April 1987

D. C. CREAGH, Chairman

#### *Commission on Crystallographic Computing*

##### *1. Closed Meetings of the Commission*

The Commission met during the XIII Congress in Hamburg in 1984 and the Summer School in Leipzig, German Democratic Republic, in 1986, and an unofficial meeting was held in Torino, Italy in 1985.

These meetings included plans for the organization and scientific programme of the International School on Computing Methods in Crystallography and an Open Meeting of the Commission at the XIV Congress in Perth. There was also close cooperation with other IUCr Commissions on common problems. The other Commission activities for the triennium are outlined below.

##### *2. Publication of the 1984 Mulheim Computing School Proceedings*

The proceedings of the 1984 International Summer School on Crystallographic Computing, held at the Max-Planck Institut in Mülheim/Ruhr, Federal Republic of Germany, 30 July–8 August 1984, were published in 1985 by Clarendon Press, Oxford, under the title *Crystallographic*

*Computing 3-Data Collection, Structure Determination, Proteins, and Databases.* G. M. Sheldrick, C. Krüger and R. Goddard are the editors of the proceedings.

### 3. The 1985 Torino Workshop

The Pre-Meeting Workshop of ECM-9 on Direct Methods and Their Application to Structures Showing Superstructure Effects was held in Torino, Italy, 29-31 August 1985 under the auspices of the Commission and organized by R. Böhme and D. Viterbo. Theoretical and practical aspects of the solution of superstructures by direct methods were considered. Computer programs were demonstrated and the participants were invited to provide their own data to be used during practical sessions. All the facilities were offered by the computing centre CSI-Piemonte (Torino). Lectures were held during the morning sessions. Particular emphasis was placed on the afternoon practical laboratories.

There were 37 participants, including 11 lecturers. Lecture notes were published in the form of a booklet. Sponsorship was given by local Italian institutions. The informal environment and excellent facilities helped to ensure the high level of the workshop.

### 4. The 1986 International Summer School on Crystallographic Computing-Leipzig

The school was held in Karl-Marx-Universität, Leipzig, German Democratic Republic, 11-20 August 1986, i.e. after ECM-10 in Wrocław. The Commission and two local crystallographers acted as the Programme Committee for the school and selected the topics and lectures. This school was intended mainly for participants in the Central and East European regions. The emphasis was on graphics, powder methods and data bases.

Twenty-six lectures were held during the morning sessions. However, the main strength of the school was the afternoon tutorials selected according to the interests of the students. There were 107 participants from 17 countries and 18 lecturers. The proceedings of the school were edited by P. Paufler, V. Geist and D. Klimm and published by Karl-Marx-Universität Leipzig Press under the title *Crystallographic Computing*. The school was financially supported by the IUCr, by Fachinformationszentrum Energie, Physik, Mathematik GmbH Karlsruhe, and by the Karl-Marx-Universität, Leipzig. Special funds were used specifically to help young scientists attend the school.

### 5. The 1987 International School on Crystallographic Computing-Adelaide

The school will be held in Adelaide, Australia, 22-29 August 1987, as an associated meeting of the XIV Congress. It will provide expert tuition on a range of crystallographic computing techniques of interest to 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. There will be lectures and small group tutorials or workshops, with material for these practical sessions provided by the lecturers to illustrate their topics. The school has received financial support from the IUCr and sponsors. Limited financial assistance towards travel and living expenses in Adelaide may be available to students, particularly those from developing countries.

### 6. Open Commission Meeting-Perth

During the XIV Congress in Perth the Commissions on Crystallographic Computing and on Crystallographic Teaching are jointly organizing a meeting on Crystallographic Micro-computing.

### 7. Computer Program Abstracts in the Journal of Applied Crystallography

The Commission finalized the guidelines and format for Computer Program Abstracts in the *Journal of Applied Crystallography*. It is a way of distributing up-to-date information on programs to the whole crystallographic community. H. D. Flack was the member of the Commission most involved in this project.

14 April 1987

K. HUML, Chairman

### Commission on Crystallographic Data

1. *Closed Meetings of the Commission.* The Commission met during the Hamburg Congress in 1984 and some members met during ECM-9 in Torino, Italy, in 1985. Topics discussed included recommendations to editors of non-IUCr journals, quality of structural work, standardization of structural results, transfer of numerical data in machine-readable form, and accessibility of databases.

2. *Open Commission Meetings.* The Commission organized two Open Commission Meetings at the XIII Congress in 1984 on Obtaining Structural Data from Computer Databases and on the Role of Crystallographic Data in Systematic Crystal Chemistry. Two joint meetings with the Commission on Journals will be held at the XIV Congress in Perth on Accuracy of Crystallographic Data and on the Future of Crystallographic Journals and Databases.

3. *Database demonstrations.* Database demonstrations were organized more or less by the Commission or its members at many meetings, including the XIII and XIV IUCr Congresses, ECM-9 in Torino, Italy, in 1985, the meetings of the Arbeitsgemeinschaft Kristallographie in Cologne, Federal Republic of Germany, in 1985 and in Giessen, Federal Republic of Germany, in 1986, the workshop at the American Crystallographic Association meeting in Hamilton, Canada, in 1986, and the schools on crystallographic computing organized by the Commission and held in Mülheim, Federal Republic of Germany, in 1985, in Leipzig, German Democratic Republic, in 1986, and in Adelaide, South Australia, in 1987.

4. *Reports of the Commission for publication.* The Commission prepared three reports:

(a) *The Deposition of Crystallographic Results: Current Problems and Their Causes* [*Acta Cryst.* (1986), C42, 1671-1675].

(b) *Recommendations for the Standardization of Unit Cell Descriptions* (not yet published, still in discussion).

(c) *Standard Crystallographic File Structure.* Prepared by former Chairman I. D. Brown and distributed in several expanded versions (including aspects of the Molecular Graphics File Structure).

#### 5. Internal Reports.

(a) *Accessibility of Databases.* Report by the Chairman on the results of a questionnaire to National Committees (14 June 1985).

(b) *Proposal to the Executive Committee for further activity in the field of numeric data and more efficient database production* (14 June 1986).

(c) Discussion on cooperation in producing databases and *Structure Reports* (22 July 1986).

6. Publication on Crystallographic Databases. For the Perth Congress the Commission will publish a booklet with the title: *Crystallographic Databases: Information Content-Software Systems-Scientific Applications*. Thirteen contributions by 26 contributors will describe the field as a whole.

1 May 1987

G. BERGERHOFF, Chairman

#### *Commission on Crystallographic Nomenclature*

The principal activities of the Commission over the last triennium have been directed through the work of its three committees. The *ad-hoc* Committee on the Nomenclature of Symmetry [see *Acta Cryst.* (1986), **A42**, 64 for the membership] has maintained an active correspondence during the period and has further refined its definition of terms related to symmetry elements in space and point groups. An Open Commission Meeting will be held at the XIV Congress in Perth, in the form of a semi-microsymposium organized by P. M. de Wolff, to discuss the present proposals concerning symmetry nomenclature.

The Sub-committee on Statistical Descriptors in Crystallography [see *Acta Cryst.* (1987), **A43**, 143 for the membership] has now produced a second draft of a report on statistical descriptors and is considering a new series of proposed revisions. Aspects of the revised report will be presented from several points of view for public discussion at another Open Commission Meeting in Perth, organized by D. Schwarzenbach, in the form of a semi-microsymposium.

The Sub-committee on the Nomenclature of Inorganic Structure Types [see *Acta Cryst.* (1986), **A42**, 64 for the membership] has held three most useful meetings, in Lisbon, Portugal, Marburg, Federal Republic of Germany, and Geneva, Switzerland, during the triennium, at no cost to the IUCr. An advanced version of the resulting report has been produced and this will be presented for public discussion at a third Open Commission Meeting in Perth, organized by J. Lima-de-Faria.

Congress registrants interested in the areas covered by these Open Commission Meetings are urged to participate and make their views known, since the final resulting nomenclature will become binding on all IUCr publications following their appearance in the IUCr journals.

Contact has been maintained throughout the triennium with a number of international bodies, particularly various committees and commissions of IUPAC, the International Mineralogical Association and several National Committees.

20 April 1987

S. C. ABRAHAMS, Chairman

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

Initially, members were solicited by the Chairman for suggestions concerning an appropriate activity for the Commission during its triennial period. At the same time, the Chairman proposed that the Commission undertake a round-robin study on ZnS, to investigate the potential for providing a fixed point on the pressure scale for use at elevated temperatures (<573 K). Such a calibration point, if well characterized, would satisfy a critical need in the high-pressure community. Since no other suggestions from

members of the Commission were forthcoming, the Chairman initiated a round-robin study to determine the temperature dependence of the high-pressure phase transition in zinc sulfide, which occurs at 15 GPa at room temperature. A well characterized determination of the phase boundary as a function of pressure and temperature was the goal.

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. In our laboratory, experiments were performed in a diamond anvil cell using the ruby fluorescence method of pressure measurement to determine the effect of temperature on the transition pressure. Preliminary results of those measurements indicate that the phase-transition pressure in ZnS is either independent of temperature or slightly negative in its dependence (lowering the pressure of the transition with increasing temperatures to 500 K). However, the experiments were found to be very difficult to carry out 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 overshot 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 and the results so far are inconclusive. More data need to be obtained and analysed before reporting a definitive result.

10 July 1987

G. J. PIERMARINI, Chairman

#### *Commission on Crystallographic Teaching*

The Commission tries to set up new activities relating to the teaching of crystallography apart from its already longer-established activities. In summary, the following activities took place or are in progress:

1. *Schools*. A highly successful winter school was held in Madras, India, in December 1985. The Proceedings of the school have been published, in cooperation with COSTED, by World Scientific, Singapore. The next school will be held in the People's Republic of China in September 1988. The Commission is trying to hold more schools in other parts of the world as well.

2. *Activities at Congresses*. The Commission organized several activities at the XIII Congress in Hamburg in 1984, such as a book exhibition, a non-commercial exhibition and a crystallographic film show. At ECM-9 in Torino, Italy, in 1985 a one-day tutorial meeting was organized, together with the Commission on Small Molecules. At the XIV Congress in Perth there will be a computer laboratory where teaching and scientific software can be demonstrated permanently.

3. *Historical Atlas of Crystallography*. The Editor, J. Lima-de-Faria, finished work on the *Atlas* and possible ways of publishing it are currently being explored.

4. *Pamphlets*. The Commission intends to continue the pamphlet project and is searching for new topics and authors. Readers of this report are encouraged to contact the Chairman of the Commission with suggestions.

5. *Crystallographic Book List*. The possibility of making available regular updates of the Book List, as appeared a

few years ago in *J. Appl. Cryst.*, is being discussed with the Book-Review Editor of *Acta Cryst./J. Appl. Cryst.*

6. *Film List.* H. von Philipsborn is currently undertaking the job of compiling a list of scientific films on crystallography. The first draft will be ready at the XIV Congress.

7. *Newsletter.* For several reasons it has not been possible to initiate a Commission newsletter, most probably because crystallography is such a small field and teaching is just part of it. The Commission strongly suggests that, instead of several Commission newsletters, there should be a general IUCr Newsletter since postage is the main source of costs.

8. *IUCr Visiting Professors.* The Commission is developing the idea of visiting professors as an alternative to summer schools. In many countries the infrastructure is not present to organize a full school with about 15 lecturers and 150 participants. Smaller-scale events, with 30 to 50 students and 1 or 2 lecturers, are much easier to arrange. The IUCr Visiting Professor scheme is intended to fulfil this objective.

10 May 1987

H. SCHENK, Chairman

#### *Commission on Electron Diffraction*

The XIII General Assembly in Hamburg in 1984 approved the application of the Commission for an increase in its membership from 9 to 10 to take into account new developments in the field. The Commission now has five HEED (high-energy electron diffraction) members, three GED (gas electron diffraction) members and two LEED (low-energy electron diffraction) members.

The Commission is responsible for advising the Editors of Volumes B and C of *International Tables for Crystallography* on the sections dealing with electron diffraction and microscopy, and various members of the Commission have written articles for *International Tables*. There has been considerable correspondence between the Editors, the Chairman of the Commission and authors of the various sections.

Preparations of the Commission for the XIV Congress in Perth have included suggesting to the Organizing Committee topics and names of speakers for Main Lectures, Micro-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 range of incident electron energies. The Commission is also supporting two Satellite Meetings connected with the Perth Congress: the Symposium on Validity of Structures from Electron Microscopy, and the Symposium on Accuracy in Structure Factor Measurements.

Major discoveries have occurred in the last three years in which crystallography plays a leading role, and these have gripped the imagination of scientists throughout the world. First came the totally unexpected discovery of quasi-crystals with fivefold symmetry, and the Commission has advised the inclusion of this topic in *International Tables*. Second came the news, which leaked out towards the end of 1986, of the discovery of relatively high-temperature ceramic superconductors. Members of the Commission are now actively studying the local crystallography of these materials using electron diffraction techniques. There can

be no doubt that while exciting discoveries like these continue to be made the Commission on Electron Diffraction will have an active role to play in the IUCr.

18 May 1987

C. J. HUMPHREYS, Chairman

#### *Commission on Neutron Diffraction*

The Commission has sponsored the following activities, of which those marked with an asterisk \* are new activities.

##### 1. *Newsletter*

This appears twice a year and is distributed to over 850 individual scientists. The editor changes after the publication of each issue, and is usually selected from the membership of the Commission. By this means not only international news but also regional news reflecting the geographical interest of the editor are covered.

The editors of the Newsletters since 1984 were: March 1984, B. T. M. Willis (UK); October 1984, M. S. Lehmann (France); April 1985, R. Chidambaram (India); October 1985, K. Hennig (German Democratic Republic); June 1986, H. G. Smith (USA); October 1986, T. J. Hicks (Australia); May 1987, B. T. M. Willis (UK).

##### 2.\* *Compilation of temperature factors of cubic elements*

A compilation has been made of the temperature factors of twenty-two cubic elements. It is based on data from X-ray and neutron diffraction,  $\gamma$ -ray diffraction and high-voltage electron diffraction. Recommended values are given of the r.m.s. thermal displacement at room temperature and of the Debye temperature. The compilation is published in the report PINSTECH/NPD-120 of the Pakistan Atomic Energy Commission (December 1986).

##### 3.\* *Fifty Years of Neutron Diffraction*

This is the title of a book published by Adam Hilger Ltd in 1987 and edited by G. E. Bacon. It forms a trilogy with the earlier volumes: *Fifty Years of X-ray Diffraction* (1962) edited by P. P. Ewald, and *Fifty Years of Electron Diffraction* (1981) edited by P. Goodman.

The Commission has assisted in the preparation of this book. Chapter 6 by B. T. M. Willis summarizes the activities of the Commission in the period 1969-1985.

##### 4.\* *Symposium on Neutron Scattering and Applications, Sydney, 8-10 August 1987*

This will be held just prior to the Congress in Perth. Topics to be covered include *ab initio* structure determination from powders, neutron optics, zeolite catalysts, and perovskite superconductors.

##### 5. *Articles for Volume B and Volume C of International Tables*

A series of articles on neutron techniques have been contributed by authors suggested by the Commission.

1 May 1987

B. T. M. WILLIS, Chairman

#### *Commission on Small Molecules*

##### *Establishment and goals*

The Commission was established at the XIII Congress in Hamburg in 1984. It aims to represent the broad field of small-molecule crystallography both within the IUCr

and in the scientific community at large in several ways, for example,

(a) by encouraging colleagues to encourage the inclusion of micro-symposia dealing with crystallographic topics in the framework of meetings organized by societies (national and international) representing other disciplines,

(b) by organizing international meetings with IUCr sponsorship where the emphasis is on the contributions of small-molecule crystallographers to the understanding of broader phenomena,

(c) by providing a forum for small-molecule crystallographers to express their concerns and wishes with respect to the IUCr and the scientific community at large,

(d) by serving as a vehicle for the dissemination of information to the small-molecule community at large, and

(e) by assisting colleagues to pursue significant research in the field.

#### Activities

1. *Micro-symposia*. Resulting from efforts of Commission members, several micro-symposia dedicated to the efforts of small-molecule crystallographers have been included in the framework of meetings sponsored by non-crystallographic scientific societies, including the Chemical Institute of Canada, the International Congress of Heterocyclic Chemistry, Western Pharmacology Meeting (Banff, Canada), and the International Congress of Steroid Hormones (Madrid, Spain). The Commission also had some input in a Symposium on Three-Dimensional Structure and Drug Action organized by the Crystallographic Society of Japan.

2. *Meetings sponsored by the IUCr*. The Commission supported applications for IUCr sponsorship of four international meetings and helped organize these meetings, namely (i) Steric Aspects of Biomolecular Interactions, Sopron, Hungary, 1985, (ii) Symposium on Organic Crystal Chemistry, Poznań-Rydzyňa, Poland, 1986, (iii) International Symposium on Molecular Structure, Beijing, People's Republic of China, 1986, and (iv) Symposium on Computational Methods in Chemical Design, Schloss Elmau, Federal Republic of Germany, 1986. The proceedings of the last two meetings will be published in the new IUCr/OUP Crystallographic Symposia Series. The commission also encouraged the publication in this series of *Patterson and Pattersons*, the proceedings of a meeting in Philadelphia to mark the 50th anniversary of the Patterson function.

3. *Forum*. The Commission has sought contact with the small-molecule community by holding Open Commission Meetings at ECM meetings, the XIII Congress in Hamburg, and at the meeting in Hungary. Each was well attended and topics of current interest were the subject of lively discussion.

At the request of the Executive Committee, the Commission conducted a survey of a sample (about 100 colleagues) of the international small-molecule crystallographic community concerning the editorial policies and structures of *Acta Crystallographica* Sections B and C.

4. *Information dissemination*. The Commission publishes a newsletter in an effort to provide the small-molecule community with up-to-date information concerning its activities, events of interest (e.g. future meetings) etc. The newsletter is distributed without charge with the understanding that it will be copied and distributed further.

5. *Research assistance*. The Commission has initiated a programme to assist scientists who do not have access to state-of-the-art data-collection facilities to come together with colleagues who are willing to measure at least one data set per year. This programme has been operational since June 1986. The Secretary of the Commission (W. L. Duax) plans to survey participants prior to the XIV Congress in Perth, in an effort to assess the effectiveness of the programme.

The Commission solicited colleagues to organize workshop-tutorials entitled Molecular Systematics and Inorganic Molecular Crystals, the day before the ECM-9 and ECM-10 meetings, respectively.

27 April 1987

J. J. STEZOWSKI, Chairman

#### Appendix F: Reports of the Representatives on Scientific and Regional Associates

##### *International Organization of Crystal Growth (IOCG)*

According to its Statutes, the main activities per triennium of the IOCG are the organization of an international school and an international conference on crystal growth. In the past triennium both events have been hosted by the British Association for Crystal Growth.

The Sixth International Summer School on Crystal Growth (ISSCG-6) was held in Edinburgh, Scotland, 5–11 July 1986, and was attended by about 120 delegates. The Eighth International Conference on Crystal Growth (ICCG-8) followed immediately, in York, England, 13–18 July 1986, and was attended by about 530 delegates. The Proceedings have already been published as an issue of *J. Crystal 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, incorporated in *J. Crystal Growth* and edited by B. Cockayne;

(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 cared for by the Japanese Association for Crystal Growth.

Finally, the composition of the new IOCG Council for the triennium 1986–1989, as approved in York after postal ballot, is: President, R. Kern (France); Co-Vice Presidents, R. F. Sekerka (USA) and B. Cockayne (UK); Secretary, M. Schieber (Israel); Treasurer, E. Kaldis (Switzerland); Past-President, R. A. Laudise (USA); Members, F. Ainger (UK), K. W. Benz (Federal Republic of Germany), A. Chernov (USSR), J. Giling (Netherlands), H. Komatsu (Japan), I. Sunagawa (Japan), B. T. J. Hurle (UK; representative of IOCG to IUCr), C. Paorici (Italy; representative of IUCr to IOCG).

10 March 1987

C. PAORICI, Representative

##### *European Crystallographic Committee*

The IUCr representative attended the meetings of the European Crystallographic Committee held in August 1984 during the XIII IUCr Congress in Hamburg, Federal Republic of Germany, in September 1985 during ECM-9 in Torino, Italy, and in August 1986 during ECM-10 in Wrocław, Poland. During these meetings the representative participated in the discussions of various topics, particularly

those concerning the affiliation of the European Crystallographic Committee to the IUCr as a Regional Associate.

The organization of the European Crystallographic Meetings (ECM) is one of the main topics considered by the Committee. They are successful and receive the appreciation of the whole crystallographic community.

During the Wrocław meeting the organization of ECM-11 (Vienna, Austria, 28 August–2 September 1988) was examined, and the proposals to hold ECM-12 in Moscow, USSR (August 1989) and ECM-13 in Ljubljana, Yugoslavia, (1991) were accepted.

The ECC officers for 1984–1987 are: President, K. Łukaszewicz (Poland), Vice-President, G. S. D. King (Belgium), and Secretary, G. Filippini (Italy). For the elections of officers for 1987–1990, the principles that West and East Europe should be equally represented and that all the three offices should not change at the same time have been approved.

The ECC has actively sought information on low-price travel for European crystallographers to the XIV IUCr Congress in Perth.

27 April 1987

M. NARDELLI, Representative

#### Appendix G: Reports of the Representatives on bodies not belonging to the Union

##### *IUPAP Commission on the Structure and Dynamics of Condensed Matter*

The main activity of this Commission is to examine preliminary applications by conferences, falling within its domain, to be sponsored and supported by IUPAP and make appropriate recommendations. The conferences are divided into three categories: (1) *General Conferences* on the entire field of interest to a Commission, normally occurring triennially with attendance in the range of 750–2000; (2) *Topical Conferences* concentrated on broad subfields of the area of the particular Commission's interest, and scheduled in the years between the General Conferences with attendance in the range of 300–600; (3) *Special Conferences* restricted on specialized topics with attendance in the range 50–200.

The following criteria are considered by the Commission in formulating its recommendation to the Executive Council of IUPAP: (1) *scientific value* based on the need for the proposed conference, the calibre of the invited speakers and the accepted papers, and refereeing for accepting papers; (2) *international character* based on the composition of the Programme Committee and on the nationalities of the participants. In this respect free circulation of *bona fide* scientists must be assured in agreement with the ICSU resolution (Helsinki, 1972); (3) *organization* defining the precise dates, location of the conference, name and address of the organizer, approval of the relevant International Commission of IUPAP, approval of the Liaison Committee for IUPAP in the host country, topics covered in the scientific sessions, information on budget, plans for dissemination of the proceedings *etc.* April of the year preceding the proposed conference is the target date by which the request should be made to Commissions.

In 1986 the number of applications for conferences in the field of the Commission to be held in 1987 was ten. Five of these were approved. Some of the topics of these meetings were related to crystallography. Information on

the proceedings is circulated through the IUPAP News Bulletin.

27 April 1987

M. NARDELLI, Representative

##### *Conference Committee of the European Physical Society*

During the meeting held on 13 September 1985 in Bucharest, Romania, the Committee discussed many aspects of the EPS conferences, such as the problems created by visas not given in time to invited scientists from some countries, the treatment of the participants in the NATO-supported EPS-sponsored conferences which have to follow the EPS rules, and the opportunities for young scientists to have discussions with leading scientists during conferences. Suggestions were made about speakers for plenary sessions and for improvement of Study Conferences. The IUCr representative explained the IUCr's policy aimed at increasing the participation of young scientists in IUCr-sponsored meetings.

In 1985 the Committee approved 9 EPS-organized conferences, 25 sponsored conferences, 11 schools (3 EPS organized) and 4 study conferences.

At the meeting held in Bad Honnef, Federal Republic of Germany on 5 September 1986, the preparations for the 7th (Helsinki, Finland, 1987) and 8th (Amsterdam, Netherlands, 1990), EPS General Conferences were discussed. During the same meeting J. Heijn, delegate of the Dutch Physical Society, and D. Hommel, delegate of the Physikalische Gesellschaft der DDR, were nominated as the new Chairman and Vice-Chairman of the Committee, respectively. It was decided that one of the main duties of the Vice-Chairman will be that of assisting the Chairman in improving the balance of the EPS activities in East and West Europe.

In 1986 the Conference Committee approved 10 EPS-organized conferences, 24 sponsored conferences, 11 schools (2 EPS organized) and 4 study conferences.

The IUCr representative was also invited to attend, as a guest, the meeting of the Condensed Matter Division of the EPS, held in Pisa, Italy, on 5 December 1986. During that meeting he had the opportunity of explaining the general organization of the IUCr and its policy for promoting scientific developments in the field of crystallography.

27 April 1987

M. NARDELLI, Representative

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

The triennium 1984–1986 has seen major changes: the constitutional reorganization whereby the Abstracting Board of the International Council of Scientific Unions (ICSU AB) became the International Council for Scientific and Technical Information (ICSTI), and the resumption of a substantial technical programme by ICSTI. This report focuses on the reorganization and on those aspects of the technical programme that appear to be of greatest interest to the IUCr.

##### *Reorganization during the triennium*

Two matters had preoccupied the ICSU Abstracting Board during the preceding triennium (1981–1983): its restructuring to meet the current needs of the users, producers, and distributors of scientific and technical information; and its relations with ICSU. In recent years the distinction between primary producers and secondary and

tertiary services, once sharp, has tended to become blurred or even to disappear. At the General Assembly in 1980, therefore, the Board decided that its membership classifications (member countries, member unions, member secondary services) no longer reflected current needs, and set up a committee to consider revision of the purposes and structure of the Board. In parallel with this, the Board's Sub-committee on Statutes and By-Laws was asked to prepare a thorough revision of the Statutes and By-Laws, eliminating as far as possible ambiguities, repetitions and obsolete provisions. Both Committees reported to the regular triennial General Assembly of the Board held in May 1983, and after full discussion it was decided to hold an Extraordinary General Assembly in June 1984. This General Assembly adopted a new set of Statutes and By-Laws that incorporated the recommendations of the committees. The major changes from the previous Statutes are:

1. The name of the organization became the International Council for Scientific and Technical Information (ICSTI).

2. There are two classes of Full Members, Class A consisting of bodies primarily concerned with the production and utilization of information, and Class B of bodies primarily concerned with the distribution of information. The IUCr falls into Class A.

3. In each Class there are three Categories of dues on a basis similar to that of the five IUCr categories. On major financial matters the number of votes depends on the dues Category; on other matters each Full Member has one vote. The dues for Class B members are about twice as great as those for Class A in each Category.

4. In addition to the Full Members, there is provision for Associate Members (organizations) and Honorary Members (persons). Such members have the right to participate in meetings of ICSTI, but have no vote. Union and Country membership, as such, has disappeared, but all existing members in these classes automatically became members in Class A.

Since the reorganization there has been a considerable increase in membership in all classes.

*Relations with ICSU.* For several years before 1984 ICSU had been expressing dissatisfaction with the ICSU Abstracting Board, though the reasons for the dissatisfaction were never made clear. This dissatisfaction was known to ICSU AB/ICSTI and fully discussed in various contexts. However, the Board/Council saw no reason from its side to propose substantial changes in its relations with ICSU, and the Statutes described above retained ICSU as the Sponsoring Body of ICSTI and as a Member in Class A. The matter has finally been resolved by a change in the listing of ICSTI in the ICSU Year Book from a 'Permanent Service' (a non-statutory classification) to a 'Scientific Associate' (a status recognized in the ICSU Statutes).

#### *Activities since reorganization*

The 1985 Council in Baden-Baden, Federal Republic of Germany, was largely concerned with implementing the reorganization, though several new members were elected. Active work began with the General Assembly and associated meetings held in York, England, in May 1986. This was the first General Assembly since the transition from the Abstracting Board of the International Council of Scientific Unions became fully operative, and was marked by greater emphasis on technical and less on organizational

matters than in recent years. This welcome trend is likely to continue.

*Compact-disk read-only memories.* There was a discussion of the possible impact of the 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 the 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. 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. The membership of the Executive Board elected at the General Assembly will serve until 1989. 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.

*Groups.* ICSTI has decided to set up five special cross-disciplinary groups, namely Economic Issues, Electronic Publishing, Primary/Secondary Relations, Numeric Data, and Education and User Needs.

The representative of the IUCr has been actively engaged with the Group on Education and User Needs (of which he is the Chairman) and the Numeric Data Group. 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. Among the topics discussed were Reports on data activities in astronomy, crystallography, materials performance, and physics; CODATA Referral Database; Data tagging; the 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*.

The next meeting of the Council will take place in New York, USA, 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.

18 March 1987

A. J. C. WILSON, Representative

*ICSU Committee on Data for Science and Technology (CODATA)*

The Executive Committee of CODATA decided to form a strong collaboration with ICSTI (International Council for Scientific and Technical Information). In the long term this could help to bring crystallographic results to scientists of other fields. This is a continuation of the main activities of CODATA which tries to transfer experience in and results of modern data handling - this means computerized data management - from one scientific field to another.

Current or proposed activities of interest to crystallographers include:

1. *ad hoc* group to discuss data dissemination and/or training activities;
2. *ad hoc* group to deal with the broad problems of computer handling of data;
3. working group to prepare a glossary of terms and acronyms used in scientific and technical data handling;
4. workshop on nucleic acid and protein sequence data banks;
5. preparation of computer-searchable directories of data sources.

The IUCr representative attended the CODATA meeting at Ottawa, Canada, 1986. Exchange of information on progress of numeric data handling in all branches of science was the most important result of the meeting. CODATA installed an electronic mailbox system with DIALCOM for faster correspondence, completing the existing electronic mail possibilities by EARN, BITNET *etc.* The representative holds a user identification (CDT0078).

1 May 1987

G. BERGERHOFF, Representative

*ICSU Committee on Science and Technology in Developing Countries (COSTED)*

COSTED was established by the International Council of Scientific Unions (ICSU) in 1966 to address specifically the problems of science and technology in developing countries. Over the years COSTED has carried out a number of activities, *e.g.* the sponsorship of various meetings and courses, with scientists in developing countries. The IUCr has had beneficial interactions with COSTED through its support for scientists from developing countries to attend IUCr-sponsored meetings, schools and workshops. Recently, the Executive Board of ICSU in the interest of enhancing ICSU's work in developing countries decided, with the support of the General Assembly, to locate regional offices of COSTED in many areas throughout the world. This involved the establishment of five Regional Secretariats, the specification of seven categories which will form the basis for the programmes and activities of COSTED, the preparation of detailed descriptions of the seven categories and the establishment of administrative processes for coordinating and carrying out the activities.

25 February 1987

J. KARLE, Representative

*ICSU Committee on Space Research (COSPAR)*

It has been the most important and dramatic triennium for materials science in space. Following the Spacelab-1

flight in 1983, two other flights took place in 1985: the NASA Spacelab-3 flight and the D-1 Mission, a flight of Spacelab chartered by the Federal Republic of Germany. The many successful experiments supported clearly the idea that, some time in the future, materials science in space will be a most interesting scientific field with direct impact to many important applications. The adherence of the IUCr to COSPAR since 1976 has been based on this assumption. Unfortunately, just at the time when materials science in space accelerated its development and the planning for the Space Station gathered momentum, the catastrophe of Challenger abruptly halted these plans. To bridge the gap and to enable the commitment of young scientists in this field, in spite of the great delay in space experimentation, ESA, NASA, NASDA and other national organizations in many western countries are pumping appreciable funds into materials science in space.

COSPAR, following this general trend, has successfully become a forum of the scientific community in this field. The only COSPAR meeting in the triennium, in Toulouse, France, 30 June-12 July 1986, contained highlights of numerous investigations in crystal growth, metallurgy, glasses, ceramics, and related fluid physics problems. Work of particular interest to crystallographers included dislocation-free solution-grown crystals, enhanced growth rate of protein crystals, and GaAs crystals with a high degree of perfection.

At present the only country which has, potentially, flight opportunities is the USSR. After a long lethargic period, their materials science in space programme started evolving, but the communication of results with the rest of the scientific community is inadequate. To improve the international scientific communication in this field, COSPAR intends to organize the first international symposium on materials science in space at its next meeting, in Helsinki, Finland, 18-29 July 1988. The IUCr is adequately represented in the programme committee, so that subject and speaker choice will be oriented towards crystallographic interests. The support of this symposium by the international Unions will strongly influence its degree of success.

24 July 1987

E. KALDIS, Representative

*ICSU Committee on the Teaching of Science (CTS)*

The Committee has had two meetings in the last three years, one in Bangalore, India, in 1985 and one in Paris, France, in 1987. The IUCr representative only attended the second one.

The main activities of the CTS are teaching activities for developing countries, popularizing science teaching in general, and stimulating contacts between the teaching Commissions of individual Unions. In fact, these Commissions can learn significantly from each other by sharing ideas and results. The main efforts of the CTS in the last three years were the following: a large conference on Science Teaching in relation to Society in Bangalore, India, in 1985 and regional follow-up activities, workshops on primary science, technician training in developing countries, and low-cost equipment. The CTS also tries to set up new activities such as microcomputers for teaching. Much of the work is sponsored by Unesco. Since the CTS meets only once every 18 months, the representative of the IUCr can only attend two such meetings in a triennium. I strongly suggest another arrangement, so that IUCr representation

on the CTS has more continuity. At present, the Chairman of the IUCr Commission on Crystallographic Teaching is (*ex officio*) the IUCr representative on the CTS. Perhaps a member of the Commission should take this job for six or nine years, to establish better contacts with the CTS and Unesco than can be established now.

10 May 1987

H. SCHENK, Representative

*IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS)*

The IDCNS is the central committee through which all provisional recommendations on nomenclature and symbols generated by any IUPAC divisional committee or commission pass for approval. The IUCr appointed S. C. Abrahams its first representative to the IDCNS in 1984, with A. J. C. Wilson as alternate, in order to strengthen the existing ties between the IUCr Commission on Crystallographic Nomenclature and the IDCNS. Copies of all such recommendations are now regularly received and, where a crystallographic input appears advisable, commented upon. One recent nomenclature publication that is likely to be of interest to many crystallographers is the *Abbreviated List of Quantities, Units and Symbols in Physical Chemistry*, published in 1987 for IUPAC by Blackwell Scientific Publications. The IDCNS meets annually. The IUCr was not represented at the 1985 meeting in Lyon, France, but A. J. C. Wilson attended the 1986 meeting in Witney, England. The 1987 meeting will be held in Boston, Massachusetts, USA, at the time of the XIV Congress.

16 April 1987

S. C. ABRAHAMS, Representative

**Appendix H: Summary of the activities of the Sub-committee on the Union Calendar**

The Sub-committee on the Union Calendar is a Sub-committee of the Executive Committee and therefore, according to Statute 8.1, has no obligation to report to the General Assembly. However, a summary of its activities is given in this Appendix for the information of delegates.

During the period since the XIII General Assembly the Sub-committee has considered many requests for sponsorship and financial support by the IUCr, and has made recommendations accordingly to the Executive Committee. From 1985 the new policy, decided by the Executive Committee, of giving financial support specially devoted to help young scientists was successfully applied. An important aspect that must be guaranteed by the organizers of all meetings sponsored by the IUCr is the free circulation of *bona fide* scientists.

The following meetings on topics of crystallographic significance have received IUCr sponsorship. \* indicates that financial support was given for organization, while † indicates financial aid to young scientists. The IUCr also provided financial support to the XIV International Congress of Crystallography.

\* Static and Dynamic Implications of Precise Structural Information, Erice, Italy, 24 May–6 June 1985.

\* Sagamore VIII Conference on Charge, Spin and Momentum Densities, Sanga-Säby, Sweden, 28 July–3 August 1985.

VI International Meeting on Ferroelectricity, Kobe, Japan, 12–16 August 1985

\* Steric Aspects of Biomolecular Interactions, Sopron, Hungary, 26–29 August 1985

\* Crystal Deposition and Dissolution in Tissues, Lugrin, France, 29–31 August 1985

\* Pre-meeting Workshop on Direct Methods and their Application to Structures Showing Superstructure Effects, Torino, Italy, 29–31 August 1985 (satellite meeting of ECM-9).

† Ninth European Crystallographic Meeting, Torino, Italy, 2–6 September 1985.

\*† School on Direct Methods, Macromolecular Crystallography and Crystallographic Statistics, Madras, India, 9–19 December 1985.

\*† Winter School on Teaching, Characterization and Properties of Epitaxial Electronic Materials, Trieste, Italy, 13–24 January 1986.

† Gordon Research Conference on Electron Distribution 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, Pouchchino, 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.

† Symposium on the Validity of Structures from Electron Microscopy, Melbourne, Australia, 8–9 August 1987 (satellite meeting of XIV IUCr Congress).

† Symposium on Neutron Scattering, Lucas Heights, Australia, 8–10 August 1987 (satellite meeting of XIV IUCr Congress).

† Symposium and Workshop on X-ray Powder Diffraction, Perth, Australia, 20–22 August 1987 (satellite meeting of XIV IUCr Congress).

\*† International Winter School on Crystallographic Computing, Bedford Park, Australia, 22–29 August 1987 (satellite meeting of XIV IUCr Congress).

- † Symposium on Accuracy in Structure Factor Measurements, Lorne, Australia, 23–26 August 1987 (satellite meeting of XIV IUCr Congress).
- \*† International School on Crystal Growth and Characterization of Materials for Electronics, La Habana, Cuba, 30 November–11 December 1987.
- \*† School on Crystallography of Molecular Biology, Erice, Italy, 29 May–7 June 1988.
- \*† International Conference on Defects in Insulating Crystals, Parma, Italy, 22–26 August 1988.
- \*† Summer School on Neutron Diffraction, Oxford, UK, 18–30 September 1988.

Financial support for young scientists attending satellite meetings of ECM-10 and the XIV IUCr Congress has been given to the organizers of the main meetings, for them to allocate.

According to recent decisions of the Executive Committee about the publishing policy of the IUCr, the organizers of IUCr-sponsored meetings are requested to recommend the journals of the IUCr as a suitable channel of publication for the original papers presented in the meetings. The IUCr's new Crystallographic Symposia series has to be considered in cases where the organizers intend to publish the proceedings of the meeting.

#### Appendix I: Budget estimates for the period to the Fifteenth General Assembly; determination of the unit contribution

##### (a) Budget estimates

Previously budget estimates have been prepared only for the General Fund (GF) for the period until the next General Assembly. This time, the likely income and expenditure for the Publications and Journals Development Fund (PJDF) account, the Research and Education Fund (REF) account and the Ewald Fund (EF) account are also considered, because these funds receive transfers from the GF and because their uses are parallel to the uses of the GF. Since the budget estimates had to be prepared at a time when the decisions on many activities were still to be made, these estimates should be considered with due reserve. In particular, no real budget could be prepared for the PJDF or the REF because of their special nature. With this proviso, and in accordance with Statute 9.3, the Executive Committee presents to the General Assembly the following estimates for the three-year period 1 January 1987–31 December 1989.

##### General Fund

<i>Income</i>			
Subscriptions from Adhering Bodies	392 490		
Yield from investments and banking accounts	580 000		
Subventions from Unesco through ICSU	60 000	1 032 490	
<hr/>			
<i>Expenditure</i>			
Administration	401 100		
Subscriptions to ICSU/ICSU bodies	16 500		
Administrative meetings	206 000		
Scientific meetings	278 000		
Transfers to other accounts	130 000	1 031 600	
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<i>Estimated profit</i>			CHF 890
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##### Ewald Fund

Balance at 31 December 1986		120 884	
<i>Income</i>			
Ewald Bequest	33 600		
Transfer from the General Fund	62 000		
Interest	44 800	140 400	
<hr/>			
<i>Expenditure</i>			
Award	33 600		
Other costs (medal, travel, administration etc.)	11 600	45 200	
<hr/>			
<i>Excess of income over expenditure</i>			95 200
<hr/>			
<i>Estimated balance at 31 December 1989</i>			CHF 216 084
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The exchange rate at 1 January 1987, CHF 1 = USD 0.5952, has been applied to convert sums defined in US dollars into Swiss Francs.

The income from subscriptions from Adhering Bodies has been determined on the basis of a unit contribution of CHF 890 for all three years 1987, 1988 and 1989 and on 147 membership units, valid at the date of the estimate.

The total yield from investments and banking accounts, which now includes the interest income credited to the EF account, is CHF 624 800, and is smaller than the amount received in the previous triennium (CHF 847 961). The estimate is based on the present interest rates of the deposit and savings accounts and on the projected yield from the investments (see the comments in Appendix B under the heading *The assets*).

The administrative expenses in the GF account include the cost of the work of the Executive Secretary and his office and of the General Secretary and Treasurer. In 1987 there are also costs for the office refurbishment, part of which was paid in 1986. As in the past, 30% of the total administrative expenses of CHF 573 000 will be charged to the publication accounts, reducing the charge to the GF to CHF 401 100.

Expenses under 'Administrative meetings' are those of the Executive Committee and the Finance Committee meetings, IUCr representation on other bodies and the printing of the Report of the General Assembly. The estimate of CHF 206 000 is higher than in the previous triennium (CHF 143 804). This is due to the high travel costs of the present year and to the transfer of the publication costs of the Report of the XIII General Assembly from the previous triennium, which alone causes CHF 34 000 of the difference.

The Executive Committee is conscious of the need to keep administrative expenses to a minimum. However, the Executive Committee is required to meet at least twice during the period between the General Assemblies (By-Law 2.1), and it is felt that these annual meetings and the meetings of the Finance Committee are necessary if effective control is to be maintained over the financial affairs of the IUCr, particularly with regard to the very large publishing activities.

The heading 'Scientific meetings' includes financial support for scientific meetings organized or sponsored by the IUCr as well as the expenses of the non-publishing Commissions, the Commission Chairmen and the Scientific Programme Committee for the triennial Congresses of Crystallography. In particular, the estimate includes substantial support for the XIV Congress and associated meetings, namely USD 35 000 for the Congress, USD 6000 for the

School on Crystallographic Computing, and the travel grants totalling USD 15 000 to the Chairmen of the non-publishing Commissions and USD 1500 to the three Sub-committees of the Commission on Crystallographic Nomenclature. The annual support for the non-publishing Commissions has been budgeted at a higher level than in the previous triennium. The support for IUCr-sponsored meetings is budgeted to remain at the level reached in 1986, at about CHF 60 000 annually in non-Congress years. In addition, CHF 160 000 can be given during the triennium as the young scientists' support from the REF, including USD 15 000 for the XIV Congress and associated meetings.

The expenses of the publishing Commissions are charged to the relevant publication funds, including the total of USD 20 000 travel support for the Editors and Co-editors for the XIV Congress.

The transfers to other fund accounts include the estimated costs of the first Ewald Prize, plus USD 10 000 to match the donation from the Ewald family. The transfers to the PJDF and the REF are assumed to satisfy the need for the capital in these funds to earn interest in order not to lose value.

The budgeted income in the Ewald Fund account includes the remaining part of the Ewald Bequest (USD 20 000), the transfers from the GF already mentioned, and 8% annual interest on the capital. The other costs include expenses for preparation of the medal, travel costs of the awardees, and administrative work, mainly in the Executive Secretary's office, to assist the Selection Committee for the first Ewald Prize.

Little can be predicted about the costs of projects to be funded from the REF and the PJDF during the triennium, except for the young scientists' support. Sometime during the triennium it is expected to replace the present office computer, which serves mainly the journals at present. This will be a major cost to be paid from the PJDF, but it is too early to estimate the date or the amount.

*(b) Unit contribution*

According to Statute 5.10(k) the General Assembly has to determine the unit contribution from the Adhering Bodies for the period to the next General Assembly.

The Executive Committee recommends to the General Assembly that the unit contribution be retained at its present level, CHF 890, for the years 1988-1990.

**Appendix J: IUCr/Oxford University Press Book Series**

There have been discussions between the IUCr and the Oxford University Press (OUP) since 1985 on the development of an IUCr/OUP Book Series, and most of the details have now been finalized.

The series will, in fact, consist of two sub-series:

(i) *IUCr Crystallographic Symposia*. These will generally be proceedings of meetings which have been sponsored by the IUCr.

(ii) *IUCr Monographs on Crystallography*. These will be textbooks on specific subjects.

A Book Series Selection Committee has been established, under the chairmanship of Dr J. H. Robertson (UK), who is retiring as Book-Review Editor for *Acta Crystallographica* and the *Journal of Applied Crystallography*, a position he has held since 1975. This Committee will consider all proposals for new publications, whether the proceedings of schools and symposia or monographs and textbooks on crystallography, and make recommendations to the IUCr Executive Committee and to the Delegates of the Press (the body responsible for approving all publications handled by the OUP).

Organizers of schools and symposia receiving IUCr sponsorship, who wish to publish the lectures presented there, will be encouraged to consider the IUCr/OUP Book Series as an appropriate vehicle for publication, and to submit a proposal to the Committee Chairman.

The forerunners of the Crystallographic Symposia series were the several proceedings of summer schools on crystallographic computing, organized by or with the assistance of the Commission on Crystallographic Computing. The first publication in the series will be *Patterson and Pattersons: Fifty Years of the Patterson Function*, the proceedings of a meeting held in Philadelphia, Pennsylvania, USA, in November 1984 to celebrate this anniversary.

## ANNEX II

**Statutes and By-Laws of the International Union of Crystallography**

**as Adopted by the Fourth General Assembly in 1957 and Amended by the Fifth General Assembly in 1960, the Sixth General Assembly in 1963, the Seventh General Assembly in 1966, the Eighth General Assembly in 1969, the Ninth General Assembly in 1972, the Tenth General Assembly in 1975, and the Eleventh General Assembly in 1978**

**Statutes****1. Objects of the Union**

1.1. The objects of the Union are

- (a) to promote international cooperation in crystallography;
- (b) to contribute to the advancement of crystallography in all its aspects, including related topics concerning the non-crystalline states;
- (c) to facilitate international standardization of methods, of units, of nomenclature and of symbols used in crystallography;
- (d) to form a focus for the relations of crystallography to other sciences.

1.2. For these purposes the Union shall have the power (a) to adhere to the International Council of Scientific Unions;

- (b) to organize international meetings and conferences on subjects falling within the purview of the Union;
- (c) to promote international publication of crystallographic research and of crystallographic works;
- (d) to set up Commissions or other bodies for special objects;
- (e) to initiate, promote and coordinate crystallographic research requiring international cooperation;
- (f) to organize Special Projects which shall be financed independently of the regular operations of the Union;
- (g) to participate in Joint Commissions with other Unions or other scientific bodies in matters of interest to the Union;
- (h) to perform all such other legal acts as are essential for or conducive to the objects of the Union including the constitution or organization of separate or independent bodies having an appropriate legal status;
- (i) to receive into association existing regional organizations of crystallographers having substantially the same aims and objects as the Union; these organizations shall be known as Regional Associates of the Union;
- (j) to receive into association existing international scientific organizations whose interests overlap with the aims and activities of the Union; these organizations shall be known as Scientific Associates of the Union.

**2. Organization and Legal Domicile**

2.1. Under the name of International Union of Crystallography an Association has been organized and incorporated; it is governed by Articles 60 and following of the Swiss Civil Code and by the present Statutes of Incorporation.

2.2. The duration of the Union is not limited.

2.3. The legal domicile of the Union is in Geneva, Switzerland.

**3. Membership**

3.1. The members of the Union are its Adhering Bodies.

3.2. There shall be only one member for each Country.

3.3. In a Country the Adhering Body can be a National Academy, National Research Council or similar body, or a scientific society or group of such societies. Each Adhering Body shall form a National Committee for Crystallography to represent it in the Union.

3.4. Any number of Countries may agree to form a group in order to name or establish a single Adhering Body. This Body shall form a joint National or Regional Committee for Crystallography. Wherever the terms Country and National Committee for Crystallography are used in these Statutes or in the By-Laws, they shall be taken to include such groups of Countries and joint National or Regional Committees for Crystallography.

3.5. Membership in the Union shall be fully effective when the nature of the Adhering Body and the membership of the National Committee have been reported to and accepted by the General Assembly. Any replacement of an Adhering Body is subject to the approval of the Executive Committee and acceptance by the General Assembly. Any major change in the nature of an Adhering Body shall be considered valid only after it has been reported to and accepted by the General Assembly.

3.6. Adherence to the Union shall be in one of five Categories I-V with corresponding voting powers and contributions as set out in Statutes 5.5 and 9.4. A Body applying for adherence to the Union shall specify in which Category it wishes to adhere; this choice of Category, or any desired change in the Category, is subject to the approval of the Executive Committee and confirmation by the General Assembly.

3.7. Any extension of a joint adherence formed in accordance with Statute 3.4 is subject to the approval of the Executive Committee and acceptance by the General Assembly.

3.8. Participation in Special Projects [Statute 1.2(f)] shall not be obligatory. The extent of financial participation shall be a matter for special negotiation for each such project, except that the relationship between contribution and voting power within the project shall be that of the Category scheme defined in Statutes 5.5 and 9.4 to determine this relationship in the General Assembly.

3-9. Each National Committee has the right to submit to the Union through the General Secretary questions within the competence of the Union.

3-10. Any Adhering Body may withdraw from the Union if it has given notice of withdrawal at least six months before the end of the current financial year; it is required to fulfil its obligations relating to the time period when it was a member of the Union. Its membership and any further obligations shall then be suspended by the Executive Committee at the expiry of the notice of withdrawal. The withdrawal shall take effect when it has been reported to the General Assembly.

3-11. An Adhering Body which withdraws from the Union in accordance with Statute 3-10, or any Adhering Body whose membership is cancelled in accordance with Statutes 5-12 or 9-6, loses all rights in connexion with the Union.

3-12. If the Countries of a group formed in accordance with Statute 3-4 agree that the group should be dissolved, or if a Country wishes to withdraw from such a group, with or without the agreement of the other Country or Countries of the group, the adherence of the original group shall be suspended by the Executive Committee at the expiry of an appropriate notice, provided that the original group has fulfilled its obligations. The termination of the original adherence shall take effect when the matter has been reported to the General Assembly. Pending this report, the Countries of the group, or any of them, may submit proposals for the continuation of their representation in the Union. In each of such proposals the nature of the Adhering Body, the membership of the National Committee and the desired Category of adherence shall be specified. These proposals are subject to the approval of the Executive Committee, which shall then make *ad interim* arrangements concerning these adherences. These arrangements are subject to acceptance by the General Assembly.

#### 4. Administration

4.1. The work of the Union shall be conducted by

- (a) the General Assembly;
- (b) the Officers of the Union, constituting the Executive Committee;
- (c) the Commissions as defined in Statute 8-1.

The composition and function of these bodies are defined in the following paragraphs, whose application is governed by the By-Laws.

#### 5. General Assembly

5-1. The work of the Union shall be directed by the General Assembly which is composed of delegates appointed by the Adhering Bodies.

5-2. The Executive Committee is responsible to the General Assembly and shall participate in its deliberations. Members of the Executive Committee have no voting power in the General Assembly, except for the casting vote of the Chairman [Statute 5-8].

5-3. The General Assembly shall, as a rule, hold an ordinary meeting once every three years. The date and the place of the meeting, unless determined by the previous General Assembly, shall be determined by the Executive Committee. The General Secretary shall communicate the date and the place of the meeting to the National Commit-

tees and to the Commissions at least twelve months in advance.

5-4. In special cases, the President of the Union, with the consent of the Executive Committee, may call an extraordinary meeting of the General Assembly. He shall do so at the request of one-fifth of the Adhering Bodies. The routine business of a General Assembly prescribed in Statute 5-10 shall normally be omitted, unless specifically included in the agenda; but an extraordinary General Assembly shall have the same powers, and be subject to the same rules, as an ordinary General Assembly, except where otherwise is stated in the Statutes and By-Laws. The General Secretary shall communicate the date and the place of the extraordinary General Assembly to the National Committees and to the Commissions at least eight months in advance if amendment of the Statutes is contemplated, or at least four months otherwise.

5-5. The voting power of an Adhering Body at General Assemblies shall be in accordance with its Category of adherence, as follows

Category	I	II	III	IV	V
Number of votes	1	2	3	4	5.

5-6. Each Adhering Body, through its National Committee, shall make known to the General Secretary before the opening of each General Assembly the names of its delegates (and of their alternates, if any), and also the name of the chairman of the national or regional delegation. No Officer of the Union may be a member of any delegation, nor shall any person serve as a member of more than one delegation.

5-7. Normally each of the delegates present at a General Assembly shall have one vote only, but when for special reasons an Adhering Body cannot be fully represented at a General Assembly it may distribute its votes among a number of delegates smaller than the number of votes which that Adhering Body has in accordance with the Category in which it adheres; such a decision has to be made known to the General Secretary before the opening of the General Assembly concerned. Any Adhering Body not represented at a General Assembly may forward its views to the General Secretary by letter, and such views shall be made known to the General Assembly if received before voting takes place.

5-8. Except where otherwise provided in the Statutes and By-Laws, decisions of the General Assembly are taken by a majority of the votes cast. In the event of an equal division of votes the Chairman shall take the final decision.

5-9. No question which has not been placed on the agenda of business to be transacted at the General Assembly shall be discussed or put to the vote unless a proposal to that effect be approved by at least two-thirds of the votes there represented.

5-10. The General Assembly shall

- (a) take appropriate action on any matters concerning membership in the Union [Statutes 3-5, 3-6, 3-7, 3-10, 3-12 and 5-12];
- (b) elect the President, the Vice-President, the General Secretary, the Treasurer and the other Officers of the Union [Statutes 6-1 and 6-3];
- (c) consider, and make decisions regarding, the confirmation of the appointments of Editors of publications of the Union [Statute 7-1];

- (d) determine the number of elected members of each Commission set up by the General Assembly [Statutes 5·11(c) and 8·2];
- (e) elect the Chairmen and members of the Commissions [Statute 8·2];
- (f) elect representatives of the Union on Joint Commissions with other Unions, and on other scientific bodies [Statutes 1·2(g) and 8·5];
- (g) receive the reports on the activities of the Union and of its Commissions [Statutes 6·8 and 8·4];
- (h) receive the audited accounts for the years elapsed since the previous General Assembly [Statute 9·1];
- (i) on receipt of satisfactory reports or accounts, release the Treasurer, or any other Officer, or the Chairman or any member of any Commission or other body, from financial or other liability to the Union;
- (j) determine the budget for general expenditure for the period to the next General Assembly, on the basis of the estimate prepared by the Executive Committee [Statutes 9·2 and 9·3];
- (k) determine the unit contribution for the period to the next General Assembly [Statute 9·5];
- (l) determine the general policy and the timetable for the period to the next General Assembly;
- (m) give preliminary consideration to the activities of the Union for the three-year period following the next General Assembly.

5·11. The General Assembly shall have the power

- (a) to amend these Statutes in accordance with Statute 13·1;
- (b) to formulate and amend By-Laws on any matters not covered by these Statutes;
- (c) to set up any Commission or other body it may deem necessary for the administrative and scientific work of the Union, and to determine the terms of reference of such a body [Statute 1·2(d)];
- (d) to dissolve any Commission or other body set up in accordance with Statute 5·11(c) when its existence is deemed no longer necessary;
- (e) to determine the nature of Special Projects which shall be financed independently of the regular operations of the Union [Statute 1·2(f)];
- (f) to accept Regional Associates, to determine the nature of the association in each case, and to determine any mutual financial commitments;
- (g) to accept Scientific Associates, to determine the nature of the association in each case, and to determine any mutual financial commitments;
- (h) to decide on all other questions falling within the competence of the Union.

5·12. The General Assembly may cancel the membership of any Adhering Body of the Union for any serious cause; such a decision may only be taken after the member in question has been previously given an opportunity to furnish an explanation to the Executive Committee for forwarding to the General Assembly. At least three-fourths of the total number of the votes of all Adhering Bodies are required for cancellation.

## 6. Executive Committee

6·1. The Officers of the Union constituting the Executive Committee are

- (a) the President;
- (b) the Vice-President;
- (c) the General Secretary;
- (d) the Treasurer;
- (e) the immediate Past President;
- (f) six ordinary members.

6·2. The election of Officers of the Union shall be arranged in such a way that there will not be more than two Officers from any one Country. A person is regarded as belonging to the Country in which he is normally resident and where he conducts the main part of his work. In cases of doubt the General Assembly shall decide to which Country a person is considered to belong.

If during the period between General Assemblies the number of Officers from a Country is increased above two because of any change of Country of residence, the Officer or Officers who changed his or their Country of residence may continue his or their service until the close of the next General Assembly. If at that time the number of Officers from the Country concerned would remain above two, one or more of the Officers who changed his or their Country of residence shall be considered to have resigned.

6·3. The offices of General Secretary and Treasurer may be combined and shall then be considered as a single office. Otherwise no person shall hold more than one office simultaneously. The voting power of the Officer holding the combined office of General Secretary and Treasurer shall not be more than that of either the General Secretary or the Treasurer.

6·4. The President holds office as President until the close of the ordinary General Assembly following his election, and continues as a member of the Executive Committee until the close of the ordinary General Assembly next but one following that of his election. He is not then eligible for immediate re-election to the office of President, nor to any other office in the Executive Committee.

The Vice-President holds office until the close of the ordinary General Assembly following his election. He is not eligible for immediate re-election to the same office.

The General Secretary and the Treasurer hold office until the close of the ordinary General Assembly following that of their election. They are eligible for immediate re-election to the same office, but shall not serve in that office for more than three full consecutive terms.

Three ordinary members are elected at each ordinary General Assembly and hold office until the close of the ordinary General Assembly next but one following that of their election. They are not eligible for immediate re-election to the same office.

In the event of a vacancy, through resignation, death or other cause, any Officer elected by the General Assembly to fill the unexpired term of office shall serve only to the end of the normal term of the Officer he replaces; at the end of this service he may be nominated for re-election for a full term to the same office.

6·5. The Executive Committee shall carry out the decisions of the General Assembly and give effect to the general policy of the Union as determined by the General Assembly.

6·6. During the periods between General Assemblies the Executive Committee shall have full power to carry on the business of the Union in all matters not specifically assigned by the Statutes, the By-Laws or the General Assembly to individuals or to Commissions or other bodies. If necessary,

it may make *ad interim* arrangements in all matters assigned by the Statutes and By-Laws to the General Assembly.

6-7. In the event of an individual, a Commission or another body of the Union failing to act in any matter assigned to him or it by the Statutes, By-Laws or the General Assembly, the Executive Committee may, after reasonable notice to the individual or body in question, take action on behalf of the Union.

6-8. The Executive Committee shall report on its activities to the General Assembly. The action taken by the Executive Committee in accordance with Statutes 3-5, 3-6, 3-7, 3-10, 3-12, 6-6, 6-7, 7-1, 7-2, 8-2, 9-6 and 9-9 shall be included in this report. The report to the General Assembly shall be dispatched by the General Secretary to the National Committees and to the Commissions at least ten weeks before the meeting.

### 7. Publications of the Union

7-1. The Editors of the publications of the Union are appointed by the Executive Committee for initial terms extending through not more than six years beyond the ordinary General Assembly following the appointment. Each initial appointment is subject to confirmation by that General Assembly. Reappointments may be made by the Executive Committee for terms of not more than three years, and are subject to confirmation by the ordinary General Assembly following the reappointment.

7-2. Co-editors and Assistant Editors are appointed by the Editors for terms of not more than three years, but they may be reappointed immediately for terms of the same length. The appointments and reappointments are subject to the approval of the Executive Committee.

7-3. Editors and Co-editors are members of the Commissions set up for their respective publications.

### 8. Commissions and Joint Commissions

8-1. The term 'Commission' shall be understood to include all Commissions, Committees, and other bodies of the Union with the exception of National Committees for Crystallography, and the Executive Committee and its subcommittees.

8-2. The Chairmen and members of the Commissions are elected at each General Assembly. Subject to the approval of the Executive Committee, Commissions may co-opt further members during the periods between General Assemblies, and may fill vacancies arising from resignation, death or other cause. Members (but not Chairmen) may be nationals of or residents in a Country not adhering to the Union.

8-3. The Commissions shall be responsible to the General Assembly. They shall generally have full freedom in arranging their internal structure and work. They may formulate their own Rules of Procedure within the framework of the Statutes and By-Laws of the Union, and within their terms of reference.

8-4. The Chairmen shall report on the activities of the Commissions to the General Assembly. These reports shall reach the General Secretary at least fourteen weeks before the General Assembly and shall be dispatched by him to the National Committees and the Commissions at least ten weeks before the meeting.

8-5. The representatives of the Union on Joint Commissions and on other scientific bodies [Statute 1-2(g)] are elected at each General Assembly. For each such body one representative shall be designated as the chief representative of the Union. His obligations to report are the same as those of the Chairmen of the Commissions.

### 9. Finance

9-1. The Executive Committee shall be responsible to the General Assembly for all the financial affairs of the Union.

9-2. The Chairman of each Commission (or other member approved by the Executive Committee) shall be responsible to the Executive Committee for any expenditure of funds by his Commission. Five months before each General Assembly he shall submit to the Executive Committee an estimate of the budget of his Commission for the period between that General Assembly and the one following it. He shall submit annually to the Executive Committee a revised budget for the ensuing year and a statement of accounts for the preceding year. His accounts shall be available for audit by the Executive Committee or its appointees.

9-3. The Executive Committee shall prepare an estimate of the budget for the period between the next General Assembly and that following it. This estimate shall be dispatched by the General Secretary to the National Committees and to the Commissions at least ten weeks before the meeting.

9-4. Each Adhering Body shall pay an annual subscription in accordance with its Category of adherence, as follows:

Category	I	II	III	IV	V
Number of unit contributions	1	3	6	10	15.

The annual subscriptions are payable during the calendar year to which they apply.

9-5. The unit contribution, stated in terms of a currency to be designated by the Executive Committee, shall be determined by the General Assembly for the period to the next General Assembly.

9-6. Any Adhering Body which is in arrears with its subscription for two years shall be warned and shall be deprived of its voting power. The membership of any Adhering Body which is in arrears for four years shall be automatically suspended and may be cancelled by the General Assembly under Statute 5-12. An Adhering Body whose membership has been suspended shall receive no privileges of the Union and incur no further responsibility for dues; it may be reinstated by action of the Executive Committee.

9-7. The financing and management of publications of the Union shall be kept distinct from general expenditure. Editors and Co-editors shall be responsible to the Executive Committee for any receipts or expenditure of funds by them with respect to their publications.

9-8. The financing and management of Special Projects of the Union shall be kept distinct from the regular operations of the Union.

9-9. No funds may be solicited or accepted on behalf of the Union or any of its Commissions from any international, governmental or other agency or person without the prior approval of the Executive Committee. Any National Committee for Crystallography may however solicit funds within

its own Country for the support of its own activities or in its capacity as host for a General Assembly, Congress or other meeting sponsored by the Union. Any funds, in the form of donations, legacies, or grants, accepted by the Executive Committee shall be used so far as is possible in accordance with the wishes of the donors.

#### 10. Liability

10·1. The Union is liable only to the extent of its assets, and the Adhering Bodies are not individually liable for its corporate debts and liabilities.

10·2. The liabilities of the Adhering Bodies are limited to the payment of their annual subscriptions and to such contributions to the Special Projects of the Union as they may have pledged.

10·3. No Officer of the Union shall be individually liable for the corporate debts and liabilities of the Union. The Union shall indemnify any Officer or former Officer in respect of any claims laid against him in respect to his authorized actions on behalf of the Union. At its discretion the Executive Committee may extend this indemnity to other persons in respect of their authorized actions on behalf of the Union.

10·4. The Union shall not accept any liability for any personal loss, damage or accident sustained by an individual, not being an employee of the Union, engaged in any activity, including travel, on behalf of the Union.

#### 11. Auditor and Representation of the Union

11·1. The Auditor of the Union shall be a person or corporation authorized to act as a public accountant. The Auditor shall be appointed by the Executive Committee on the recommendation of the Treasurer and maintained thereafter subject to the approval of the General Assembly.

11·2. With the exception of cheques, all contracts and formal agreements involving the Union shall be signed by two Officers of the Union. The Executive Committee may restrict the power to sign a particular document or type of document to specific persons among the Officers; and it shall determine rules for the signing of cheques.

11·3. The President shall be the official representative of the Union on all other civil and legal occasions and in dealing with other organizations. He may in this respect delegate his powers to another Officer of the Union, or, with approval of the Executive Committee, to any other person.

#### 12. Dissolution of the Union

12·1. The Union shall not be dissolved except on a motion presented at a General Assembly. If a motion to

dissolve is to be presented, the notice for that General Assembly as given under Statute 5·3 or 5·4 shall include a statement of the motion to dissolve and shall refer specifically to this Statute. Such a motion shall be presented to the General Assembly without amendment and at least three-fourths of the votes there represented shall be required for dissolution.

In the event that less than three-fourths of the total number of the votes of all Adhering Bodies are represented at the General Assembly, a postal ballot may be arranged, and in such a postal ballot at least three-fourths of the total number of the votes of all Adhering Bodies shall be required for dissolution.

12·2. In the event of dissolution of the Union in accordance with Statute 12·1, the General Assembly shall appoint a special Committee, reporting to the International Council of Scientific Unions, for the liquidation of the assets of the Union. The net assets shall be given to one or more, preferably international, organizations or institutions which shall spend the assets for purposes so far as is possible in accordance with the objects of the Union.

#### 13. Statutes

13·1. Amendments to the Statutes require action at a General Assembly. An amendment is adopted at such an Assembly only if (i) at least two-thirds of the votes represented at the General Assembly are affirmative and (ii) if these affirmative votes amount to more than half the total number of the votes of all Adhering Bodies. In the event that the vote on a proposed amendment satisfies condition (i) but not condition (ii), the Executive Committee may refer the proposed amendment to a postal ballot of the Adhering Bodies. If the proposed amendment then obtains affirmative votes amounting to more than half the total number of the votes of all Adhering Bodies, the amendment is adopted.

Proposals for amendments may be made by the Executive Committee or by any National Committee. Such proposals made by National Committees shall reach the General Secretary at least six months in advance of the General Assembly. The General Secretary shall dispatch these proposals, and those made by the Executive Committee, to the National Committees and to the Commissions at least four months before the meeting.

13·2. The present English text shall be considered the authoritative text in the interpretation of these Statutes. Where disputes arise concerning this interpretation, the matter shall be decided by the General Assembly, or, during the periods between General Assemblies, by a ruling of the President of the Union.

### By-Laws

#### 1. General Assembly

1·1. The agenda of business to be transacted at a General Assembly shall be determined by the Executive Committee and shall be dispatched by the General Secretary to the

National Committees and to the Commissions at least ten weeks before the meeting.

1·2. Any National Committee and any Commission the Union may propose business to be transacted at a General Assembly. Such proposals shall reach the General

Secretary at least four months before the meeting, and shall be included in the agenda of the General Assembly.

1-3. The General Assembly may provisionally determine the date and the place of the next but one ordinary meeting of the General Assembly.

1-4. Chairmen of the National Committees and of the Commissions, and representatives of Regional Associates and Scientific Associates may attend the General Assembly and take part in the discussions but shall have no voting power. The President may invite representatives of scientific bodies, or individuals, to attend the General Assembly; such invited guests may take part in the discussions but shall have no voting power. Other interested persons may also attend the General Assembly but they shall not take part in the discussions, unless specifically invited or permitted to do so by the Chairman, and they shall have no voting power.

At the discretion of the Chairman any or all of the persons attending the General Assembly under this By-Law may be required to withdraw.

1-5. If a delegate to a General Assembly is absent from a session of the Assembly, his place may be taken by any of the alternates nominated to the Assembly under Statute 5-6 provided that the Secretary of the Assembly is notified before the beginning of the session of the name of the delegate and of the name of the alternate, either by the delegate or by the chairman of his delegation. In general no such substitution may take place during a session of the Assembly, but the Chairman of the Assembly may permit substitution to be made under special circumstances.

1-6. The names of the representatives of a Body whose application for adherence to the Union has been received and declared in good order by the Executive Committee under By-Law 2-9(a) shall be made known to the General Secretary as prescribed in Statute 5-6. These representatives shall be seated with the delegates of the Adhering Bodies during the preliminary ceremonies and the initial business of the General Assembly. At the discretion of the Chairman or by a vote of the Assembly, the representatives may be required to withdraw during the discussion of and voting on matters concerning adherence to the Union. The delegates of a new member may take their seats among the other delegates as soon as the General Assembly has accepted their Adhering Body as a member of the Union.

1-7. Unless decided otherwise by the General Assembly, matters concerning adherence to the Union shall take precedence over all other business at the first business session of the General Assembly, and shall normally precede the reading of the minutes and the discussions of matters arising therefrom.

1-8. Delegates of an Adhering Body may not vote on any matter concerning its membership in the Union.

1-9. In the event of the General Assembly considering a change in a group of Countries according to Statute 3-12, the delegates from the Countries belonging or previously belonging to the group may not vote on any matters concerning the representation in the Union of any of these Countries. After acceptance of the *ad interim* arrangements made by the Executive Committee under Statute 3-12, these delegates have full voting power.

1-10. The delegates of new members may not vote on any matters concerning adherence to the Union, nor on any matters concerning the adoption of the minutes of the

previous General Assembly, during the General Assembly at which they themselves are admitted.

1-11. The General Secretary shall post on the official bulletin board of the General Assembly the names of the Chairmen and members (and alternates, if any) of the delegations and the numbers of votes represented by them.

1-12. During the General Assembly any delegate (or alternate) and any Officer of the Union is considered to have been notified of any action of the General Assembly, or of the Executive Committee, or of any Commission, if one of the two following procedures is adopted

- (a) a notice is placed in the mail box or other location at which the delegate (or alternate) or the Officer is accustomed to receive his mail during the course of the General Assembly, or
  - (b) a notice is handed to the designated Chairman of each delegation with the specific request that he communicate its contents to his delegation, and to the General Secretary with the specific request that he communicate its contents to the Executive Committee,
- provided that in either case a similar notice is posted on the official bulletin board.

1-13. Minutes of the meetings of the General Assembly shall be made. Copies of the draft minutes shall be communicated by the General Secretary to the National Committees, to the Officers of the Union and to the Chairmen of its Commissions. After approval at a subsequent General Assembly, two copies of the definitive minutes shall be signed by the Chairman and the Secretary of the session at which they are approved, and shall be kept by the President and the General Secretary.

## 2. Executive Committee

2-1. The Executive Committee shall meet at each General Assembly. There shall be at least two additional meetings during the period between General Assemblies, unless the Executive Committee by a postal vote decides otherwise.

2-2. The Executive Committee shall make nominations to the General Assembly for the Officers of the Union, for the Chairmen and members of the Commissions, and for representatives on Joint Commissions and on other scientific bodies. Normally these nominations shall be made after a preceding postal communication with the National Committees. In each case in which an Officer of the Union is nominated for another office, either by the Executive Committee or by delegates to the General Assembly [By-Law 7-2], the Executive Committee shall also include a nomination for the office which would be vacated if the election to the other office occurs. If the election to the other office does not occur and if the Officer's term has not expired, the nomination to the office which would have been vacated shall not be considered.

2-3. In the event of the resignation, death or disability of the President, the Vice-President shall assume the office of President until the close of the next ordinary General Assembly.

In the event of the resignation, death or disability of the Vice-President, the Executive Committee may appoint one of its members to serve as Vice-President until the close of the next ordinary General Assembly.

In the event of such circumstances that the General Secretary or the Treasurer cannot carry out his duties, the

other shall assume those duties until the Executive Committee has considered the situation. In that event the Executive Committee may, but need not, appoint a new General Secretary or Treasurer to serve until the close of the next ordinary General Assembly.

In the event of the resignation, death or disability of an ordinary member of the Executive Committee, the Executive Committee may co-opt a new member to serve until the close of the next ordinary General Assembly.

The accession of an Officer of the Union to a new office under the conditions of this By-Law shall be accompanied by his resignation from the office to which he was previously elected, but service under this By-Law shall not affect his eligibility for immediate re-election to the new office.

2.4. Any Officer unable to attend a meeting of the Executive Committee may designate a deputy to attend that meeting. Such a deputy shall be named in writing to the President or the General Secretary. He shall have no voting power and shall not be counted as part of a quorum.

2.5. The President, on his own initiative or at the request of the Executive Committee, may invite any individual to be present at a meeting of the Executive Committee; such an invited guest may take part in the discussions but shall have no voting power.

2.6. At a meeting of the Executive Committee two-thirds (fractional parts neglected) of the Officers specified by Statutes 6.1 and 6.3, excluding any who have resigned or died, shall constitute a quorum; and decisions shall be taken by a simple majority of the Officers present and voting. The Chairman of the meeting shall not vote in open ballots; but in the event of an equal division of votes the Chairman may take the final decision. In secret ballots required by the Statutes or By-Laws or ordered by the Chairman he may vote at his discretion. If he does not vote and there is an equal division of votes he may take the final decision. If he has voted in a secret ballot he may not take the final decision, and must leave it to further discussion and ballot.

2.7. During the period between meetings of the Executive Committee, voting may take place by post. Adoption of a proposal shall require affirmative votes from two-thirds (fractional parts neglected) of the Officers specified by Statutes 6.1 and 6.3, excluding any who have resigned or died. No decision on any proposal other than calling or cancelling a meeting of the Executive Committee shall be made by postal vote in the event that at least two Officers express the wish that the matter concerned should first be given more or further consideration, either by correspondence or at a meeting of the Executive Committee.

2.8. Minutes of the meetings of the Executive Committee shall be made. Two copies of the minutes shall be signed by the Chairman and the Secretary of the meeting at which they are approved, and shall be kept by the President and the General Secretary. A summary of the draft minutes of meetings of the Executive Committee shall be despatched by the General Secretary to the National Committees within ten weeks of the conclusion of each meeting.

2.9. In addition to the obligations described in the Statutes and elsewhere in these By-Laws, the Executive Committee shall

- (a) receive and report on applications for adherence to the Union if the nature of the applying Body and the membership of the National Committee have been duly reported to and considered to be in good order by the Executive Committee; pending the next General

Assembly the Executive Committee may in the case of such applications provide such services of the Union as it deems proper;

- (b) consider and report on any other questions concerning adherence to the Union;
- (c) present an annual report, including an audited statement of receipts and expenditure, to the National Committees;
- (d) report to the Commercial Registry of Geneva any changes in the registered information concerning the Union;
- (e) have the power to appoint representatives on scientific bodies not belonging to the Union.

### 3. President

3.1. The President of the Union is Chairman of the General Assembly and of the Executive Committee. In the absence of the President from a session or meeting, the Vice-President, or if he is not present another Officer of the Union designated by the Executive Committee, shall act as Chairman.

3.2. The President of the Union is an *ex officio* member, with voting power, of all Commissions of the Union.

### 4. General Secretary

4.1. The General Secretary of the Union is Secretary of the General Assembly and of the Executive Committee. In his absence from a session or meeting, another Officer of the Union designated by the Executive Committee shall act as Secretary.

4.2. The General Secretary of the Union is an *ex officio* member, with voting power, of all Commissions of the Union.

4.3. The General Secretary is responsible for conducting the ordinary business of the Union, with the exception of the financial administration, and for keeping its records.

### 5. Treasurer

5.1. The Treasurer of the Union is responsible for the financial administration of the Union and for keeping its accounts.

5.2. The Treasurer is an *ex officio* member of all Commissions of the Union, with voting power only for those questions which may involve the Union in financial commitments.

### 6. Commissions of the Union

6.1. The Chairmen of the Commissions and the chief representatives on Joint Commissions or other bodies shall forward records of all meetings of the Commissions to the President and the General Secretary. They shall report annually on the activities of these bodies to the Executive Committee.

6.2. If funds are provided for the use of a Commission, it may make its own financial arrangements, with the prior approval of the Executive Committee and subject to the provisions of the Statutes and By-Laws. In cases where the Executive Committee has given prior approval, payments toward travelling expenses of Chairmen and members of

Commissions may be made from the general funds of the Union.

6.3. No person who has served for three consecutive full terms of office on a Commission is eligible for nomination for a fourth consecutive term of service on the same Commission except as Chairman. In no case is any person eligible for more than four consecutive full terms of service on the same Commission. These limitations do not apply to Editors [Statute 7-1], Co-editors [Statute 7-2] and *ex officio* members. Any Commission, in its Rules of Procedure, may reduce the length of service specified here.

6.4. In the event of the resignation, death or disability of the Chairman of any Commission, the Executive Committee shall appoint a member of that Commission to serve as Chairman until the close of the General Assembly following this appointment.

### 7. Nominations and Elections

7.1. All delegates (and alternates) shall be notified of the nominations presented by the Executive Committee under By-Law 2-2 for the Officers of the Union as early as possible and at least ninety-six hours before the scheduled commencement of the session of the General Assembly at which the vote is to be taken.

7.2. After the delegates have been notified of the nominations by the Executive Committee as prescribed in By-Law 7-1, other nominations for Officers of the Union may be made by any six or more delegates. Such nominations shall be made in writing to the General Secretary not less than thirty-six hours before the voting session and shall be accompanied by a written statement that the consent of the nominees has been obtained. These nominations shall be posted by the General Secretary on the official bulletin board not less than twenty-four hours before that session.

7.3. Recommendations from each Commission for the Chairman and members of the Commission shall be made in writing to the General Secretary not less than seventy-two hours before the voting session of the General Assembly. These recommendations shall be approved by a majority of the members of the Commission and shall be accompanied by a written statement that the consent of the persons recommended has been obtained. All delegates (and alternates) shall be notified of the nominations presented by the Executive Committee under By-Law 2-2 for the Chairman and members of each Commission at least forty-eight hours before the voting session.

7.4. After the delegates have been notified of the nominations by the Executive Committee as prescribed in By-Law 7-3, other nominations for the Chairman and members of each Commission may be made by any six or more delegates. Such nominations shall be made in writing to the General Secretary not less than twenty-four hours before the voting session and shall be accompanied by a written statement that the consent of the nominees has been obtained. These nominations shall be posted by the General Secretary on the official bulletin board not less than twelve hours before that session.

7.5. In voting for the President, Vice-President, General Secretary and Treasurer of the Union, each of these offices shall be taken separately and voting shall be by secret ballot. A simple majority of the votes represented by the delegates present at the voting session shall be required for election.

If there is only one candidate for one of these offices, his nomination shall be presented to the General Assembly and the candidate concerned shall be considered as elected. If there are two candidates or more, and an election is not achieved after two ballots, the candidate receiving the smallest number of votes in the second ballot shall be removed from the list. If an election is not achieved after a third ballot, this procedure shall be repeated until an election is achieved. Any ballot form showing more than one mark shall be invalid. Any contingency arising during the balloting shall be resolved by a ruling of the Chairman of the General Assembly.

7.6. The election of the ordinary members of the Executive Committee shall be by secret ballot, the ballot form showing the nominations presented by the Executive Committee and the nominations made by delegates. A simple majority of the votes represented by delegates present at the voting session shall be required for election. If there are not more candidates than vacancies, the nominations shall be presented to the General Assembly and the candidates shall be considered as elected. If there are more candidates than vacancies and all vacancies are not filled by election at the first ballot, a second ballot shall be arranged containing the names of the candidates not elected. If there are vacancies after the second ballot, the balloting procedure shall be repeated until all vacancies are filled; for each of these subsequent ballots the name of the candidate receiving the smallest number of votes on the preceding ballot shall be removed from the list. Any ballot form showing more marks than the appropriate number of vacancies shall be invalid. Any contingency arising during the balloting shall be resolved by a ruling of the Chairman of the General Assembly.

7.7. In the event that an election must be held to fill the unexpired term of an office vacated by an ordinary member [Statute 6-4], the nominations for this office shall be distinct from the nominations for ordinary members for full terms. A person may be nominated for both categories, but can be elected to only one office [Statute 6-3]. If ballots are required in the elections for both categories, the ballots for the full-term offices shall take place first. A person who has been elected to two consecutive non-full terms is not eligible, on completion of his second term, for immediate re-election as an ordinary member of the Executive Committee.

7.8. In voting for the Chairmen and members of the Commissions each Commission shall be considered separately. For the election of the Chairmen the procedure described in By-Law 7-5 shall be followed. For the election of the members of the Commissions the procedure described in By-Law 7-6 shall be followed except that no more than two ballots shall be held. Any vacancies still remaining may be filled as provided in Statute 8-2.

7.9. The procedure for the nomination and election of representatives of the Union on Joint Commissions and on other scientific bodies is so far as is possible the same as that for the nomination and election of the Chairmen and members of the Commissions.

### 8. By-Laws

8.1. These By-Laws may be amended or suspended at any General Assembly and at least two-thirds of the votes

there represented are required for an amendment or suspension. A motion to amend or suspend, if not already included in the agenda of business of the General Assembly, may be placed there by the procedure of Statute 5·9. No notice is required for a proposal to suspend the time limits prescribed by By-Laws 7·2 and 7·4. Notification of any other motion to amend or suspend the By-Laws must be given by its originators to all delegates (and alternates) and to all Officers of the Union in accordance with the procedure prescribed in By-Law 1·12, at least forty-eight hours before

the session of the General Assembly at which the motion is to be considered.

8·2. Words importing the male sex in the Statutes and By-Laws shall include the female sex.

8·3. The present English text shall be considered the authoritative text in the interpretation of these By-Laws. Where disputes arise concerning this interpretation, the matter shall be decided by the General Assembly, or during the periods between General Assemblies, by a ruling of the President of the Union.

## APPENDIX

### *Timetable in Preparation for General Assembly*

		Statute	By-Law
12 months	Notice of date and place of ordinary General Assembly to National Committees and Commissions	5·3	—
8 months	Notice of date and place of extraordinary General Assembly to National Committees and Commissions, if amendment of Statutes is contemplated	5·4	—
6 months	Proposals for amendments to Statutes to General Secretary	13·1	—
5 months	Estimated budgets from Commissions to Executive Committee	9·2	—
4 months	Proposals for agenda of General Assembly to General Secretary	—	1·2
4 months	Notice of date and place of extraordinary General Assembly to National Committees and Commissions, if amendment of Statutes is not contemplated	5·4	—
4 months	Proposals for amendments to Statutes to National Committees and Commissions	13·1	—
14 weeks	Reports of Commissions to General Secretary	8·4	—
10 weeks	Report of Executive Committee to National Committees and Commissions	6·8	—
10 weeks	Reports of Commissions to National Committees and Commissions	8·4	—
10 weeks	Budget to National Committees and Commissions	9·3	—
10 weeks	Agenda to National Committees and Commissions	—	1·1

### *Timetable during General Assembly*

'Before'	Notice by National Committees to General Secretary of names of delegates, alternates and chairmen of delegations, and of distribution of votes if not one per delegate	5·6, 5·7	—
96 hours	Nominations by Executive Committee for Officers of Union	—	7·1
72 hours	Recommendations by Commissions to General Secretary for Chairmen and members of Commissions	—	7·3
48 hours	Nominations by Executive Committee for Chairmen and members of Commissions	—	7·3
48 hours	Notification of motion to amend or suspend By-Laws	—	8·1
36 hours	Notice to General Secretary of nominations by delegates for Officers of Union	—	7·2
24 hours	Posting of nominations by delegates for Officers of Union	—	7·2
24 hours	Notice to General Secretary of nominations by delegates for Chairmen and members of Commissions	—	7·4
12 hours	Posting of nominations by delegates for Chairmen and members of Commissions	—	7·4

## ANNEX III

## Committees, Commissions and Representatives on Regional and Scientific Associates and Bodies not belonging to the Union

### Membership of Bodies belonging to the Union

## EXECUTIVE COMMITTEE

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*Immediate Past President*

Th. Hahn\* (Federal Republic  
of Germany)

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P. Coppens† (USA)  
R. Diamond† (UK)  
A. Kálmán\* (Hungary)  
E. N. Maslen\* (Australia)  
S. A. Semiletov† (USSR)

*Executive Secretary*

J. N. King  
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\* Until the close of the  
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† Until the close of the  
Sixteenth General Assembly  
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## ANNEX IV

### Adhering Bodies

<i>Country</i>	<i>Category*</i>	<i>Adhering Body</i>	<i>Secretary of National Committee</i>
Argentina	I	Consejo Nacional de Investigaciones Científicas y Técnicas	M. A. R. DE BENYACAR, División Física del Sólido, 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, GPO Box 783, Canberra City, ACT 2601
Austria	I	Österreichische Akademie der Wissenschaften	A. PREISINGER, Institut für Mineralogie, Kristallographie und Strukturchemie, Technische Universität Wien, Getriedemarkt 9/171, A-1060 Vienna
Belgium	II	Académie Royale des Sciences, des Lettres et des Beaux-Arts de Belgique	E. LEGRAND, Materials Sciences Department, Studiecentrum voor Kernenergie, B-2400 Mol
Brazil	III	Conselho Nacional de Desenvolvimento Científico e Tecnológico	S. CATICHA ELLIS, DESCM, Instituto de Física, Universidade Estadual de Campinas, Campinas, São Paulo 13100
Bulgaria	I	Bulgarian Academy of Sciences	J. MACIČEK, Bulgarian Academy of Sciences, Institute of Applied Mineralogy, Rakovskyst. 92, 1000 Sofia
Canada	III	National Research Council	J. T. SZYMAŃSKI, CANMET, Department of Energy, Mines and Resources, 555 Booth St, Ottawa, Ontario K1A 0G1
Chile	I	Comisión Nacional de Investigación Científica y Tecnología	D. BOYS, Departamento de Física, 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. PETŘIČEK, Institute of Physics, 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. VAHVASELKÄ, Department of Physics, University of Helsinki, Siltavuorenpenger 20 D, SF-00170 Helsinki 17
France	IV	Académie des Sciences (Institut de France)	Y. EPELBOIN, Association Française de Cristallographie, Tour 26, 4 place Jussieu, 75230 Paris CEDEX 05
German Democratic Republic	I	Vereinigung für Kristallographie in der GGW der DDR	P. RUDOLPH, Sektion Physik, Humboldt-Universität-Berlin, 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	K. SIMON, Physical Chemistry Department, Chinoin Pharmaceutical and Chemical Works, POB 110, H-1325 Budapest
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, CS Relaz. Strutt. Reatt. Chim., CNR, 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 Tecnología	L. E. RENDÓN DÍAZMIRÓN, Instituto de Investigaciones en Materiales, UNAM, Delegación Coyoacán, 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

\* 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.

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Norway	I	Det Norske Videnskaps-Akademi	B. F. PEDERSEN, Institute of Pharmacy, University of Oslo, PO Box 1033, Blindern, 0315 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 Física	M. M. R. R. COSTA, Departamento de Física, Universidade de Coimbra, 3000 Coimbra
South Africa	II	South African 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, Department of Structural Chemistry, 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	N. I. SOROKINA, 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, 41 000 Zagreb

\* See footnote on preceding page.

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