

**International Union of Crystallography**  
**Sixteenth General Assembly and International Congress of Crystallography**  
**Beijing, China, 21–29 August 1993**

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### Introduction and Opening Ceremony

By invitation of China's National Committee for Crystallography and the Chinese Association for Science and Technology (CAST), the Sixteenth General Assembly and International Congress of Crystallography were held at the Beijing International Convention Center, China, 21–29 August 1993.

The meetings were attended by 1167 scientists and 218 accompanying members from 53 countries.

The General Assembly and Congress were opened on the afternoon of 21 August at the Beijing International Convention Center. Professor X.-J. XU, Chairman of the Organizing Committee, chaired the ceremony. The welcoming addresses and the opening address by Professor A. AUTHIER, President of the IUCr, were followed by a general lecture on *Crystallography and the Crystallographic Community in China* by Professor Y. TANG. The Ewald Prize was presented to Professor N. KATO. There then followed a show of Chinese folk music and dances performed by the Central Song and Dance Ensemble of the Nationalities of China. The evening ended with a welcoming reception.

### Sixteenth International Congress

#### Scientific programme

18 Main Lectures and 48 Microsymposia and Open Commission Meetings were held during the morning and late afternoon sessions. The early afternoons were reserved for poster sessions, with discussion sessions in the late afternoons to discuss the results presented in the posters and to extend the discussions on the Microsymposia. The 1259 abstracts in the published book of Collected Abstracts were prepared largely from camera-ready copy and these abstracts also appeared as a Supplement to *Acta Crystallographica*, Volume A49, dated 1 September 1993.

#### Exhibitions

A commercial exhibition was organized jointly with the 34th IUPAC Congress (15–20 August 1993). The total exhibition comprised 15 industrial companies, four book exhibitions and two databank and software demonstrations.

#### Social events

In addition to the opening reception, there was a banquet and a visit to the Great Wall of China. Optional tours in Beijing and post-Congress tours were also organized.

### Minutes of the Sixteenth International Congress

These Minutes have been prepared by M. H. Dacombe, Executive Secretary, under the authority of A. I. Hordvik, 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 Sunday 22 August, Monday 23 August and Thursday 26 August. It was not found necessary to meet on Saturday 28 August, as originally planned. The following attendance list

gives the names of official delegates appointed by the Adhering Bodies and of the alternates who substituted at one or more sessions. Dates of attendance are given in parentheses for those who were not present at every session. 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 where they are known; those of alternates are marked by an asterisk. There were no delegates from Argentina, Bulgaria, Mexico, Portugal or Ukraine.

*Australia* (3): D. C. Creagh, I. E. Grey\* (26 August), H. C. Freeman, **J. W. White** (23 August)  
*Austria* (1): A. Preisinger  
*Belgium* (2): **G. H. Evrard**, G. S. D. King  
*Brazil* (3): L. Q. D. Amaral, Y. P. Mascarenhas, **I. C. Torriani**  
*Canada* (3): I. C. Bassignana, **M. N. G. James**, Y. Le Page  
*Chile* (1): J. L. Garin  
*China* (4): **J.-I. Huang**, K.-z. Pan, D.-c. Xie (26 August), X.-j. Xu  
*Croatia* (1): B. Kamenar  
*Czech/Slovak Republics* (1): K. Huml  
*Denmark* (1): N. Thorup  
*Egypt* (1): M. S. Ahmed  
*Finland* (1): T. Paakkari  
*France* (4): B. Capelle, Y. Epelboin, **R. Fourme**, G. Precigoux  
*Germany* (4): **J. Felsche**, H. R. Hoeche\*, H. Küppers (22 and 26 August), P. Paufler  
*Hungary* (1): K. Simon  
*India* (2): **K. K. Kannan**, K. Lal  
*Israel* (1): F. H. Herbstein (22 and 23 August), M. Kaftory\* (26 August)  
*Italy* (3): G. Ferraris, G. Filippini, **G. Gilli**  
*Japan* (4): O. Nittono, Y. Ohashi, **M. Tanaka**, M. Tokonami (22 August), T. Yamanaka\* (23 and 26 August)  
*The Netherlands* (2): P. T. Beurskens (22 and 26 August), **D. Feil**, G. A. Wieggers\* (23 August)  
*New Zealand* (1): W. T. Robinson  
*Norway* (1): B. Fjaertoft  
*Poland* (1): K. Łukaszewicz  
*Russia* (4): L. A. Aslanov, D. M. Kheiker, W. R. Melik-Adamyan\* (23 August), V. I. Simonov (22 and 26 August), **B. K. Vainshtein**  
*Serbia* (1): S. Stanković  
*Slovenia* (1): I. Leban  
*South Africa* (2): **J. C. A. Boeyens**, G. J. Kruger  
*Spain* (3): **S. García-Granda**, F. Lahoz (22 and 26 August), A. López-Castro  
*Sweden* (2): J. Albertsson, **I. Olovsson**  
*Switzerland* (2): **G. C. Chapuis**, H. D. Flack  
*UK* (5): A. C. Bloomer, J. B. Forsyth, **J. A. K. Howard**, A. J. Smith, D. J. Watkin (23 and 26 August)  
*USA* (5): **R. F. Bryan**, W. L. Duax, J. Flippen-Anderson, K. Watenpaugh, B. Wuensch  
*Venezuela* (1): M. V. Capparelli (22 and 23 August), D. Gomez de Andere\* (26 August)

*Present as members of the Executive Committee:* A. Authier (President), A. Kálmán (Vice-President), A. I. Hordvik (General Secretary and Treasurer), M. Nardelli (Immediate Past President), R. Chidambaram, P. W. Coddington, P. Coppens, R. Diamond, J. Harada and Yu. T. Struchkov (Ordinary Members). M. H. Dacombe was in attendance as Executive Secretary.

**First Session, Sunday 22 August 1993, 8.05 p.m.****(1) Introductory remarks by the President**

Professor AUTHIER welcomed the delegates and observers. The President began by recalling the names of crystallographers who had died during the last triennium. To this list was added the name of Jim King, who had been the Executive Secretary of the IUCr since 1969. The President said what a great pleasure it had been to work with Jim and that his untimely death was a great loss to the IUCr. He asked Professor Cruickshank, who had recruited Jim, to say a few words. D. W. J. CRUICKSHANK then gave a very moving account of Jim's personal qualities which made him so suited to his work, and emphasized his dedication to the IUCr and his enormous contribution to the whole crystallographic community. The General Assembly expressed its appreciation for all that Jim had done.

The President then reported that M. H. Dacombe had been appointed as the new Executive Secretary.

**(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. D. Flack (Switzerland) and K. Łukaszewicz (Poland), were appointed to act as tellers when votes had to be counted during the Assembly.

**(3) Approval of agenda**

The Agenda and the Appendices to the Agenda had been distributed to Secretaries of National Committees in June 1993. The Agenda were approved.

**(4) Applications for membership of the Union**

Applications for membership of the IUCr had been received from Croatia (Category I), the Regional Committee of Czech and Slovak Crystallographers (Category I), Germany (Category IV), Russia (Category IV), Slovenia (Category I), Ukraine (Category I), Venezuela (Category I) and Serbia (Category I) and the Executive Committee recommended to the General Assembly that these be accepted. All applications were accepted by the General Assembly and the delegates from these countries took their seats.

The President reported that Armenia, Latvia, Moldavia and Uzbekistan had applied for membership but were not yet in a position to pay the annual subscription. They had been informed that they would be able to take part in discussions of the General Assembly, without voting power.

**(5) Changes in names of Adhering Bodies**

The changes in names of the Adhering Bodies of South Africa [to the Foundation for Research Development (FRD)] and Spain [to the Comisión Interministerial de Ciencia y Tecnología (CICYT)] were accepted by the General Assembly.

**(6) Approval of Minutes of Fifteenth General Assembly**

The Minutes, which were contained in the published Report of the Fifteenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (1992), A48, 353–405], 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.

**(7) Report of Executive Committee**

The Report of the Executive Committee on the activities of the IUCr since the Fifteenth General Assembly had been submitted to the National Committees and the Commissions in June 1993, in accordance with Statute 6·8 and, with subsequent corrections, follows these Minutes as Annex I, Appendix A. The report was accepted with minor modification.

**(8) Financial Report**

A Financial Report, covering the calendar years 1990, 1991 and 1992, had been prepared by the Treasurer and had been submitted to the National Committees and the Commissions in June 1993. The Report, with subsequent corrections, follows these Minutes as Annex I, Appendix B.

The Treasurer reported that the financial state of the IUCr was healthy. He explained the structure and uses of the various Funds, grouping these into 'money earning' Funds (for example, *Acta Crystallographica*, *Journal of Applied Crystallography*, *International Tables*, *Structure Reports*), a 'sleeper' Fund (the General Fund) and 'expense' Funds (Publications and Journals Development Fund, Research and Education Fund, Ewald Fund, President's Fund). The intention was that the 'expense' Funds should be built up to be self-supporting and transfers to and grants from these Funds during the triennium were detailed. He showed a graph illustrating the growth in total balance (excluding fluctuations in exchange rates) during the triennium until June 1993.

The General Assembly accepted the Financial Report with acclamation.

**(9) Ewald Prize**

The General Assembly applauded Professor N. Kato, to whom the third Ewald Prize had been presented at the Opening Ceremony. Details of the Prize and the citation are given in Annex I, Appendix C.

The President reported that there had been a suggestion to introduce a 'junior prize'. This suggestion had been studied by the Finance Committee and the Executive Committee who felt that this would devalue the main prize and the proposal was not approved.

**(10) Commission on Journals. Report by Chairmen and review of activities**

The report of the Commission on Journals had been distributed to the National Committees and the Commissions in June 1993 and is reprinted in Annex I, Appendix D. The Chairman of the Commission, C. E. BUGG, summarized the report and also announced that a new journal, the *Journal of Synchrotron Radiation*, would be launched in 1995. A preliminary flyer announcing this major new initiative was then distributed.

The report was accepted by the General Assembly.

Note: Item (10) actually took place in the Second Session.

**(11) Commission on Structure Reports. Report by Chairman and review of activities**

The report of the Commission on *Structure Reports* had been distributed to the National Committees and the Commissions in June 1993 and is reprinted in Annex I, Appendix D. The

Chairman of the Commission, G. FERGUSON, confirmed that the final volumes were with the printer and that the work of the Commission was therefore complete. D. W. J. CRUICKSHANK noted that the Commission had been in existence since the founding of the IUCr.

The General Assembly accepted the report and thanked with acclamation the dedicated work of Professor Ferguson and all the editors of this series.

(12) *Commission on International Tables. Report by Chairman and review of activities*

The President reported that the Chairman of the Commission, A. J. C. Wilson, had decided that he wished to retire as Chairman and was not present in Beijing. The President further noted that there was probably no period since the creation of the IUCr when Professor Wilson had not been involved with some aspect of the IUCr's activities. The General Assembly warmly thanked Professor Wilson for his significant contribution to the IUCr.

The President announced that Th. Hahn had been appointed as the new Chairman of the Commission.

The report of the Commission on *International Tables* had been distributed to the National Committees and the Commissions in June 1993 and is reprinted in Annex I, Appendix D.

TH. HAHN summarized the report and mentioned some future plans. Discussions were under way concerning the possibility of putting the three-dimensional space-group diagrams into computer graphics to give a three-dimensional representation. This study might extend to cover colour groups and even four-dimensional groups.

The report was accepted by the General Assembly.

(13) *Report of Director of Archiving and Crystallographic Information*

The President reported that the Director of Archiving and Crystallographic Information, E. N. Maslen, had found that the work involved was too much for one person. The Executive Committee had therefore decided to provide help and replace the Director by an advisory Committee on Electronic Publishing, Dissemination and Storage of Information with Dr Maslen as the Chairman. This Committee would be a Sub-committee of the Executive Committee.

The report of the Director of Archiving and Crystallographic Information had been distributed to the National Committees and the Commissions in June 1993 and is reprinted in Annex I, Appendix E. E. N. MASLEN had nothing to add to the report, which was accepted by the General Assembly.

(14) *Non-publishing Commissions. Reports by Chairmen and review of activities*

The reports of the Commissions on their activities since the Fifteenth General Assembly had been distributed to the National Committees and the Commissions in June 1993. The reports are reprinted in Annex I, Appendix D. 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. W. SCHÜLKE (Commission on Charge, Spin and Momentum Densities) noted that although his Commission had applied for five Microsymposia at this Congress they had received only one. D. C. CREAGH (Commission on Crystallographic Apparatus) reported that in future the Commission would be concentrating more on the apparatus side and would try to link in with the work of the Commission on Powder Diffraction. F. H. ALLEN (Commission on Crystallographic

Data) reported that a technical sub-committee (COMCIFS) had been established to supervise the maintenance of standards in CIFs. This sub-committee would report to the Executive Committee. He added that contact with the crystallographic databases (which now contained some 200 000 structures) was continuing.

W. T. ROBINSON encouraged others to participate in the IUCr Visiting Professorship Programme (coordinated by the Commission on Crystallographic Teaching) as he had found this very rewarding. J. M. COWLEY (Commission on Electron Diffraction) reported that the Summer School on Electron Crystallography held the previous week in Beijing had been very successful. S. A. MASON (Commission on Neutron Diffraction) similarly reported that the Satellite Meeting on Neutron Scattering held at Beidaihe, 17–19 August, had been successful. R. A. YOUNG (Commission on Powder Diffraction) also expressed support for the Visiting Professorship Programme, which had been of great benefit for his Commission. J. R. HELLIWELL (Commission on Synchrotron Radiation) noted that his Commission had had a major input in connection with the launch of the *Journal of Synchrotron Radiation* and that S. S. Hasnain had been particularly active in canvassing the major synchrotron facilities throughout the world. He added that the European Synchrotron Radiation Source in Grenoble had now passed its commissioning.

The President summarized the background to the establishment of the *ad interim* Commission on Aperiodic Crystals. J. M. PÉREZ-MATO then summarized his report.

The General Assembly accepted all the reports that had been received on the activities of the non-publishing Commissions.

(15) *Possible confirmation of Commission on Aperiodic Crystals, established ad interim in 1991*

The President reported that the *ad interim* Commission had been very active and that the Executive Committee was very satisfied with its work. The Commission was established. J. M. PÉREZ-MATO then explained that because of the level of work involved he would like the number of members of this Commission to be increased by three.

(16) *Determination of 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 Seventeenth General Assembly; these numbers did not include Chairmen, Co-editors or *ex officio* members.

The Executive Committee now proposed that the membership of (1) the Commission on Aperiodic Crystals be increased from four to seven members, and (2) the Commission on Crystallographic Computing be increased from seven to eight members.

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>International Tables</i>	0
3. Commission on Aperiodic Crystals	7
4. Commission on Biological Macromolecules	8
5. Commission on Charge, Spin and Momentum Densities	9
6. Commission on Crystal Growth and Characterization of Materials	8
7. Commission on Crystallographic Apparatus	7
8. Commission on Crystallographic Computing	8

9. Commission on Crystallographic Data	9
10. Commission on Crystallographic Nomenclature	9
11. Commission on Crystallographic Teaching	0
12. Commission on Electron Diffraction	7
13. Commission on Neutron Scattering	9
14. Commission on Powder Diffraction	9
15. Commission on Small Molecules	9
16. Commission on Synchrotron Radiation	8

(17) *Proposal to change name of Commission on Neutron Diffraction*

The Chairman of the Commission on Neutron Diffraction explained that the Commission felt that its title should be changed to the slightly more general Commission on Neutron Scattering because it wished to represent and serve all neutron scatterers who consider that they use crystallographic techniques. The General Assembly approved the change.

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

In accordance with Statute 8.5 the reports of the Representatives on Regional and Scientific Associates had been circulated with the Agenda papers in June 1993. These reports are reprinted as Annex I, Appendix F. The reports were accepted by the General Assembly. In particular, it was noted that the Inaugural Conference of the Asian Crystallographic Association, AsCA '92, had been an important milestone which had provided a sound foundation for AsCA.

The President then adjourned the session at 10.15 p.m.

**Second Session, Monday 23 August 1993, 8.00 p.m.**

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

The President reported that as the Condensed Matter Division of the European Physical Society (EPS CMD) was a regional, European, body the Executive Committee had decided that it would be more appropriate to stop the IUCr's one-way representation and for the IUCr's European Regional Associate (the European Crystallographic Committee) to have representation on EPS CMD.

In accordance with Statute 8.5 the reports of the Representatives had been circulated with the Agenda papers. These reports are reprinted as Annex I, Appendix G. The reports were accepted by the General Assembly.

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

Since this is a sub-committee of the Executive Committee, the Assembly is not formally required to approve its report, which is reprinted as Annex I, Appendix H.

The Chairman of the Sub-committee explained the procedure for applying for sponsorship and noted that this support was of two types. The first was support for young scientists from the Research and Education Fund and the second was support for the organizers from the General Fund. The young scientists' support was in the form of travel grants and the awardees received a letter informing them that the support was from the IUCr. The Chairman also noted that Commissions were encouraged to apply for support of meetings which they organized.

The number of applications was increasing as other organizations were reducing their support but the IUCr was able to satisfy this increase in demand.

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

The report on this Book Series was accepted by the Assembly without comment. It is reprinted as Annex I, Appendix I.

(22) *Determination of general policy and timetable for period to Seventeenth General Assembly*

It was noted that several meetings to be held in this period had already requested IUCr sponsorship and financial support. The delegates made no further observations or comments.

(23) *Preliminary consideration of activities for period 1996-1999*

There were no comments on this item.

(24) *Budget estimates for period to Seventeenth General Assembly: determination of unit contribution*

These budget estimates had been distributed with the Agenda papers and are reprinted as Annex I, Appendix J.

R. DIAMOND, the Convener of the Finance Committee, presented a diagram summarizing the income and expenditure of the IUCr. He pointed out that the income from the subscriptions of members was disproportionately small compared with the other sources of income. The tax status of the IUCr in some countries was based on the IUCr being substantially supported by members' contributions and this was the only source of income over which direct control was with the IUCr. The contribution should be made more realistic and appropriate to the scale of the IUCr's operations.

The General Assembly accepted the budget estimates and approved by a large majority (only three delegates from Canada voted against and there were no abstentions) the recommendation that the unit contribution, which had remained at SwFr 890 since 1981, be increased to SwFr 1000 for the years 1994, 1995 and 1996.

The President took the opportunity to explain that the Finance Committee had been established in 1981 as a result of the poor state of the IUCr's finances at that time. He noted that the Finance Committee consisted of the President, the General Secretary and Treasurer, two members from the country in which the IUCr had its office (*i.e.* the UK) and the Chairman of the Commission on Journals. If possible, one of the two UK members should be a member of the Executive Committee. There had been two Conveners – the first was M. M. Woolfson and the second was R. Diamond, who was now finishing his term after nine years. The Convener was a member of the Executive Committee as this was the only way that a suitable liaison could be established. The President asked Dr Diamond to sum up the role played by the Finance Committee since 1981.

R. DIAMOND reported that in 1981 the financial state of the IUCr was in a perilous situation and the first Finance Committee had taken three important steps: (1) the prices for the IUCr's publications were changed to the currency of production, (2) the printing was tendered, and (3) large price rises were imposed on the publications. These three actions turned *Acta Crystallographica* into a large profit-maker and meant that there was then no need to increase the price of *Acta Crystallographica* again until 1990. This period provided the main source of the IUCr's wealth and made possible all the good work of the IUCr. The members of this first Finance Committee were J. Karle,

K. V. J. Kurki-Suonio, D. W. J. Cruickshank, M. M. Woolfson and S. C. Abrahams. Together with the late J. N. King they deserved the warm thanks of the IUCr.

Dr Diamond went on to explain why it was important for the Convener to be someone who lived in the UK (the country where the IUCr had its office). The IUCr had a major responsibility as an employer and the Convener needed to be actively involved with taxation, pension schemes and permanent disability schemes. All of these aspects were complex and the Convener needed ready access to the Chester office and familiarity with UK rules and regulations. These special responsibilities made a UK Convener essential.

Dr Diamond was thanked with acclamation for his tremendous work over the past nine years.

*(25) Confirmation of date and place of Seventeenth General Assembly*

The President read out a letter which he had received from the Foreign Secretary of the US National Academy of Sciences. This letter confirmed the invitation from the US National Committee for Crystallography, on behalf of the US National Academy of Sciences and in collaboration with the American Crystallographic Association, to hold this General Assembly and Congress in Seattle in 1996. The meeting would be hosted in accordance with ICSU policies, in particular with regard to free circulation of scientists. The President reported that the Executive Committee had met the Organizing Committee Chairman and the Programme Committee Chairman and found their reports very satisfactory and proposed acceptance of the invitation.

The invitation, which had been preliminarily accepted in 1990, was formally accepted.

*(26) Preliminary consideration of date and place of Eighteenth 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 Eighteenth General Assembly to be held in 1999. The President announced that invitations had been received from the Israel Crystallographic Society to hold the Congress in Jerusalem, Israel, and from The Royal Society to hold the Congress in Glasgow, UK. He reported that the Executive Committee had considered both applications and found them to be in order.

F. H. HERBSTEIN (Israel) presented the formal invitation for Israel and C. J. GILMORE (UK) and J. A. K. HOWARD (UK) presented the formal invitation for the UK.

A decision on which invitation to accept was delayed until the next session to give the delegates time to consider the choice.

The President adjourned the session at 10.15 p.m.

**Third Session, Thursday 26 August 1993, 8.05 p.m.**

*(26) Preliminary consideration of date and place of Eighteenth General Assembly (continued)*

The General Assembly gave preliminary acceptance to the invitation to hold the Eighteenth General Assembly in 1999 in the UK.

*(27) Confirmation of appointments of Editors of publications of the Union*

In accordance with Statute 7-1, the initial appointments and the reappointments of the Editors of the publications of the Union were made by the Executive Committee and were subject to confirmation by the General Assembly.

In addition to the appointments and reappointments notified to the delegates in the Agenda papers, the Executive Committee had appointed the following Editors for the separate Sections of *Acta Cryst*: A. Authier for Section A, F. H. Allen for Section B, S. R. Hall for Section C and J. P. Glusker for Section D. It had appointed S. S. Hasnain, J. R. Helliwell and H. Kamitsubo as Editors of the *Journal of Synchrotron Radiation*. It had also reappointed the following Editors for *International Tables*: Th. Hahn for Volume A, U. Shmueli for Volume B, A. J. C. Wilson for Volume C, A. Authier for Volume D and V. Kopsky and D. B. Litvin for Volume E.

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

Editor-in-Chief of *Acta Crystallographica*: C. E. Bugg (USA)

Editor of Section A of *Acta Crystallographica*: A. Authier (France)

Editor of Section B of *Acta Crystallographica*: F. H. Allen (UK)

Editor of Section C of *Acta Crystallographica*: S. R. Hall (Australia)

Editor of Section D of *Acta Crystallographica*: J. P. Glusker (USA)

Editor of *Journal of Applied Crystallography*: A. M. Glazer (UK)

Editors of *Journal of Synchrotron Radiation*: S. S. Hasnain (UK), J. R. Helliwell (UK) and H. Kamitsubo (Japan)

General Editor of *International Tables* and Editor of Volume A: Th. Hahn (Germany)

Editor of Volume B: U. Shmueli (Israel)

Editor of Volume C: A. J. C. Wilson (UK)

Editor of Volume D: A. Authier (France)

Editors of Volume E: V. Kopsky (Fiji) and D. B. Litvin (USA)

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

The nominations made by the Executive Committee for the Chairmen and elected members of Commissions, after consultation with the Commissions through their Chairmen, had been notified to delegates. This list of nominations included *ex officio* members of the non-publishing Commissions, for information.

Since no other nominations had been made by the delegates, the persons nominated by the Executive Committee were considered elected.

The current full memberships of all the Commissions, including the *ex officio* members, together with the addresses of the Chairmen, are given in Annex III.

*(29) 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 were made, these persons were considered elected.

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

*(30) Election of Officers of the Union*

The nominations made by the Executive Committee for Officers of the Union had been included in the Agenda papers distributed in June 1993. P. Coppens was nominated for President, Yu. T. Struchkov for Vice-President and A. I. Hordvik for General Secretary and Treasurer. For the first time six nominations were made for the three vacancies for Ordinary Members for the normal six-year term: E. N. Baker (New Zealand), M. Hart (UK), K. Huml (Czech Republic), Y. Mascarenhas (Brazil), I. Olovsson (Sweden) and H. Schenk (The Netherlands). No other nominations were made by the delegates. Elections for the three Ordinary Members were held by secret ballot. The following nominees were elected:

**President:**

P. Coppens (USA)

**Vice-President:**

Yu. T. Struchkov (Russia)

**General Secretary and Treasurer:**

A. I. Hordvik (Norway)

**Ordinary Members (six years):**

E. N. Baker (New Zealand)

M. Hart (UK)

H. Schenk (The Netherlands)

The newly elected President congratulated the new members of the Executive Committee. He said that he had first attended an IUCr Congress in 1960 as a PhD student and that he now had many friends and colleagues in the IUCr and was much indebted

to it. He invited crystallographers with professional problems or with new ideas for projects or publications to come to him or to any member of the Executive Committee. He commented that the last triennium had been very productive and thanked the retiring members of the Executive Committee for all that they had done. In particular, he thanked the retiring President for his leadership which had resulted in the IUCr becoming more vibrant. There being no further business, and therefore no need for the final session of the General Assembly which had been scheduled for Saturday 28 August, the President declared the Sixteenth General Assembly closed at 9.25 p.m.

**Closing Ceremony, Sunday 29 August 1993**

X.-J. XU, Chairman of the Congress Organizing Committee, thanked the Executive Committee, the Programme Committee and the Congress staff for all their hard work.

A. AUTHIER, the retiring President, said that this had been a very successful well organized Congress with good scientific sessions. He thanked all his Chinese colleagues for making the Congress a very rewarding experience for everybody coming to China and seeing its new openness. He then introduced the newly elected President.

The new President, P. COPPENS, said that this Congress would be a yardstick against which future Congresses would be measured.

Prizes for the best posters were then awarded and the Sixteenth General Assembly and Congress officially closed.

## ANNEX I

## Appendices to the Agenda of the Sixteenth General Assembly

## Appendix A: Report of the Executive Committee

*Executive Committee and Finance Committee meetings*

The Executive Committee met in Bordeaux in July 1990 before and during the General Assembly, in Chester, England, in August 1991 and in Pittsburgh, USA, in July 1992 at the time of the ACA annual meeting. 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 dealt with by the Executive Committee during the triennium at these meetings, and in postal ballots between meetings, were:

- (1) Editorial policy, pricing policy and subscription rates, approval of appointments of Co-editors, Section Editors for *Acta Crystallographica*, and other matters concerning the IUCr journals.
- (2) Appointment of new staff in the IUCr office in Chester.
- (3) Upgrading of office technology in the IUCr office in Chester and expansion of this office.
- (4) Publication of a new Section (*Section D*) of *Acta Crystallographica* on Biological Crystallography.
- (5) Consideration of the possible publication of a new journal, the *Journal of Synchrotron Radiation*.
- (6) Future of *Structure Reports* and cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and the International Centre for Diffraction Data.
- (7) The implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* papers and other uses of CIF, patent application and adoption of the STAR file and CIF by other bodies.
- (8) Progress with Volumes B, C, D and E of *International Tables for Crystallography* and consideration of possible further volumes.
- (9) *Historical Atlas of Crystallography*.
- (10) Establishment of an international crystallographic newsletter, the *IUCr Newsletter*.
- (11) Approval of publications, jointly with the Oxford University Press, in the IUCr/OUP Book Series.
- (12) *World Directory of Crystallographers*.
- (13) Approval of the audited accounts.
- (14) The General Fund estimates and the level of the unit contribution.
- (15) Investment policy.
- (16) UK taxation considerations.
- (17) Funding and uses of the Publications and Journals Development Fund and the Research and Education Fund.
- (18) Consolidation of the Ewald Fund and appointment of the Selection Committee for the third Ewald Prize.
- (19) Sponsorship of meetings and possible financial support for meetings.
- (20) Young scientists' support to meetings.
- (21) Free circulation of scientists.
- (22) Approval of the membership of the Programme Committee for the Beijing Congress.
- (23) Discussion of the arrangements for the Beijing General Assembly and Congress.
- (24) Level of financial support for the Beijing Congress and its Satellite Meetings.
- (25) Review of the activities of the Commissions.
- (26) Establishment of an *ad interim* Commission on Aperiodic Crystals.
- (27) Review of IUCr representation on the Regional and Scientific Associates and on other bodies.
- (28) Nominations for Officers of the IUCr and for Chairmen and members of Commissions, and proposals from the National Committees for these positions.

*Publications*

The subscription prices (in Danish kroner) of *Acta Crystallographica* and the *Journal of Applied Crystallography* were increased each year during the triennium. The new *Section D* of *Acta Crystallographica* is supplied free of charge in 1993 to all subscribers to *Acta Crystallographica* (except those taking only *Section C*).

The total annual number of pages published in 1990, 1991 and 1992 were:

	1990	1991	1992
<i>Acta Cryst. Section A</i>	998	860	954
<i>Acta Cryst. Section B</i>	864	1030	856
<i>Acta Cryst. Section C</i>	2500	2740	2280
<i>J. Appl. Cryst.</i>	560	1102	812
Total	4922	5732	4902

In addition, in 1990 *Acta Cryst. Section A* included a Supplement of 540 pages of abstracts communicated to the Bordeaux Congress. The October 1991 issue of *J. Appl. Cryst.* included 68 papers (465 pages) contributed to the Eighth International Conference on Small-Angle Scattering, Leuven, Belgium, 6–9 August 1990. New procedures for the submission and publication of papers in *Section C* of *Acta Cryst.* were instituted in January 1992. This led to a temporary drop in submissions for this Section in 1992 but the level of submissions has since returned to its previous high level. More details are given in the Report of the Commission on Journals.

The Fast Communications section in *Acta Cryst. Section A* was extended to *Section B* (and *Section D* on its launch in 1993) and to *J. Appl. Cryst.* Lead Articles in *Acta Cryst.* and *J. Appl. Cryst.* are actively encouraged. Colour diagrams are printed free of charge in all IUCr journals.

Full details on the publication of volumes of *Structure Reports* and of *International Tables for Crystallography* are given in the Reports of these Commissions.

The Eighth Edition of the *World Directory of Crystallographers*, edited by E. N. Maslen, was published in 1990. Y. Epelboin has been appointed Editor of the Ninth Edition. The Ninth Edition will be held as an electronic database in STAR file format which will also allow the automated typesetting of the *Directory*. Details of the electronic data entry form appeared in *Acta Cryst.* (1993), A49, 222–225. Work is progressing well and it is planned to have a preliminary demonstration of the database in Beijing.

The establishment, jointly with Oxford University Press, of the IUCr/OUP Book Series has been very successful. Details are given in the relevant Appendix to the Agenda.

The *IUCr Newsletter* was launched in January 1993 and by the time of the Beijing meeting three issues will have appeared. W. L. Duax is the Editor and receives editorial help from the American Crystallographic Association. The American Institute of Physics handles the production and distribution.

#### *Sponsorship of meetings*

The Executive Committee has a Sub-committee on the Union Calendar to consider and to advise the Executive Committee on requests for IUCr sponsorship and financial support of meetings. The Chairman of the Sub-committee has been P. Coppens in this triennium. Because of its healthy financial status, the IUCr has been able to increase its support for young scientists attending meetings. A list of IUCr-sponsored meetings is given in the Report of the Calendar Sub-committee.

Applications for sponsorship and financial support are considered if they are submitted at least nine months in advance of the date of the meeting. Requests from Satellite Meetings must be submitted, and possible financial support requested, through the organizing committee of the main meeting. Meetings (other than Satellite Meetings) scheduled to be held within two months before or after an IUCr Congress will not be considered for sponsorship. For any meetings scheduled to be held between two and three months before or after a Congress, the application for sponsorship requires the approval of the Chairman of the Congress Programme Committee.

The IUCr continues to support and uphold ICSU's policy of non-discrimination and adheres to its decisions and procedures concerning free circulation of scientists. Organizers of any meetings seeking IUCr sponsorship or support must assure the Calendar Sub-committee that the authorities of the country in which the meeting is to take place guarantee free entrance of *bona fide* scientists from all countries.

#### *Commissions of the IUCr*

Each Commission Chairman is required to provide a written triennial report to the General Assembly. These reports are included as Appendices to the Agenda. Financial assistance has again been offered to the Commission Chairmen, to enable them to attend the General Assembly for the presentation and discussion of their reports and to meet the Executive Committee prior to the General Assembly.

In 1991 the Executive Committee approved the establishment of a Commission on Aperiodic Crystals, *ad interim* until the Beijing General Assembly. J. M. Pérez-Mato kindly accepted the Executive Committee's invitation to chair this Commission and to draft its terms of reference.

#### *Regional Associates, Scientific Associates, and other bodies*

The reports of the Representatives on these bodies are given as separate Appendices to the Agenda.

#### *IUCr staff*

There have been some staff changes during the triennium. In particular, it is with deep regret that the death of Dr J. N. King, the Executive Secretary, is recorded. The present members of staff in the IUCr office in Chester are: Mr M. H. Dacombe (Acting Executive Secretary and Technical Editor), Mrs A. Cawley (Administrative Assistant to the Executive Secretary), Mrs S. E. King and Mr P. R. Strickland (Assistant Technical Editors), Mr B. McMahon (Research and Development Officer), Dr M. A. Hoyland (Research and Development Assistant), Dr

A. S. Berry, Dr M. Hurst and Mr S. Westrip (Senior Editorial Assistants), Ms L. E. Jones, Dr G. F. Holmes, Miss C. A. Moore, Mr S. Conway, Miss A. M. K. Monahan and Miss J. K. Stoddard (Editorial Assistants), Ms L. Allsop and Mrs A. Whitehead (Secretaries) and Mrs C. Cook (Part-time Keyboard Operator).

Additional editorial staff were appointed during the triennium to handle the increased workload resulting from (1) the transfer of the consistency and duplication checking from the journals' Co-editors to the Chester office, (2) the increased number of manuscripts being submitted for publication in *Acta Cryst.* (including the new *Section D*) and *J. Appl. Cryst.*, (3) the introduction of the facility for the submission of manuscripts in electronic form, and (4) the archiving of structural data in connection with (3) above.

#### *Acknowledgements*

On behalf of the IUCr, the Executive Committee wishes to express its deep gratitude to the Chinese National Committee for Crystallography and the China Association for Science and Technology (CAST) for the invitation to hold the Sixteenth General Assembly and International Congress of Crystallography in Beijing. It particularly wishes to thank the Chairman of the Programme Committee, Professor Xiao-jie Xu, and the Chairman of the Organizing Committee, Professor Xiang-lin Jin.

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 1990 and 1991 have already been published [*Acta Cryst.* (1991), A47, 606–630 and (1992), A48, 922–946]. The accounts for 1992 have been audited and will be published in due course in *Acta Crystallographica Section A*. The accounts for the three years 1990, 1991 and 1992 are summarized in Tables 1–14. All amounts are expressed in Swiss Francs. The notations used in this report for the various currencies of the IUCr's activities are CHF = Swiss Franc, GBP = Pound Sterling, USD = US Dollar, NLG = Netherlands Guilder, DKK = Danish Krone.

### *General Financial Development*

Table 1 shows a comparison of the fund accounts at the beginning and the end of the triennium. No new funds were established in this period. The total assets of the IUCr have increased by CHF 142 741, or 2.7%, over the triennium. One should note that the fluctation in rates of exchange during this period has been CHF –714 856.

Table 2 shows the distribution of the assets. The amount of CHF 356 679 for debtors at 31 December 1992 is normal. It includes, in part, the IUCr's funding of the XVI General Assembly and Congress paid in advance, but the largest part relates to amounts due at that date in respect of the publishing operations during 1992, from Munksgaard for the journals and from Kluwer for *International Tables*, *Structure Reports* and other publications. These amounts, due in early 1993, and the

Table 1. *Balance Sheet, Fund Accounts (Swiss Francs)*

	31 December 1989	Fluctuations in rates of exchange	31 December 1992
General Fund	1 170 342	-152 914	1 053 301
President's Fund	16 686	-6 123	36 114
<i>Acta Crystallographica</i>	2 090 433	-226 056	1 783 370
<i>Journal of Applied Crystallography</i>	442 674	-64 296	435 705
<i>Structure Reports</i>	134 260	-17 716	134 055
<i>International Tables</i>	176 773	-21 436	164 550
Book Fund	11 989	-1 825	11 435
<i>Molecular Structures and Dimensions</i>	6 120	-805	—
Publications and Journals Development Fund	543 020	-107 975	745 264
Research and Education Fund	372 377	-84 784	700 989
Ewald Fund	218 494	-30 926	261 126
TOTAL ACCUMULATED BALANCE	5 183 168	-714 856	5 325 909

great majority of the other amounts under debtors and creditors, have since been settled.

The total investments at 31 December 1992 are CHF 4 583 625, as shown in Table 2, of which 30.7% is held by Merrill Lynch, 51.5% by Foreign & Colonial and 17.8% is a one-year National Westminster (CI) deposit. The IUCr bank accounts and short-term deposits are held with the Union Bank of Switzerland, the National Westminster Bank, the Amsterdam-Rotterdam Bank, and Merrill Lynch, involving the currencies CHF, GBP, NLG and USD.

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 is not subject to United Kingdom tax. Investment income received from other countries with which Switzerland has a Double Taxation Agreement is also 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.

#### *General Fund*

Table 3 shows the accounts for the General Fund (GF) and Table 4 compares these accounts for the triennium with the budget approved by the Bordeaux General Assembly. This fund carries the income and expenditure related to the IUCr's administration and its regular scientific activities other than publications. The income has two main sources, the subscriptions from Adhering Bodies and the interest income from investments and bank accounts. The subscriptions from Adhering Bodies are based on the unit contribution, which has been CHF 890 for all three years. The total number of membership units was 150 for 1990, 149 for 1991, and 148 for 1992, while the budget was based on 150 units for each year. The yield from investments exceeds the budgeted amount by CHF 263 597. This positive difference makes it possible for the IUCr to expand its scientific activities somewhat faster than planned.

The amount charged to the journals is calculated as 30% of the general administration costs of the IUCr, including the work of the Executive Secretary and his office and of the General Secretary and Treasurer. The Executive Committee met annually, while the Finance Committee held two meetings each year. The cost of these meetings varies, as seen from Table 3, depending on the location and the circumstances. In Table 4 they are

Table 2. *Balance Sheet, Assets (Swiss Francs)*

	31 December 1989		31 December 1992	
CURRENT ASSETS				
Cash at banks				
Current Accounts	44 190		40 935	
Deposit and Savings Accounts	555 883	600 073	452 834	493 769
Cash with Union officials		11 123		17 405
Debtors		342 577		356 679
Subscriptions due		8 900		30 260
		962 673		898 113
Deduct Creditors and accrued charges		277 063		171 776
NET CURRENT ASSETS		685 610		726 337
INVESTMENTS				
At market value	4 748 245		4 904 653	
Change in value	-270 633		-321 028	
At revalued cost		4 477 612		4 583 625
FIXED ASSETS				
Office equipment at revalued cost, less depreciation		19 946		15 947
TOTAL ASSETS		5 183 168		5 325 909

included in the expenses of administrative meetings, together with the costs of the report of the Perth General Assembly and Congress in 1987 and the IUCr representatives on other bodies. The expenses of scientific meetings in Table 4 include the travel grants for the Bordeaux Congress in 1990, the cost of the meeting in 1992 of the Programme Committee for the Beijing Congress, the expenses of the non-publishing Commissions and the Working Party on Crystallographic Information, and financial support to meetings and Schools. The financial support for young scientists attending meetings and Schools is charged to the Research and Education Fund, see Table 13.

During the triennium CHF 20 000 was transferred to the Ewald Fund.

Table 3. *General Fund (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Subscriptions from Adhering Bodies	133 500	132 610	131 720
Yield from investments and bank accounts	533 335	350 620	199 642
Grants from Unesco to ICSU and from ICSU	21 234	16 740	16 632
Amount charged to:			
<i>Acta Crystallographica</i>	53 882	59 492	68 473
<i>Journal of Applied Crystallography</i>	17 961	19 830	22 824
<i>Molecular Structures and Dimensions</i>	166	—	—
	760 078	579 292	439 291
<b>EXPENDITURE</b>			
Administration	239 644	264 408	304 323
Subscriptions to ICSU/ICSU bodies	4 602	4 860	4 394
Executive Committee	—	31 070	37 528
Finance Committee	6 813	21 938	15 701
XV General Assembly and Congress:			
Travel grants	49 245	—	—
Travel grants to Commissions	20 841	—	—
Executive Committee	42 159	—	—
Finance Committee	4 888	—	—
Expenses	1 028	—	—
XVI General Assembly and Congress:			
Programme Committee	202	—	30 218
IUCr Representatives on other bodies	3 677	6 161	7 314
Newsletter	—	—	5 040
Working Party on Crystallographic Information	8 003	19 650	—
STAR/CIF	—	—	21 570
Expenses of Commissions	2 937	12 367	2 849
Sponsorship of meetings	18 515	1 500	19 343
Transfers to other Funds:			
President's Fund	25 000	10 000	25 000
Research and Education Fund	200 000	100 000	150 000
Ewald Fund	—	—	20 000
	627 554	471 954	643 280
EXCESS OF INCOME OVER EXPENDITURE	132 524	107 338	-203 989
FLUCTUATIONS IN RATES OF EXCHANGE	-171 282	89 872	-71 504
ACCUMULATED BALANCE AT THE END OF THE YEAR	1 131 584	1 328 794	1 053 301

Table 4. *General Fund. Comparison of budget and accounts for the years 1990-1992 inclusive (Swiss Francs)*

	Budget	Accounts	Difference
<b>INCOME</b>			
Subscriptions from Adhering Bodies	400 500	397 830	-2 670
Yield from investments and bank accounts	820 000	1 083 597	+263 597
Grants from Unesco, ICSU and COSTED	38 000	54 606	+16 606
	1 258 500	1 536 033	+277 533
<b>EXPENDITURE</b>			
Administration (net)	546 700	565 747	+19 047
Subscriptions to ICSU/ICSU bodies	13 100	13 856	+756
Administrative meetings	209 000	177 249	-31 751
Scientific meetings	189 000	213 308	+24 308
Transfers to other fund accounts	270 000	530 000	+260 000
	1 227 800	1 500 160	+272 360
FAVOURABLE VARIANT FROM BUDGET			5 173
ESTIMATED PROFIT	30 700		30 700
EXCESS OF INCOME OVER EXPENDITURE		35 873	35 873

Table 5. *President's fund (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Donations, transfers and interest	26 336	11 947	26 005
<b>EXPENDITURE</b>			
Grants	1 524	23 395	13 818
<b>EXCESS OF INCOME OVER EXPENDITURE</b>	24 812	-11 448	12 187
<b>FLUCTUATIONS IN RATES OF EXCHANGE</b>			
	-5 456	1 783	-2 450
<b>ACCUMULATED BALANCE AT THE END OF THE YEAR</b>	36 042	26 337	36 114

*President's Fund*

Table 5 gives the account for the President's Fund. It is intended mainly for use in emergencies and under special or difficult circumstances, to help crystallographers from countries with currency problems to take part in the activities of the IUCr

*The Journals Funds*

Tables 6 and 7 give the accounts for *Acta Crystallographica* (AC) and the *Journal of Applied Crystallography* (JAC). One

notes from the numbers there that the profit for both journals has stayed rather constant during the triennium, if one takes into account the transfers to other funds. The Finance Committee (FC) and the Executive Committee (EC) have monitored the financial development for both journals very closely and, according to the predicted number of printed pages for AC in 1989, considered that the journal would operate at a loss in 1990. The EC therefore decided to increase the AC subscription rates by 10% for 1990. Subscription rates had not been increased since 1983. In order to maintain a sound economy for the journals, subscription rates were increased by 15% for AC and 5% for JAC in 1991 and by 7% for both journals in 1992.

There was a small decrease in the number of subscriptions (about 7% for AC and 2.5% for JAC) during the triennium. For further details see the Triennial Report by the Chairmen of the Commission on Journals.

*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.* Volume 55A in 1990, Volume 56A in 1991 and Volumes 51B and 57A in 1992. The other expenses of a year always include editorial work for several volumes yet to be published.

In 1986 the EC decided to discontinue the publication of the Organic Compounds volumes of *Structure Reports* after the publication of the volume for 1985 (Volume 52B). In 1991 the

Table 6. *Acta Crystallographica (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Subscriptions	1 582 371	1 697 994	1 850 963
Sale of back numbers and single copies	19 102	18 556	23 308
Airfreight charges to subscribers	51 278	52 180	52 636
Profit on reprints	10 944	-4 589	4 855
Royalties, copyright fees	1386	—	964
	1 665 081	1 764 141	1 932 726
Less Publisher's commission	112 080	120 158	131 199
Yield from advertisements	1 170	1 960	1 433
	1 554 171	1 645 943	1 802 960
<b>EXPENDITURE</b>			
Printing and binding	586 118	592 323	565 172
Distribution and postage	127 753	125 894	121 224
Airfreight costs	41 604	48 078	41 747
Annual Index	14 886	19 074	22 558
<i>Acta</i> Supplement	28 594	—	—
Biological Crystallography Section	3 767	4 006	8 910
Computer hardware/software	17 758	16 118	17 024
Editorial expenses	455 519	561 394	682 713
Administration expenses	53 882	59 492	68 473
Transfers to other Funds:			
Publications and Journals			
Development Fund	500 000	35 000	150 000
Research and Education Fund	100 000	—	—
Ewald Fund	—	—	—
	1 929 881	15 000	1 476 379
<b>EXCESS OF INCOME OVER EXPENDITURE</b>	-375 710	169 564	125 139
<b>FLUCTUATIONS IN RATES OF EXCHANGE</b>			
	-225 427	+120 335	-120 964
<b>ACCUMULATED BALANCE AT THE END OF THE YEAR</b>	1 489 294	1 779 195	1 783 370

Table 7. *Journal of Applied Crystallography (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Subscriptions	281 415	304 301	335 730
Sale of back numbers and single copies	9 400	5 400	5 128
Airfreight charges to subscribers	7 428	7 732	7 753
Royalties, copyright fees	691	—	1 300
	<u>298 934</u>	<u>317 433</u>	<u>349 911</u>
Less Publisher's commission	20 368	21 679	23 860
	<u>278 566</u>	<u>295 754</u>	<u>326 051</u>
Yield from advertisements	—	817	—
Contribution towards cost of printing Conference Proceedings	—	20 433	—
	<u>278 566</u>	<u>317 006</u>	<u>326 051</u>
<b>EXPENDITURE</b>			
Printing and binding	86 948	149 977	85 991
Distribution and postage	14 792	23 754	24 373
Airfreight costs	6 324	9 811	7 865
20-Year Index	11 669	—	—
Loss on reprints	1 283	470	1 431
Editorial expenses	63 956	118 689	131 346
Administration expenses	17 961	19 830	22 824
Transfers to other Funds:			
Publications and Journals	—	—	50 000
Development Fund	—	—	—
Ewald Fund	15 000	—	—
	<u>217 933</u>	<u>322 531</u>	<u>323 830</u>
EXCESS OF INCOME OVER EXPENDITURE	60 633	-5 527	2 221
FLUCTUATIONS IN RATES OF EXCHANGE	-66 168	31 425	-29 553
ACCUMULATED BALANCE AT THE END OF THE YEAR	<u>437 139</u>	<u>463 037</u>	<u>435 705</u>

Table 8. *Structure Reports (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Sale of copies	71 821	58 239	193 476
Less Publisher's commission	18 673	15 142	50 304
	<u>53 148</u>	<u>43 097</u>	<u>143 172</u>
<b>EXPENDITURE</b>			
Printing and binding new volumes	7 062	6 722	45 413
Typing of manuscripts	7 804	5 507	16 928
Editorial expenses	28 612	13 670	90 188
	<u>43 478</u>	<u>25 899</u>	<u>152 529</u>
EXCESS OF INCOME OVER EXPENDITURE	9 670	17 198	-9 357
FLUCTUATIONS IN RATES OF EXCHANGE	-18 922	10 311	-9 105
ACCUMULATED BALANCE AT THE END OF THE YEAR	<u>125 008</u>	<u>152 517</u>	<u>134 055</u>

EC agreed that the A Series (Metals and Inorganic Compounds) of *Structure Reports* should be terminated with the volume for 1990 and the Ten-Year Cumulative Index for 1981-90. For further details see the Triennial Report by the Chairman of the Commission on *Structure Reports*.

#### *International Tables*

The *International Tables* accounts are shown in Table 9. The sales figures there show that there have been rather constant

sales of Volume A, the Brief Teaching Edition of Volume A, and Volumes II, III and IV during the triennium. Volume C came out in 1992 and sells well.

The costs connected with the printing and reprinting of Volume A are charged to the 1992 accounts. The editorial expenses for the triennium are mostly related to the work on the two new volumes, Volumes B and C. The accounts for 1992 also include expenditure on the typesetting/printing of these two volumes. For further details see the Triennial Report by the Chairman of the Commission on *International Tables*.

Table 9. *International Tables (Swiss Francs)*

	1990		1991		1992	
<b>INCOME</b>						
<b>Sales</b>						
Volume A	67 573		65 044		87 410	
Teaching Edition of Volume A	6 428		3 111		5 939	
Volumes II, III and IV	27 762		30 309		17 032	
Volume C	—		—		121 674	
	<hr/>		<hr/>		<hr/>	
Less Publisher's commission	101 763		98 464		232 055	
	26 458	75 305	25 600	72 864	60 334	171 721
	<hr/>		<hr/>		<hr/>	
<b>EXPENDITURE</b>						
Printing/Reprinting Volume A	—		—		40 471	
Typesetting Volume B	15 150		9 515		—	
Printing/Typesetting Volume C	24 350		1 216		48 364	
Editorial expenses	67 966	107 466	67 396	78 127	36 249	125 084
	<hr/>	<hr/>	<hr/>	<hr/>	<hr/>	<hr/>
EXCESS OF INCOME OVER EXPENDITURE		-32 161		-5 263		46 637
		<hr/>		<hr/>		<hr/>
FLUCTUATIONS IN RATES OF EXCHANGE		-19 012		8 725		-11 149
		<hr/>		<hr/>		<hr/>
ACCUMULATED BALANCE AT THE END OF THE YEAR		125 600		129 062		164 550
		<hr/> <hr/>		<hr/> <hr/>		<hr/> <hr/>

Table 10. *Book Fund (Swiss Francs)*

	1990		1991		1992	
<b>INCOME</b>						
Transfer from <i>Molecular Structures and Dimensions</i> Fund	—		5 315		—	
<b>Sale of copies (net):</b>						
<i>Historical Atlas of Crystallography</i>	7 922		6 776		4 550	
<i>Escher Kaleidozyklen</i>	170		—		—	
<i>Crystallographic Databases</i>	813		256		179	
<i>Fifty Years of X-ray Diffraction</i>	133		—		—	
<i>Escher Drawings</i>	787		-52		389	
<i>Early Papers</i>	103		30		99	
<i>Fifty Years of Electron Diffraction</i>	56		39		124	
<i>World Directory of Crystallographers:</i>						
7th edition	151		—		—	
<i>World Directory of Crystallographers:</i>						
8th edition	136		44 658		960	
Sundry publications	245		66		22	
<i>Molecular Structures and Dimensions</i>	—		1 381		382	
<b>Royalties:</b>						
<i>Escher Drawings</i>	300		400		400	
Book Series. IUCr Crystallographic Symposia	742	11 558	1 040	59 909	3 777	10 882
	<hr/>	<hr/>	<hr/>	<hr/>	<hr/>	<hr/>
<b>EXPENDITURE</b>						
<i>Escher Kaleidozyklen</i>	36		—		—	
<i>Crystallographic Databases</i>	—		—		—	
Book Series expenses	187		57		735	
<i>Historical Atlas of Crystallography</i>	12 019		16 136		1 183	
<i>World Directory of Crystallographers:</i>						
8th edition	1 270		48 937		242	
Sundry publications	259	13 771	11	65 141	6	2 166
	<hr/>	<hr/>	<hr/>	<hr/>	<hr/>	<hr/>
EXCESS OF INCOME OVER EXPENDITURE		-2 213		-5 232		8 716
		<hr/>		<hr/>		<hr/>
FLUCTUATIONS IN RATES OF EXCHANGE		-1 285		236		-776
		<hr/>		<hr/>		<hr/>
ACCUMULATED BALANCE AT THE END OF THE YEAR		8 491		3 495		11 435
		<hr/> <hr/>		<hr/> <hr/>		<hr/> <hr/>

Table 11. *Molecular Structures and Dimensions (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Sale of copies	224	—	—
Less Publisher's commission	58	—	—
	<hr/>	<hr/>	<hr/>
<b>EXPENDITURE</b>			
Transfer to Book Fund	—	5 315	—
Salaries	—	—	—
Administration expenses	166	—	—
	<hr/>	<hr/>	<hr/>
EXCESS OF INCOME OVER EXPENDITURE	nil	-5 315	nil
FLUCTUATIONS IN RATES OF EXCHANGE	-805	nil	nil
ACCUMULATED BALANCE AT THE END OF THE YEAR	5 315	nil	nil

Table 12. *Publications and Journals Development Fund (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Transfers from other Funds:			
General Fund	—	—	—
<i>Acta Crystallographica</i>	500 000	35 000	150 000
<i>Journal of Applied Crystallography</i>	—	—	50 000
Interest	36 027	49 011	44 134
	<hr/>	<hr/>	<hr/>
<b>EXPENDITURE</b>			
Refurbishment of Chester office	62 500	—	—
Computer expenses:			
Purchase of equipment and software	175 113	59 867	36 924
Programming and development	57 857	75 976	85 716
	<hr/>	<hr/>	<hr/>
EXCESS OF INCOME OVER EXPENDITURE	240 557	-51 832	121 494
FLUCTUATIONS IN RATES OF EXCHANGE	-103 014	45 589	-50 550
ACCUMULATED BALANCE AT THE END OF THE YEAR	680 563	674 320	745 264

### *The Book Fund*

Table 10 gives the accounts of the Book Fund. The increase in the accumulated balance of this fund during the triennium is small, and the numbers are compatible with those given for the 1987-89 triennium [*Acta Cryst.* (1992), A48, 367].

### *Molecular Structures and Dimensions*

The *Molecular Structures and Dimensions* accounts are shown in Table 11. The accumulated balance at the end of 1990 has been transferred to the Book Fund.

### *Publications and Journals Development Fund*

Table 12 shows the accounts of the Publications and Journals Development Fund (PJDF). The fund was established in 1984 and has been built up through transfers from other funds, such as AC and JAC. In order to build up the fund further and in a systematic way, with the goal to make it self-supporting, the EC decided to increase its balance by crediting it with interest calculated as 8% of the balance in the fund, from 1989 onwards, as shown in Table 12. Furthermore, one notes from that table that the main expenses during the triennium are

related to the purchase of computer hardware and software and to programming and development.

It is the EC's policy to support and encourage the IUCr's highly qualified staff by supplying them with the best equipment.

### *Research and Education Fund*

Table 13 shows the account of the Research and Education Fund (REF). The fund was also established in 1984 and, like the PJDF, has been built up through transfers from other funds. As for the PJDF, the EC decided to increase this fund by 8% per year, taken from the interest income, with the goal to make it self-supporting. One notes that about CHF 220 000 was given as young scientists' support during the triennium.

### *Ewald Fund*

The accounts of the Ewald Fund are given in Table 14. The interest on the capital is intended to cover the costs of the Prize. It is calculated as 8% of the balance in the fund, and is taken from the total annual interest income received from the IUCr's investments, in the same way as for the interest credited to the PJDF and the REF. The balance of the interest

Table 13. *Research and Education Fund (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Transfers from other Funds:			
General Fund	200 000	100 000	150 000
<i>Acta Crystallographica</i>	100 000	—	—
<i>Journal of Applied Crystallography</i>	—	—	—
Interest	27 373	40 484	44 336
	<hr/>	<hr/>	<hr/>
<b>EXPENDITURE</b>			
History of the IUCr	1 976	—	—
Young scientists' support	76 145	53 804	90 850
Visiting Professorship Programme	—	145	9 665
1989 ECM Fund creditor	—	13 007	2 697
IUCr publications donated	606	202	—
	<hr/>	<hr/>	<hr/>
EXCESS OF INCOME OVER EXPENDITURE	248 946	73 326	91 124
FLUCTUATIONS IN RATES OF EXCHANGE	-81 683	44 446	-47 547
ACCUMULATED BALANCE AT THE END OF THE YEAR	<hr/> <hr/>	<hr/> <hr/>	<hr/> <hr/>

Table 14. *Ewald Fund (Swiss Francs)*

	1990	1991	1992
<b>INCOME</b>			
Interest	17 282	15 567	19 173
Transfers from other Funds:			
General Fund	—	—	20 000
<i>Acta Crystallographica</i>	—	15 000	—
<i>Journal of Applied Crystallography</i>	15 000	—	—
	<hr/>	<hr/>	<hr/>
<b>EXPENDITURE</b>			
Prize	26 582	—	—
Selection Committee and expenses	—	253	1 689
	<hr/>	<hr/>	<hr/>
EXCESS OF INCOME OVER EXPENDITURE	5 700	30 314	37 544
FLUCTUATIONS IN RATES OF EXCHANGE	-29 474	16 260	-17 712
ACCUMULATED BALANCE AT THE END OF THE YEAR	<hr/> <hr/>	<hr/> <hr/>	<hr/> <hr/>

from the investments is credited to the GF. One notes that an additional CHF 50 000 has been transferred to the fund during the triennium. This has allowed the IUCr to increase the Prize to USD 25 000 for 1993.

#### Appendix C: Ewald Prize

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 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.

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, was used as capital for the Ewald Prize. The interest from this capital is used to finance the Prize.

The Prize consists of a medal, a certificate and an award of US \$20 000 (increased to US \$25 000 for 1993). It is presented once every three years during the triennial International Congresses of Crystallography. The first Prize was presented during the Perth Congress, being awarded jointly to Professor J. M. Cowley and Dr A. F. Moodie. The second Ewald Prize was presented during the Bordeaux Congress to Professor B. K. Vainshtein.

In April 1993 it was announced that the third Ewald Prize had been awarded to Professor N. Kato for his outstanding and profound contributions to the dynamical theory of X-ray diffraction of spherical waves by perfect crystals and slightly deformed (nearly perfect) crystals, for the experimental exploitation of these theories towards the characterization of the defect structure of single crystals and for his extraordinary achievements in X-ray diffraction topography. Professor Norio Kato works at the Department of Physics of Meijo University, Nagoya, Japan.

The presentation of the Ewald Prize to Professor Kato will be made during the Congress Opening Ceremony on 21 August.

#### Appendix D: Reports of 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. The total number of papers in *Acta Cryst.* during this period decreased slightly to 3274, while the papers in *J. Appl. Cryst.* increased slightly to 408. Papers were received from 50 countries. Median publication times for Full Articles were up slightly for Sections A and B, to 5.2 months and 5.6 months, respectively, and were up approximately 50% for Section C, from 4.9 months during the last triennium to 7.5 months. This increase is due to the backlog of Section C papers that occurred in 1990 but which has since been cleared with the installation of new computer facilities, centralized checking procedures, and an expanded editorial staff in the Technical Editor's office.

Commitments have been made by selected authors for publication of 19 future Lead Articles in *Acta Cryst.* and seven in *J. Appl. Cryst.* In addition to these invited Lead Articles, the Commission approved the submission of unsolicited review articles covering topics of general interest to the crystallographic community.

Subscription rates for *Acta Cryst.* and *J. Appl. Cryst.* rose each year during the triennium after having remained constant for several years. While the number of subscribers taking all three sections of *Acta Cryst.* decreased by 7%, the number of subscriptions to the individual sections increased slightly. *J. Appl. Cryst.* subscriptions declined by 2.5% during the triennium.

Revised *Notes for Authors* for *Acta Cryst.* were published in late 1991. The new *Notes* for Section C instituted new publication requirements and submission procedures in January 1992, including procedures designed to facilitate the direct transfer of text and numerical data from authors' computers to the typesetting programs in the Technical Editor's office.

The Executive Committee accepted the recommendation that the new *Acta Cryst. Section D, Biological Crystallography*, be launched, with a publication date of January 1993. This new section of the *Acta Cryst.* series will be devoted primarily to macromolecular crystallography, especially the structural aspects of these crystallographic studies. J. P. Glusker was appointed Editor of this section, and she has named an Advisory Board to assist her in developing general policies and targeting appropriate audiences. All current subscribers to *Acta Cryst.* (except those taking only Section C) will receive the new Section D.

The Executive Committee also approved the appointment of individual editors for Sections A, B and C of *Acta Cryst.* The Chairman of the Commission on Journals will be Editor-in-Chief of the *Acta Cryst.* series, and will present nominations for the individual editors to the Executive Committee at the Beijing Congress.

A. M. Glazer succeeded M. Schlenker as Editor of *J. Appl. Cryst.* following the Bordeaux Congress in 1990. New *J. Appl. Cryst.* Co-editors appointed during the triennium were C. J. Howard, J. I. Langford, J. Vicat, T. C. Huang and H. Hashizume. New *Acta Cryst.* Co-editors appointed were I. D. Brown, P. W. Coddling, S. R. Hall, A. Kálmán, M. Ohmasa, M. Nardelli, D. Schwarzenbach, E. T. Adman, T. A. Jones, M. J. Adams and M. Vijayan. Co-editors who retired during the triennium were A. Gavezzotti and H. Burzlaff for *Acta Cryst.* and H. Iwasaki and B. Morosin for *J. Appl. Cryst.* R. F. Bryan was appointed the

new Book Review Editor to replace R. Gould. The Commission greatly appreciates the time spent by the Co-editors and the Book Review Editor in performing their editorial and administrative duties, and looks forward to their help with the journals during the next triennium.

The editorial staff in the Technical Editor's office in Chester was significantly expanded during the triennium. The additional staffing has been necessary due to the increased use of in-house computing facilities for the checking and archiving of structural data, and to handle the increasing numbers of electronically submitted manuscripts. The Commission commends all members of the Technical Editor's staff for their excellent and loyal work, and for their flexibility and enthusiasm throughout the major transitions that occurred in our publishing operations.

13 March 1993

C. E. BUGG, Chairman  
A. M. GLAZER, Co-Chairman

##### *Commission on Structure Reports*

Volume 55A (Metals and Inorganic Compounds for 1988), Volume 56A (Metals and Inorganic Compounds for 1989), Volume 57A (Metals and Inorganic Compounds for 1990) and Volume 51B (Organic Compounds for 1984) have been published. The Multi-Year Index for the Organic Compounds to 1980 (Volume 47B) has been completed, is with the publisher, and will appear in 1993. Co-editorial work will be completed for Volume 50B (Organic Compounds for 1983), for Volume 52B (Organic Compounds for 1985) and for the 1913–1990 Metals and Inorganic Indices (Volume 58A) – the final *Structure Reports* volumes – and they will be with the publisher before the Beijing General Assembly in August 1993. In accordance with decisions made previously, this will conclude the work of the Commission on *Structure Reports* which will then be disbanded.

3 February 1993

G. FERGUSON, Chairman

##### *Commission on International Tables*

The International Union of Crystallography held its triennial meetings in Bordeaux in July 1990, in the course of which the Commission on *International Tables* met both in a closed and in an open session. The status of the current Volumes A–D was reported on both occasions, and proposals for future volumes were outlined. The Open Meeting was well attended, but only the Editors and one *ex officio* member (out of seven) were present at the closed meeting. This is not surprising, since the tight scheduling of Commission meetings meant that most of the *ex officio* members had to choose between chairing their own Commissions or attending that on the *International Tables*. Perhaps partly because of this poor attendance, the Executive Committee decided not to appoint *ex officio* members for the period 1990–1993. However, such members were very important in planning and suggesting authors for Volumes B and C, and this decision should be reconsidered if second editions of these volumes are planned.

Discussion continued on two other proposals (*Crystallographic Computing; Mathematics for Modern Crystallography*). Such volumes would be of great value to the crystallographic community, but the appropriate format needs further consideration. The formats so far considered are (i) Volumes of the *International Tables* and (ii) Monographs, such as those of the Oxford University Press. The proposals have not progressed further during the triennium.

A. J. C. Wilson has resigned as Chairman of the Commission with effect from 1 July 1993, and will be succeeded by Th. Hahn.

Detailed reports on the Volumes of the *International Tables for Crystallography* that are currently active are given below.

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

The third, revised edition of Volume A of *International Tables* was published in November 1992. Its main feature is the incorporation of new diagrams for the tetragonal and, in particular, for the cubic space groups. Work on the remaining space-group diagrams is in progress; they will be incorporated into the fourth edition. Efforts towards a more detailed and improved presentation of the subgroups of space groups have continued throughout the triennium. A list of errata in the second edition (1987, 1989) appeared early in 1993 in *Acta Crystallographica* [(1993), A49, 592–593].

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

The report for this period concerns mainly routine, albeit lengthy, processing of the final stages of the editing of this volume. The status of Volume B, at the time of the Bordeaux Congress, in July 1990, was communicated to the Open Meeting of the Commission on *International Tables*, and was discussed with the Executive Committee. At the time of that meeting, 16 chapters of the volume were in galley-proof stage and the three remaining ones were in preparation at the Technical Editor's office. Most of the corrected galley proofs were returned for subsequent technical editing by the end of 1990. As far as Volume B is concerned, the year 1991 was devoted to the production of the page proofs, their distribution among the authors, and reviewing of some corrected page proofs that were returned by the authors. The processing of the page proofs was slower than expected, as in May 1992 corrected page proofs of some chapters were still expected at the Editor's office. However, by the end of September 1992 all the corrected page proofs were received, marked for indexing, and transferred to the Technical Editor's office. The only other subsequent contributions of the Editor were a preface to the volume and promotional text that was requested by the publishers. The last of these was acknowledged on 4 January 1993. Throughout the above period correspondence – usually by electronic mail – took place between the Editor, the authors and the Technical Editor.

Some dates may be relevant for this summarizing report: the editing of Volume B formally commenced beginning 1983, and the authors were requested to submit the final drafts of their contributions by 31 December 1985. These drafts arrived at the Editor's office between February 1986 and May 1990. This long time range was due, in part, to withdrawal of promised contributions, and consequent late invitations. The Editor looks forward to the publication of Volume B, and hopes it will be interesting and useful to the crystallographic community.

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

The first edition of Volume C was published in March 1992. It is intended to supersede Volumes II, III and IV of the previous series *International Tables for X-ray Crystallography*, and this is the last occasion for which data of sales *etc.* of these will appear in Table 1. As Volume C contains many sections contributed by many authors, it has been necessary to make the indexes more extensive than in any previous volume. An author index is included for the first time. The deaths of two contributors, Henry Lipson and William Parrish, in the course of the preparation of the volume are recorded with sorrow.

Table 1. Sales and stocks of volumes published to date

Volume	Brief					
	II	III	IV	A	A	C
Date of publication	1959	1962	1974	1983	1985	1992
Dates of reprinting	1967	1968	1989	1984	1988	—
	1972	1983	—	1986	1989	—
	1985	1985	—	1987	—	—
	1989	—	—	1989	—	—
	—	—	—	1992	—	—
Number of copies sold up to 31						
December 1989	9169	8437	3981	3612	2707	—
in 1990	83	85	82	308	341	—
in 1991	97	107	98	340	172	—
in 1992	53	53	41	394	326	450
up to 31						
December 1992	9402	8682	4202	4654	3546	450
Stock at 31						
December 1992	121	191	162	521	109	535

*Volume D. Physical Properties of Crystals; Editor A. Authier*

A. Authier was appointed Editor of Volume D in July 1990 replacing B. T. M. Willis who had resigned in March 1990. At the invitation of the new Editor, a Working Party of nine persons met in Paris in June 1991. This group redefined the outline of the volume, which will consist of three parts (Part I: *Tensorial Aspects of Physical Properties*; Part II: *Symmetry Aspects of Excitations*; Part III: *Symmetry Aspects of Structural Phase Transitions, Twinning and Domain Structures*), and proposed a list of authors. This outline and a preliminary list of potential authors was accepted by the Executive Committee in its August 1991 meeting. About three-quarters of these authors have accepted and have started the preparation of their manuscripts. New authors are being sought for the remaining parts. It had been proposed that the volume be accompanied by software to read the *Tables*, based on test software made in Czechoslovakia. It turned out subsequently, however, that due to the situation in that country, the firm which was to develop the software was no longer in a position to do so, and another solution will have to be found. It is hoped that the manuscript of Volume D can be completed in 1994.

*Volume E. Subperiodic Symmetry Groups; Editors V. Kopsky and D. B. Litvin*

The proposal for a Volume E was presented to and accepted by the Executive Committee at the time of the Bordeaux Congress. Volume E consists of three parts: Part 1 is a guide to and symmetry tables of the subperiodic groups: *Frieze Groups, Rod Groups and Layer Groups*. Parts 2 and 3 deal with the relationship between subperiodic groups and space groups. Subperiodic groups are considered as factor groups of space groups in Part 2, and as subgroups of space groups in Part 3. A document entitled *Nomenclature, Symbols and Classification of the Subperiodic Groups*, containing the standards for the nomenclature, symbols and classifications used in Volume E, was written by the authors. This was submitted to and approved by the Commission on Crystallographic Nomenclature. An Abstract will appear in *Acta Cryst.* [(1993), A49, 594].

Part 1 has been read by Professor Hahn for consistency with Volume A in content, style and presentation. Comments by Professor Hahn have been incorporated, and Part 1 is complete

except for professional redrawing of diagrams and a final section comparing the numerous sets of symbols of the subperiodic groups. A draft of Part 2 has been written and of Part 3 is partially done. It is expected that all parts will be completed in 1993.

*Volume F. Multidimensional Crystallography; no editor appointed*

No direct progress has been made with planning a volume on  $N$ -dimensional crystallography ( $N > 3$ ). An enthusiastic editor is lacking, and the great number of space groups is a problem. However, the Working Group set up in 1990 by the Commission on Crystallographic Nomenclature has in effect functioned also as a sub-committee of the Commission on *International Tables*; two editors are members of the Working Group, and the other Editors have been consulted as occasion required. It has not proved possible to reach any unanimous recommendations, but discussion within the group and with others interested in the problem has resulted in the clarification of many problems and the publication of new or revised versions of the systems favoured by some members of the group.

The Commission on *International Tables* has a problem of size on its hands. For the description of the symmetry of the complex electron density when dispersion is appreciable and related problems (the Patterson synthesis; certain magnetic properties) 'coloured' (Shubnikov) space groups are required; there are 1651 dichromatic groups. The only reasonably complete treatment of the dichromatic groups is in Russian (V. A. Koptsik, *Shubnikov Groups*. Moscow University Press, 1966) and is out of print. It is much less detailed than Volume A of *International Tables*; the entry for each space group contains little more than the equivalent of the diagrams of Volume A. Such colour groups in three dimensions are subperiodic groups of the 4895 space groups in four dimensions [H. Heesch (1930). *Z. Kristallogr.* 73, 325–345]. It takes about 800 pages to treat the 230 three-dimensional space groups in Volume A, an average of 3.5 pages per group. *Pro rata*, it would require a volume of 5800 pages to treat the colour groups in the same detail, and one of 17 000 pages for the four-dimensional space groups. 'Volumes' of such a size are not impossible – they would amount to about the complete *Oxford English Dictionary* and the *Encyclopaedia Britannica*, respectively – but are they practicable? The material could be produced largely as direct computer output and distributed as a volume of about the current size plus one or two compact disks. Readers for compact disks are not widely available as yet, but may be expected to become common within the next few years. Alternatively, computer programs for generating the space-group entries could accompany the single printed volume.

13 April 1993

A. J. C. WILSON, Chairman

*Commission on Biological Macromolecules*

The most obvious feature of the last three years is the continual acceleration in the structural determination of macromolecules – there have been some spectacular successes which will have immense impact on biochemistry, biology and medicine. This has rested on improved computing and graphics technology, on advances in crystallographic software (especially in the area of data processing and phasing calculations) and on developments in data-collection equipment, particularly image plates and the growing availability and refinements of the synchrotron centres.

There has been generally good progress with the practice of depositing crystallographic data at Brookhaven, which is

now widely accepted by the community and mostly recognized by scientific journals as a requisite for publication. With the flood of data now being published and deposited, expansions of resources and techniques (including validation tests) are being implemented at Brookhaven.

Meetings have been held in the USA and Europe to coordinate policies and compare ideas and practices in database usage and development. Another change in the offing is the introduction of the CIF format for use in macromolecular structures. Its ready acceptance by the small-molecule crystallographic community has been noted and it is hoped that the advantages of the CIF will soon be absorbed by the macromolecular community. The contribution of the IUCr Advisory Committee on the CIF has been very important in defining practices in development and how to implement them.

The publication of macromolecular structures is still being carried out in a wide variety of journals. The arrival of *Acta Crystallographica Section D* will meet a need for describing crystallographic methods and reporting detailed structures and comparisons, and will serve as a forum for reporting meetings, publishing conference proceedings and for commissioning articles of general interest.

The growth in the number of structures determined by NMR and the extension of the method to molecules of larger molecular weight is complementing X-ray crystallographic research. In addition, the NMR method is characterizing macromolecular solution properties, mobilities and solvent interactions with remarkable precision. This information again adds importantly to the crystal studies. The atomic coordinates of NMR derived structures can now be deposited at Brookhaven; discussions are in train as to the best method of depositing these data.

21 April 1993

G. G. DODSON, Chairman

*Commission on Charge, Spin and Momentum Densities*

In the triennium 1990–93, the guidelines of the Commission on Charge, Spin and Momentum Densities were to encourage all activities devoted to the accurate determination of density distributions in position and momentum space; within our scope we have also observed with special sympathy experimental and theoretical activities which have a strong influence on the physical understanding of ground-state properties as far as they are related to electron density distributions. This widespread activity is in accordance with the main aim of our Commission of bringing together crystallographers, whose principal interest is to investigate chemical bonding, with physicists and chemists, who contribute to the fundamental understanding of bonding, both from the quantum theoretical point of view and by utilizing different experimental methods that provide access to these problems.

The most important activity of the Commission in 1990 was the organization and realization of the following three Microsymposia at the Bordeaux Congress: Accuracy of Experimental Densities (Chair: J. Schneider), The Use of Charge Densities in Computer Simulation and Molecular Design (Chair: K. Hermansson), and Extinction (Chair: N. Kato), where the first was held as an Open Commission Meeting. The Microsymposia found appreciable support from the Congress attendees, so that the Commission felt justified with its choice of subjects. Additionally to the above Microsymposia, the Commission has organized a discussion session on Accurate Electron Densities devoted to a thorough discussion of the new Commission project on Quantum Mechanical Description of Electronic Structure from Experimental Charge and Momentum Densities. In a Closed

Meeting at Bordeaux, the date and subjects of the Xth Sagamore Conference were fixed.

The most important activity of the Commission in 1991 was the organization and realization of the Xth Sagamore Conference, held 1–7 September in Konstanz, Germany, where the Commission was acting as Programme Committee. The local organization was performed very successfully by W. Weyrich and his group at Konstanz University. The Conference found good support. With 160 attendees, 45 lecture contributions (including tutorials) and 100 poster presentations, the Conference has touched the upper limits of an informal meeting with much open time for discussion and scientific exchange. The topics of the Conference covered electron and spin densities in position and momentum space and their implications both for solid-state physics and structural chemistry, where new experimental techniques, for instance magnetic photon scattering, as well as properties of new materials, for example the high- $T_c$  superconductors and their Fermi surface topology investigated by positron annihilation, found special attention. Moreover, problems connected with the dynamics of ground-state properties (dynamic structure factor) were included in the programme following a recommendation of the preceding Sagamore Conference in 1988. In this context also new experimental developments such as ultrahigh energy resolution inelastic X-ray scattering and coherent inelastic X-ray scattering were demonstrated. Finally, the problem of reconstructing quantum mechanical quantities, e.g. density matrices, from experimental data, the matter of a new Commission project, were presented in oral and poster sessions. In two Closed Commission Meetings during the Sagamore Conference, further activities (Gordon Conference 1992, Beijing IUCr Congress, XIth Sagamore Conference 1994) were discussed, the new Commission project Quantum Mechanical Description of Electronic Structure from Experimental Charge and Momentum Densities was finally approved, and the nomination of new Commission members was initiated.

In 1992, members of the Commission have been active in contributing to the Gordon Conference, 20–24 July 1992, on Electron Distributions and Chemical Bonding, Co-chaired by M. B. Hall and G. T. De Titta, where these Gordon Conferences are mainly devoted to the chemical aspects of electron densities, thus being to some extent complementary to the Sagamore Conferences. During the Gordon Conference, a Closed Commission Meeting was held, where the nominations of new Commission members were fixed, two new Commission projects (High- $T_c$  Fermiology, and Multipole Refinement) were approved and the Commission project Electron Density in Perovskite Structures was dropped, since it has not found enough support.

Current Commission projects:

1. *Quantum Mechanical Description of Electronic Structure from Experimental Charge and Momentum Densities* (Project leaders: W. Weyrich, V. Smith Jr). This project was initiated during a pre-conference Workshop of the IXth Sagamore Conference, 1988, and finally approved at the Xth Sagamore Conference. The aim of this project is to investigate to what extent the combination of accurate experimental density data from both position and momentum space can enable a direct access to wave functions and density matrices, respectively. Moreover, it becomes feasible to measure on selected highly perfect crystalline solids nondiagonal elements of the density matrix in momentum space directly by means of coherent Compton scattering, so that methods for reconstructing wave functions from experimental data can be additionally controlled by experiment. The project found broad support among the attendees of the Xth Sagamore Conference in Konstanz, documented

by a long list of interested persons. A meeting will be held every year, organized by the project leaders, to report on progress.

2. *Fermiology of High- $T_c$  Superconductors via High-Resolution Synchrotron-Based Compton Scattering Spectroscopy* (Project leader: A. Bansil). This project was initiated during the Xth Sagamore Conference, 1991, in Konstanz. The project will consist of three steps, where the first is to standardize the procedures for evaluating high-resolution Compton data from synchrotron-based instruments. In the second step, the principal ability of Compton scattering to contribute to the fermiology of metallic systems should be investigated on rather simple systems by several groups, where the word fermiology means not only the Fermi surface but also the spectral properties of the electron gas near the Fermi energy more generally. In the third step, the participating groups, based on the experiences of the foregoing steps, should concentrate their effort on obtaining information both on the shape of the Fermi surface and on the discontinuity of the momentum distribution at the Fermi energy of  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , thus making possible a fundamental contribution to the knowledge of the physics of high- $T_c$  superconductors. In order to define more precisely how to proceed and to come to a first scientific exchange among the participating groups, a Workshop is planned to be held 2–4 July in Kraków, Poland, locally organized by L. Dobrzynski and chaired by W. Schülke and A. Bansil.

3. *Multipole Refinement and Properties: a Program Package for Analysing Electron Densities from Diffraction Data* (Project leader: P. Mallinson). The project was initiated at an *ad hoc* meeting during the Gordon Conference on Electron Distribution and Chemical Bonding, July 1992, and was approved in a ballot in December 1992. The purpose of the project is to prepare a unified version of *MOLLY* for analysing the electron charge distribution, where features of other currently used programs should be included. Moreover, programs for deriving properties and for analysing the topology of density distributions should be added. A comprehensive documentation of the package should be produced, and arrangements should be made for distribution and support on a continuing basis. The participation of the user community in designing updates should be invited.

1 March 1993

W. SCHÜLKE, Chairman

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

During the triennium, the Commission reconsidered its objectives. While confirming its commitments in continuing the successful series of international Schools for the benefit of young scientists of developing countries, a series that dates back more than 10 years, it was felt that a better definition of the interaction area between the crystallographic and the crystal growth communities was needed. It is now evident that, for a real expansion of the crystallographic activities in the field of crystal growth and related materials science, the new developments and trends in this field have to be carefully taken into consideration. Crystallographers must be aware that the tendency is towards ever more structurally complex materials (semiconductor multi-layer structures, superconductors, organic crystals, biomaterials and proteins *etc.*) and hence very sophisticated technologies (ultra high vacuum molecular beam epitaxy, metal-organic chemical vapour deposition, microgravity growth *etc.*), which more and more require the support of advanced characterization tools and skills, to which crystallography can largely contribute. In order to move towards a better definition of

the interdisciplinary area that both crystallographers and crystal growers share, it stressed the need of a stronger interaction with the IOCG and the national associations of crystal growth. Along these lines, the Commission undertook the following activities during the triennium.

The Commission helped organize the Third European Conference on Crystal Growth (ECCG-3), which was held in Budapest in the period 5–11 May 1991 with the sponsorship of the IUCr and the approval of the IOCG. The Commission organized a Microsymposium on crystal growth during the European Crystallographic Meeting (ECM-13, 1991), first planned in Ljubljana and later moved to Trieste because of the war in Yugoslavia. This Microsymposium, aimed at discussing various aspects of crystal growth and characterization of materials, was mainly focused on organic crystals, materials of increasing interest for their potential application in many fields.

As to the International School Programme for developing countries, the main activity of the Commission was the organization, jointly with the International Centre for Theoretical Physics (ICTP) and the International Centre for Science and High Technology (ICS) of Trieste, of the School of Materials for Electronics: Growth, Properties and Applications. The School, sponsored by the IUCr, the IAEA and UNESCO, was held in Miramare, Trieste, 18 November–6 December 1991 and was attended by 67 participants from 28 countries, selected from more than 400 applicants. During the triennium, the proceedings of the International School on Crystal Growth and Crystallographic Assessment of Industrial Materials, organized by the Commission in 1990 at Sitges, Barcelona, Spain, have been published under the title *Crystalline Materials: Growth and Characterization* (1991), edited by R. Rodriguez-Clemente & C. Paorici (Zürich: Trans Tech Publications).

15 April 1993

C. PAORICI, Chairman

#### *Commission on Crystallographic Apparatus*

Over the past triennium, the Commission on Crystallographic Apparatus has had as its primary aim the solution of problems associated with the calculation and measurement of the fundamental parameters of X-ray scattering ( $f'$ ,  $f''$  and  $s$ ). It has been actively involved in theoretical and experimental determinations of  $f'$  and  $f''$ , the measurement of X-ray absorption coefficients, and the creation of standards and criteria for XAFS experiments. In addition, it has been interested in the precise measurement of single-crystal lattice parameters and the development of criteria for correctly specifying the properties and performance of two-dimensional detectors. Its High Pressure Group has been involved in the organization of conferences and Workshops. Considerable progress has been made in most aspects of its work. Now that many of its projects have reached a satisfactory conclusion, the Commission is planning to broaden its activities, and will concentrate on the techniques of measurement in both X-ray and neutron diffraction, where these two fields have problems in common.

1. *The X-ray Attenuation Project* (D. C. Creagh). This project reached its conclusion with the publication of *International Tables for Crystallography* Volume C. The tables of X-ray absorption and related tables on X-ray spectroscopy and the dispersion corrections which were presented in that volume have been compared with existing theoretical and experimental data sets [Creagh (1990). *Nucl. Instrum. Methods*, **A295**, 417–434; Creagh (1992). Proceedings of the International Conference on Anomalous Scattering, Malente; Creagh (1992). National Sem-

inar on Recent Trends in Photon–Atom Interactions, Karnatak]. Work is proceeding on the production of parameterized fits to the X-ray attenuation data and the generation of MS DOS programs for computing  $f'$  and  $f''$ .

2. *The Single-Crystal Lattice-Parameter Project* (G. T. De Titta). This project has made slow progress this triennium. The requisition of ruby spheres of sufficiently high perfection has not been easy, and each sphere must be mounted and tested prior to distribution to laboratories participating in the project. This project has two labour-intensive phases: specimen preparation and selection, and data collation. It is recommended that funding be provided for assistance in both phases of the project.

3. *The Accuracy in XAFS Project* (D. C. Creagh, H. Oyanagi and R. Frahm). We have been involved in the development of standards and criteria for the performance, the data reduction and subsequent publication of the results from XAFS experiments. We have been concerned with the improvement of the status of XAFS research. The results of the first two Workshops which were concerned with the establishment of standards and criteria for XAFS research have been published [Lytle, Sayers & Stern (1989). *Physica (Utrecht)*, **B152**, 701–721; (1991). *X-ray Absorption Fine Structure*, edited by S. S. Hasnain, pp. 751–771. London: Ellis Horwood]. The third Workshop was concerned with the development of an International Short Course on XAFS. The instructional modules for this course are now being written. The section on X-ray optics has been written by D. C. Creagh. In addition, an XAFS data file has been set up in collaboration with the NNDC at Brookhaven, USA. It is anticipated that this data file will be as valuable to XAFS users as the JCPDS file has been to users of X-ray powder diffraction. Largely because of our involvement, the XAFS body has become a formal entity. It is now the International XAFS Society (IXS). Discussions with its President, D. Sayers, are proceeding to ascertain what kind of relationship might exist between the IUCr and the IXS.

4. *Evaluation of Two-Dimensional Detectors*. Some progress has been made on this project. Whether or not this project can proceed further depends on the response of IUCr members to papers on area detectors to be given in our Open Commission Meeting at the forthcoming Beijing Congress.

5. *The Absolute Structure Determination of Light-Atom Compounds* (L. Malakhova). Professor Malakhova has established that sufficient laboratories are interested in this project to make it viable. It has been decided to proceed with this project and funding for it has been requested in the next triennium.

6. *The High-Pressure Group Committee* (R. Nelmes). This Committee has organized two highly successful Workshops, the first at Daresbury in conjunction with the Synchrotron Radiation Instrumentation Conference (Chester, England, 1991) and the second in collaboration with the Commission on Powder Diffraction (Washington, USA, 1992). Its plans for its Microsymposium at the Beijing Congress are well advanced. The High-Pressure Group was formed from the remnants of the Commission on Crystallographic Studies at Controlled Pressures and Temperatures, which was disbanded at the Perth Congress. Since its formation, the group has been vigorous in its activities and has greatly expanded its membership. If its work continues to prosper the IUCr ought to consider reforming it as a High Pressure Commission.

The Commission is also considering the possibility of becoming involved in a project to measure X-ray wavelengths, which has been proposed by R. Deslattes (NIST). Crystallographers have long been aware of deficiencies in the tables of X-ray wavelengths printed in *International Tables for X-ray Crystallography* Volume III, which have been reprinted in *International Tables*

for *Crystallography* Volume C. The resolution in discrepancies in these tables is of great importance to all crystallographers.

10 April 1993

D. C. CREAGH, Chairman

(8) The organization and programme of an Open Meeting of the Commission with the title Crystallographic Computing for the Beijing Congress is being undertaken.

25 March 1993

H. D. FLACK, Chairman

#### *Commission on Crystallographic Computing*

In the present triennium, the Commission has been engaged in the following activities:

(1) Organization of the Microsymposium Trends in Crystallographic Computing at the Bordeaux Congress.

(2) Refereeing of the section Computer Program Abstracts in *J. Appl. Cryst.* Until July 1990 this work was undertaken by D. Viterbo and K. Watenpaugh. Currently it is carried out by A. Olson and G. Reck.

(3) The Veszprém School on Crystallographic Computing was held at Balatonfüred, Hungary, from 31 May to 6 June 1992. The School was attended by 85 participants from 20 countries. There were 20 invited lectures and about a dozen contributed posters. The School provided a balanced programme of lectures, tutorials in small groups and demonstrations of crystallographic computer programs on a plentiful array of modern computer equipment, both PCs and workstations. A noteworthy aspect of the work presented at the School was the presentation of systems using modern windowing techniques and object-oriented programming. The organization of the School was the work of two committees: (a) a Programme Committee comprised of H. D. Flack (Chair), F. H. Allen, H.-F. Fan, K. Huml, N. W. Isaacs, C. Kratky, A. J. Olson, L. Párkányi, G. Reck, H. Schenk, M. I. Sirota, I. Vicković, D. Viterbo and K. Watenpaugh and (b) a Local Organizing Committee comprised of K. Simon (Chair), Gy. Argay (Secretary), Zs. Böcskei, M. Czugler, G. Csonka, G. Náráy-Szabó, I. Sajó and G. Speier. M. Hanusz provided much technical help before and during the meeting.

(4) It has most unfortunately not been possible to organize a School on Crystallographic Computing to be held in the People's Republic of China in the summer of 1993 as a Satellite Meeting to the Beijing Congress. At each of the two choices of site, the local organization faced insurmountable difficulties. In the summer of 1992, the Chairman of the Commission, in consultation with the IUCr Executive Committee, decided to cancel the arrangements for this School.

(5) In conjunction with the European Crystallographic Committee, crystallographic news on conferences, meetings, IUCr circulars and journals has been installed since spring 1992 on the information server CONCISE of the RARE project COSINE. This server is available for consultation by e-mail, interactive session or file transfer. Connection details have been circulated by e-mail and by announcements in the *IUCr Newsletter*. Considerable experience has been gained in the use of such computerized information systems.

(6) Preliminary negotiations are under way to find a site for a School on Crystallographic Computing in the Asian area in 1994/1995. Likewise, early contacts have been made for a School to be held as a Satellite Meeting to IUCr XVII.

(7) The invited lectures and contributed posters of the Veszprém School have been prepared for publication in the IUCr series of Monographs published by Oxford University Press. The editorial work on this book was undertaken by H. D. Flack, L. Párkányi and K. Simon. M. Hanusz also participated actively in the editorial work necessary to prepare this book. At the time of writing, the manuscripts and figures have all been formatted and delivered to OUP.

#### *Commission on Crystallographic Data*

Much of the work of the Commission during the period 1990–93 has been concerned with the onward development of the crystallographic information file (CIF) and of its applications. The CIF provides a simple extensible format for the interchange of crystallographic data between individuals, journals and databases and provides a convenient archival mechanism. The CIF was adopted as the IUCr standard at the Bordeaux Congress in 1990. The work summarized below has been coordinated through the Commission on Crystallographic Data and the IUCr Working Party on Crystallographic Information, but has involved active collaboration with other Commissions (principally Journals and Computing), the IUCr Editorial Office in Chester, England, individual crystallographic program developers and the crystallographic database producers. Specific activities in this area have been:

(1) The publication of the CIF Core Dictionary in *Acta Cryst.* (1991), A47, 655–685.

(2) The development of procedures for the use of CIF for the submission of machine-readable manuscripts to *Acta Crystallographica*. CIFs prepared by the Editorial Office from hard-copy submissions are also processed through data check and evaluation software and automated typesetting procedures. These processes are summarized in *Acta Cryst.* (1993), C49, 418–424. CIFs are forwarded to the appropriate database for inclusion in their files.

(3) Extensions of the CIF Dictionary to cover powder diffraction data and macromolecular structures are due for completion by the time of the Beijing Congress.

(4) Crystallographic software developers have, in many cases, already added CIF generators to their systems. Software for the manipulation of CIFs is at an advanced stage.

(5) Discussions with the Chemical Structure Association and other interested bodies have led to a proposed integration of the Standard Molecular Data File within the STAR/CIF concept.

(6) Members of the Commission have been involved in the technical planning of the next *World Directory of Crystallographers*. This will be derived from a database created using the STAR concepts described by S. R. Hall in *J. Chem. Inf. Comput. Sci.* (1991), 31, 326–333.

(7) An independent technical committee for the maintenance of CIF standards has been established to oversee future developments and to provide up-to-date information on CIF-related software.

The Commission has organized two joint Open Meetings with the Commission on Journals at the Bordeaux and Beijing Congresses. It has also represented the data activities of the IUCr at the CODATA International Congress in Beijing in October 1992. The Commission has kept in close touch with crystallographic database activities and is pleased to record considerable activity in database development and in the software systems associated with these databases. Some 200 000 crystal structures are now recorded in the four structural databases.

19 February 1993

F. H. ALLEN, Chairman

### Commission on Crystallographic Nomenclature

The Commission conducted its work during the triennium either by letter or by fax, being able to make use of electronic mail only during the first and last days of the period. Membership of the Commission increased sharply following the Bordeaux General Assembly. All members are *ex officio* appointments as Editors of the IUCr journals, each volume of the *International Tables for Crystallography* and *Structure Reports*. In addition, the Chairs of the IUCr/OUP Book Series Committee and the Commission on Crystallographic Teaching are new appointments, resulting in a total strength of 11 members. Its principal activities have been carried out, as has been customary, by its Committees, Sub-committees and Working Groups.

The final Report of the IUCr *ad hoc* Committee on the Nomenclature of Symmetry, under the Chairmanship of P. M. de Wolff, was published in *Acta Cryst.* (1992), A48, 727–732. In addition to redefining printed symbols for symmetry elements, the Report recommends use of the letters *e* and *k* for certain glide planes that previously were without either a unique or a specific symbol.

The Sub-committee on the Nomenclature of *N*-Dimensional Crystallography, under the Chairmanship of A. J. C. Wilson and with membership as given in *Acta Cryst.* (1991), A47, 611, set up a Working Group with the limited task of comparing and evaluating the existing nomenclatures of crystal families, crystal systems and Bravais lattices in four dimensions followed by the presentation of a recommended nomenclature. The first task was completed early in the triennium. The Working Group, however, has not found it possible to resolve the differences between several widely divergent naming and notation proposals. Accordingly, the Commission is considering a temporary suspension of activity in this nomenclature area to allow fresh thought to develop in this growing crystallographic field.

A Working Group of the Commission, consisting of the Editors (V. Kopsky and D. B. Litvin) of Volume E of *International Tables for Crystallography*, has completed a Report entitled Nomenclature, Symbols and Classification of the Subperiodic Groups. The Commission accepted the final Report, which will be published in Volume E in due course, and agreed that an Abstract of the Report should be published in *Acta Cryst.* as a form of advance notice to the crystallographic community. Preprints of the Report are available from D. B. Litvin. The Report recommends symbols for the seven frieze groups, 80 rod groups, and 75 layer groups together with symmetry tables and a classification of the subperiodic groups.

The Commission is considering the establishment of a Working Group to examine the recently issued *ISO Guide to the Expression of Uncertainty in Measurement* for its possible impact on the nomenclature of statistical techniques used in crystallography and to be charged with making such recommendations as are appropriate.

15 February 1993

S. C. ABRAHAMS, Chairman

### Commission on Crystallographic Teaching

During the last three years, the Commission has concentrated on facilitating the IUCr Visiting Professorship Programme and reinitiating the Pamphlet Project.

#### Visiting Professorships

The Visiting Professorship Programme was initiated by C. H. L. Kennard of the University of Queensland, Brisbane, Australia, who gave a course at the Department of Chemistry, University of Peradeniya, Sri Lanka, 8–20 January 1991. 31

students took the basic course and nine graduate students took the advanced course on X-ray diffraction.

The second Visiting Professor was W. T. Robinson of the University of Canterbury, New Zealand, who gave a course in December 1992 at the Institute of Theoretical Chemistry, Jilin University, Changchun, People's Republic of China.

The third Visiting Professorship, also held by C. H. L. Kennard, was at the Technical University of Hanoi, Vietnam, 9–19 December 1992. This course had been delayed by visa problems that were finally resolved. The visit was successful and the organizers hope to arrange another such visit. Ten 90-minute lectures and five two-hour tutorials, together with detailed tutorial notes, were presented. Dr Kennard reports that there is a big gap in crystallography teaching in Hanoi, and hoped that books and computer software (for personal computers) would become available so that conditions could be improved. No diffraction equipment was in working order.

As a result of these three Professorships some further guidelines for future visits are being prepared.

A School on the Rietveld Method was held in conjunction with the XVI National Meeting of the Brazilian Association of Crystallography at the University of São Paulo, San Carlos, Brazil, 14–16 December 1992, and the Rietveld Summer School at the National University of La Plata, Argentina, 8–10 December 1992, immediately before the Brazil meeting. The IUCr sponsored and underwrote these Schools at which R. A. Young, A. K. Cheetham and R. B. Von Dreele were the Visiting Professors.

A 15-hour course was given as a Visiting Professorship by D. K. Smith on Geometrical Crystallography, 27 January–7 February 1993 at Ain Shams University, Cairo, Egypt. This course was given immediately after the Fourth International Workshop of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis, Aswan, Egypt, 16–26 January 1993, co-organized by the IUCr Commission on Powder Diffraction. In his role as Visiting Professor, Dr Smith also visited students and crystallographers at Asyut University (Aswan Branch), the Egyptian Geological Survey in Cairo, Cairo University, Military Technical College, Suez Canal University, Helwan University and the Egyptian Antiquities Museum. In each case he discussed techniques in powder diffraction.

#### Pamphlet Project

The Pamphlet Project has been reinstated and an arrangement has been made for Polycrystal Book Service to print and distribute the pamphlets. A set of *Notes for Authors* for pamphlets has been prepared and the IUCr technical editing staff will assist with technical editing when requested. The previous set of 19 pamphlets is still available from Polycrystal Book Service (PO Box 3439, Dayton, OH 4501, USA). Future pamphlets include:

20. *Crystals: a Handbook for School Teachers*. E. A. Wood. Permission has been obtained from the copyright owner for a reissue of this booklet as a pamphlet.

21. *Radiation Measurement and Protection in X-ray Laboratories*. H. von Philipsborn. Under review.

22. *Crystal Packing*. A. Gavezzotti. Under review.

23. *Gamma-ray Diffraction Study of Single Crystals*. A. Kurbakov. In preparation.

Several letters of invitation have been sent out, and several crystallographers have promised to write a new pamphlet.

#### International Schools

An Asian-Region Seminar on Crystallography in Molecular Biology is being planned for 9–14 December 1993 with S. Parthasarathy as the Convener and some members of this Commission on the Organizing Committee. This meeting has been

sponsored by the IUCr, which has also provided funds for young scientists to attend. Invitations to possible lecturers have been sent out and additional funds are being sought to support this meeting.

*Programmes at IUCr meetings*

A Microsymposium on Crystallographic Teaching: Practical Hints and New Concepts is planned for the Beijing Congress. At this time, the IUCr Visiting Professorship Programme and the Commission on Crystallographic Teaching Pamphlet Project will be described.

8 April 1993

J. P. GLUSKER, Chairman

*Commission on Electron Diffraction*

At the Bordeaux General Assembly in July 1990, the membership of the Commission was re-established to provide as broadly representative a group of members as possible after an unusually great number of mandatory retirements and resignations. A last-minute resignation of the member representing interests in LEED and allied surface analysis techniques required a special later election procedure and the position was filled by M. van Hove in 1991.

The proposal that the Commission should undertake the compilation of a multi-author book on electron diffraction techniques was initiated at the Perth Congress in 1987. After considerable discussion, this project was started in 1988 with a proposed deadline for submission of chapters in final form in 1989. After considerable modifications of the original plans, delays by some authors and expansions of the length and scope of some chapters, the final product is a set of two volumes published by Oxford University Press as part of the *IUCr Monographs on Crystallography* series. The first volume appeared late in 1992 and the second volume in early 1993. The main emphasis of the books is on the theory, experimental techniques and analytical methods for the determination of the structures of solids by use of high-energy electron diffraction. The principles and practice of electron microscopy are included only to the extent required for understanding the diffraction effects involved. Low-energy electron diffraction and related techniques for studying surface structure are not included, being well documented in other publications, and only one short chapter is devoted to gas electron diffraction. Otherwise, the coverage of electron diffraction techniques is made as complete as seemed reasonably possible.

Following a proposal made at the Bordeaux meeting of the Commission, plans were developed to hold Summer Schools on topics related to electron crystallography. The original intention was for two Schools, one in China and one in Europe, to allow easier access for a larger number of potential students. Because only the China School could receive support as a Satellite Meeting of the IUCr Congress in 1993, the plan for a European School was deferred. The Summer School on 'Electron Crystallography – Theory and Practice' will be held in Beijing, during the week immediately preceding the Congress. An international panel of instructors will lead discussions on the use of high-energy electrons to determine structures of gases, amorphous solids, thin crystals of biological, organic and inorganic materials and to determine accurate values for structure factors using dynamical diffraction methods.

A survey of the computer programs being used for the calculation of intensities for high-resolution electron micrographs of crystals and electron diffraction patterns has been initiated and is being coordinated by D. van Dyck, Antwerp. A proposal for

sets of calculations to be made as a basis for comparisons of accuracies has been circulated. It is anticipated that the results of the survey will be submitted for publication.

The Commission has been active in preparing proposals to the Programme Committee of the Beijing Congress for special talks and Symposia dealing with electron diffraction and related areas of crystallography.

10 February 1993

J. M. COWLEY, Chairman

*Commission on Neutron Diffraction*

Many of the Commission's activities are continuing ones, and often informal, involving communication of information, encouraging exchanges, involvement of members in organizing meetings *etc.* It was particularly pleasing to see publication in 1992 of Volume C of the new *International Tables*, which includes a wealth of pertinent information for neutron scatterers. Many of our colleagues contributed, but the efforts of B. T. M. Willis are particularly noted here. As another example, members of our Commission and of that on Powder Diffraction have helped to organize IAEA Training Courses in China and Grenoble. These courses promote the use of neutrons, *e.g.* for materials development and characterization, particularly in countries new to neutron beam research. They bring together scientists needing to use neutron beams and experienced lecturers for both in-depth course work and hands-on experience in running experiments. Typical techniques are powder diffraction, small-angle neutron scattering, and radiography. The IAEA will propose further courses where required.

The recently established *IUCr Newsletter* promises to be one of the main channels for crystallographers to exchange information about meetings, international cooperation, IUCr and Commission activities, and projects of an explicitly scientific nature. Many of these goals are shared with the Commission, which will make full use of the new *Newsletter*. Also, the Commission will continue to promote *Neutron News*, edited by G. Lander (with J. Axe and Commission member Y. Endoh), in every possible way. Since 1990, it has been a powerful means of communication among all neutron scatterers – not only diffractionists – and this wide readership is a source of strength to the neutron diffraction community. This role will remain, and it will be enhanced further by the recent inclusion within *Neutron News* of the new *Journal of Neutron Research*. The dynamism of *Neutron News* was earlier shown once again, with publication in Vol. 3, No. 3 (1992) of not only the Koester, Rauch and Seymann table of experimental values of neutron scattering lengths as a handy wall chart, but also of the latest V. F. Sears rationalized values of neutron scattering lengths and cross sections. The Commission on Neutron Diffraction thanks the *Neutron News* editors, staff and sponsors and those submitting contributions for their efforts. Again, we urge scientists to see that their library buys a copy, to ensure its continued existence. The Commission's own neutron newsletter was voluntarily discontinued when *Neutron News* started, and the Commission Chairman regularly writes a Chairman's contribution for *Neutron News*.

The next edition of the *World Directory of Crystallographers* is in preparation – the last dates from 1990 – and for the first time it will be prepared from a database maintained at the IUCr office in Chester. It is already possible to obtain by e-mail from Chester a template file for preparing your own entry – for submission to your national Sub-editor – and a list of national Sub-editors! It is important to note that the *Directory* is open to anybody working in crystallography and related topics. See the *IUCr*

*Newsletter*, Vol. 1, No. 1 and *Acta Cryst.* (1993), A49, 222–225 for details. All those using neutron diffraction, even occasionally, are urged to see that they are entered into the database, as this will help the Commission to fulfil its role. Eventually, the IUCr database should replace other less well maintained databases as the primary source for address lists for special interest groups, conference organizers, seekers of technical information *etc.*

As the mandate of the present Commission nears its end, its attention turns increasingly to the Beijing Congress and General Assembly, 21–29 August 1993. The previous scientifically very successful IUCr Congress was at Bordeaux, France, in 1990. With two parallel Main Lectures, some six parallel Microsymposia and daily poster sessions, the Beijing Congress will be a source of scientific stimulation and international contacts for all participants, as well as providing an overview of the state of the science of diffraction

The Commission proposed a number of Microsymposia for the Beijing Congress, as well as a list of suggested Plenary Lecturers. We thank those inside and outside the Commission who helped us in the preliminary stages by contacting potential contributors. The severe selection from the very large number of propositions meant that not all of our suggestions were accepted, but it was pleasing to see that the subjects chosen emphasized the complementarity of neutron scattering with other techniques. Thus there will be Main Lectures by R. K. Thomas on reflectometry and by W. I. F. David on fullerenes, and Microsymposia on magnetic scattering, on X-ray and neutron powder diffraction, and on thin-film structures. There will also be an Open Commission Meeting of the Commission on Neutron Diffraction devoted to the complementarity of neutron sources. And, of course, many of the other sessions will have contributions involving neutrons: area detectors, superconducting materials *etc.* Overall, these contributions will again demonstrate the leading role played by neutron scatterers in important areas of physics, chemistry, biology, materials science, instrumentation, computing... while at the same time emphasizing that neutrons should be used chiefly where their special features give unique information.

Before and after the main Congress, there will be five IUCr-sponsored Satellite Meetings at various sites in China, including one on neutron scattering. The Satellite Meetings complement the main IUCr Congress, and provide an opportunity for in-depth discussions. The Neutron Scattering Satellite Meeting (NSS-93) will be held at Beidaihe, about 300 km to the east of Beijing, 17–19 August 1993. Commission members are part of the International Programme Committee, and open access and balance in setting up the programme are guaranteed. Following on from the highly successful meeting at Alpe d'Huez after the Bordeaux Congress, the broad theme is the complementarity of reactor and spallation neutron scattering techniques with other techniques, especially diffraction with synchrotron and laboratory X-ray sources. As well as considering the state of development of neutron sources and instrumentation, there will be adequate time to review neutron experiments with applications in materials and engineering science, physics, and chemistry of small and large molecules. Although some areas of neutron scattering are feasible only at the highest flux sources, a surprisingly large range of science can be carried out at low- or medium-flux reactors by taking advantage of new technology and by good design. Discussion of such science is an integral part of the Satellite Meeting, as it is hoped that many participants will come from countries where neutron scattering is in its early youth. The special session on reflectometry at Beidaihe should enable neutron and X-ray specialists of this technique to demonstrate the progress made in the last three years, both in

the number of instruments available and in new results obtained. Again this session is designed to complement those at the Beijing Congress.

Every three years the membership of IUCr Commissions is modified, at the time of the IUCr Congress and General Assembly. This is also an appropriate time, for anyone who wishes to do so, to suggest new directions or new projects or simply to offer constructive remarks about the work of the Commission. This can be done through any Commission member. Finally, if agreed formally by the Beijing IUCr General Assembly, our Commission will in future be called the Commission on Neutron Scattering, to emphasize the fact that neutron diffraction flourishes by contact with scientists working with neutrons in related areas such as small-angle scattering, reflectometry, interferometry, optics, magnetism and dynamics.

7 April 1993

S. A. MASON, Chairman

#### *Commission on Powder Diffraction*

During the triennium, the CPD was actively involved in various projects, meetings and Workshops/Schools and in planning for future ones.

#### *Publications*

The CPD project to produce a book on the subject came to fruition with the publication of *The Rietveld Method* in early 1993 by the Oxford University Press as No. 5 in the series *IUCr Monographs on Crystallography*.

The Proceedings of the International Conference on Accuracy in Powder Diffraction II (see below), held 26–29 May 1992, were published as *NIST Special Publication No. 846* at the end of 1992. The editors, E. Prince and J. K. Stalick, are due special congratulations and appreciation for getting the Proceedings out in good form and substance in such a remarkably short time.

The results of the first phase of the Rietveld Refinement Round Robin (RRRR) were published: Hill (1992). *J. Appl. Cryst.* **25**, 589–611.

The project of establishing a Program Information Exchange Bank on computer programs for powder diffraction data analysis has been conducted by D. K. Smith, Consultant to the CPD. The first phase of this project came to fruition with the publication of a categorized and annotated list of more than 280 programs, with informative discussion of each category, in *J. Appl. Cryst.* (1991), **24**, 369–402, authored by D. K. Smith and S. Gorter and reviewed before publication by the entire CPD membership.

The intended two-per-year schedule for producing *CPD Newsletters* was kept: Nos. 4 and 5 were published in 1990, 6 and 7 in 1991, and 8 and 9 in 1992. More than 1000 copies of each of the later issues were distributed. A conscious effort to increase the *Newsletter* mailing list of interested persons has met with some success. A check of the mailing list against the current *World Directory of Crystallographers* (WDC) verified that our *Newsletters* reach a community not well represented in mainline crystallography: approximately one half of the names on our mailing list are not in the current WDC.

#### *Meetings/Workshops/Schools*

A Satellite Meeting on Powder Diffraction, originated by the CPD, took place in Toulouse on 16–19 July 1991. The Programme Committee was chaired by D. Louër (Rennes) and the Organizing Committee by J. Galy (Toulouse). That these Committees did outstanding jobs was attested by the facts that there were 255 scientific registrants and that enthusiasm remained high throughout the meeting. The scientific sessions

were held in an air-conditioned auditorium at the Paul Sabatier University (Université de Toulouse II) and the large lobby area (also air-conditioned) just outside it was filled mainly with posters but also provided 'coffee', social, and registration areas. The social events included a reception at City Hall in the lush 'Salle Illustré', a laboratory visit and reception with free-flowing liquids at Dr Galy's Centre d'Optique Electronique, and a chartered bus ride to Bordeaux marked by camaraderie and a box lunch.

At the Bordeaux Congress, two of the Microsymposia were engendered by the CPD, those on Advances in Structure Determination from Powder Diffraction Data (A. K. Cheetham and D. Louër) and on Powder Diffraction Studies of Fibrous, Polymeric and Similarly Imperfectly Ordered Materials (K. H. Gardner, D. Tchoubar and R. A. Young). Both session topics attracted a number of posters and a substantial and very interested audience.

The CPD also participated in the trial of a new feature for the International Congresses of Crystallography: Discussion sessions organized 'on-the-spot', or nearly so, in each of which the topic is to be the posters associated with one or two particular Microsymposia. Such a discussion session on the posters associated with the above-mentioned Microsymposia was organized, on behalf of the CPD, and moderated by R. J. Hill. The vigour of the discussions indicated that this new feature might well become a standard feature of our Congresses.

A major inter-Congress meeting was held 26–29 May 1992 at the National Institute of Standards and Technology in Gaithersburg, MD, USA, with the title Accuracy in Powder Diffraction II (APD-II). There were 175 registered participants from 18 countries. The meeting was organized by the CPD and was sponsored by the ICDD, the IUCr and NIST. Generous financial support for speakers and young scientists was received from the ICDD and the IUCr, respectively. Excellent local arrangements were made under the Co-chairmanship of E. Prince and J. Stalick of NIST. The Programme Chairman was R. J. Hill (Australia), who is also Secretary of the CPD. The participants seemed to be very satisfied with the meeting.

Four three-day Rietveld Summer Schools were organized by the CPD during the triennium: August 1990 and 1992 at the Silesian University in Cieszyn, Poland, with Z. Bojarski as head of the local organizing group; 8–10 December 1992 at the National University in La Plata, Argentina, with G. Punte leading the local organizing group; and 14–16 December 1992 at the University of São Paulo at São Paulo, with Y. Mascarenhas and L. Amaral in charge of the local organization. The Schools featured hands-on practice on PC-type computers. Student attendance ranged from 30 to 58 and was limited primarily by the number of computers available. For the two Schools in Poland, financial support was provided by the IUCr for the travel of the main lecturers (A. K. Cheetham, R. B. Von Dreele and R. A. Young) and for registration and living-costs grants for 20 students from various European countries. The December Schools received financial sponsorship from CONICET (Argentina) and CNPQ (Brazil). The full travel expenses of the three lecturers from the northern hemisphere were funded by the Cooperative Science programs that the US NSF has with CONICET and CNPQ. The Schools were also sponsored in name and underwritten by the IUCr through its Visiting Professorship Programme and Commission on Crystallographic Teaching. Although in the end no IUCr money was used, the IUCr's underwriting was crucial; the Schools could not have been held without it. The reason is that the NSF funding, welcome though it was, did not actually come through until after all plans and local arrangements, including local financial commitments, had been made, travel tickets had

been bought and one of the lecturers had already boarded his plane.

The CPD co-organized the International Workshop of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis held in Aswan, Egypt, 16–26 January 1993. Three CPD members served on the Programme Committee, one as Chairman. Funding to bring in all the needed topic-organizing Chairmen fell short. Much appreciated was the fact that the IUCr's Visiting Professorship Programme provided travel funds for D. K. Smith to give an intensive five-day course on Mineralogical Crystallography at Ain Shams University in Cairo after the Workshop. That made it possible for him to organize and conduct one of the most important teaching sections of the Workshop, that on quantitative phase analysis by diffraction means. Also placed on the teaching programme were F. R. Ahmed (NRC, Ottawa), A. Authier (IUCr President, Paris), S. Gorter (Delft), R. Jenkins (ICDD), S. E. Rasmussen (Aarhus), J. Schneider (Munich), H. Toraya (Nagoya), G. Will (Bonn), A. Wright (Reading) and CPD members J. I. Langford and D. Louër, who also served on the Programme Committee.

The Satellite Meeting on Powder Diffraction to be held in Hangzhou, China, 31 August–3 September 1993 was initiated and is being co-organized by the CPD. The Programme Committee, under the able Chairmanship of CPD member J. I. Langford, did most of its work during this reporting period. In response to a request from the CPD, the ICDD has allocated US \$5000 in support of this meeting.

#### *Other Projects*

A Task Group on Crystallite Size and Microstrain Determination has been set up jointly with the ICDD. J. Fiala (CPD) and R. L. Snyder (ICDD) are the Co-chairs. The first focus is to be a round robin, which will illuminate the current methodologies and data-interpretation models used by the participants, including strengths and weaknesses of the methods and models.

The CIF/STAR format, previously recommended by the CPD to be extended for use with powder data, has now been accepted by the ICDD. J. I. Langford chairs the CPD's development efforts and coordinates with B. Toby who chairs the ICDD's.

Phase two of the Round Robin on Rietveld Refinement is nearing completion. In mid-1993, the results will be submitted for publication in the *Journal of Applied Crystallography*. This large project is being coordinated by R. J. Hill (CPD Secretary). It is an intercomparison of 41 X-ray and neutron powder diffraction sets collected on a standard sample of monoclinic zirconia using 31 different instruments in 18 countries. The results should prove to be even more interesting than those arising from Part I of the project. Dr Hill is scheduled to present a short summary of them at the 1993 Satellite Meeting on Powder Diffraction in Hangzhou.

The ICDD's Hanawalt Award was presented to CPD member D. Louër during the opening ceremonies of the EPDIC-2 meeting in Enschede, The Netherlands. It is given for excellence in the field of powder diffraction.

23 April 1993

R. A. YOUNG, Chairman

#### *Commission on Small Molecules*

During the past triennium, the principal activity of the Commission on Small Molecules has been the organization, planning and execution of International Symposia on topics appropriate to the Commission.

A well balanced programme of sessions and poster presentations of interest to small-molecule crystallographers was scheduled for almost every day of the Bordeaux Congress in 1990. There were stimulating discussion sessions based upon the Microsymposia. The Microsymposia were attended by 150–200 people and the discussion sessions drew 75–125.

International Symposia organized during the triennium with assistance from the Commission included the following. Computational Methods in Chemical Design – Molecular Modeling – Theory and Experiment, the third in the series of meetings held in Schloss Elmau, 15–20 October 1990, brought together theoreticians and experimentalists. The unifying theme was structural chemistry. Experimental topics included X-ray crystallography, NMR spectroscopy and piezomodulation spectroscopy. Theoretical topics ranged from *ab initio* calculations to molecular dynamics. The meeting was attended by nearly 200 participants including a number of young scientists.

The Eighth Crystal Chemistry Symposium organized by R. Boese, J. Garbarczyk, Z. Kaluski and D. Jones was held in Rydzyna, Poland, 26–30 July 1992. Topics of the meeting included crystal engineering and the design of crystals with specific properties, information on crystal chemistry derived from databases and low-temperature crystal chemistry. A report from the meeting appeared in the first issue of the *IUCr Newsletter*.

A Satellite Symposium on Molecular Structure will be held in Fuzhou, China, 30 August–1 September 1993 immediately following the Beijing Congress. Details of the programme, which includes four main topics (Systematic Analysis of Molecular Geometry, Conformation and Thermal Motion; Molecular Interaction and Recognition in Crystals; Structure and Activity of Biological Molecules; and Phase Relation and Transformation in Some Small Moiety Systems), were included in the first issue of the *IUCr Newsletter*. The International Programme Committee is composed of J. A. K. Howard, W. L. Duax, H. Bürgi, M. F. Mackay, G. Gilli, L. Nassimbeni, S.-x. Liu and J.-l. Huang.

To date, the CSM proposal of International Cooperation in Intensity Data Collection has been responsible for the collection of intensity data on 35 structures. In most of these cases, structures have been solved and manuscripts are published, in press, or in preparation. An article concerning the project will appear in a forthcoming issue of the *IUCr Newsletter*.

17 May 1993

W. L. DUAX, Chairman

#### Commission on Synchrotron Radiation

The field of synchrotron radiation and its applications in crystallography in the last three years has seen further dramatic growth. This is due, of course, to the immense utility of these intense, polychromatic and collimated X-ray sources.

At the Bordeaux Congress, synchrotron radiation (SR) figured prominently and likewise in the plans for the Beijing Congress. Additionally at Beijing there is to be a Satellite Meeting on Applications of Synchrotron Radiation in Crystallography. The Commission has been actively involved in planning these conferences. Additionally, there have been Satellite Meetings of both ECM-13, held on Synchrotron Radiation in Crystallography in 1991 in Trieste, and of the Synchrotron Radiation Instrumentation (SRI) World Congress, in Manchester also in 1991. Most recently, a Workshop has been organized and held in Rome in May 1993 on CCD detectors in macromolecular crystallography to help the growth of the detector development match that of source development.

To meet the need to set standards in the field and allow comparisons between sources, global instrumentation surveys have been commissioned. The first of these, on macromolecular crystallography, was published in *Synchrotron Radiation News* in 1992. Other surveys are in preparation for EXAFS, materials science diffraction and fibre diffraction.

A proposal for a *Journal of Synchrotron Radiation* has been made to the IUCr. The Commission has had a major input to the deliberations on this. Open discussions were held at a variety of conferences, both national and international, in Europe, the USA and Japan. Representative organizations and the Directors of Synchrotron Radiation Laboratories have also been contacted.

Various representative organizations have grown up in recent years. These include BioSync in the USA, the European Synchrotron Radiation Society and the Japanese Synchrotron Radiation Society. Contact has been maintained with each. The Commission has also provided detailed technical input to an important review/policy document prepared by BioSync planning the provision and growth of SR instruments and facilities for biological synchrotron-radiation research in the USA in the next decade.

1992 has seen the commissioning of the first of the next generation of high-brilliance high-energy synchrotron-radiation sources, namely the European Synchrotron Radiation Facility (ESRF) in Grenoble. This is indeed a milestone for the field of synchrotron radiation.

10 May 1993

J. R. HELLIWELL, Chairman

#### Ad interim Commission on Aperiodic Crystals

The IUCr Executive Committee approved in April 1991 the establishment of the Commission on an *ad interim* basis with the following membership: J. M. Pérez-Mato (Chairman), G. Chapuis, M. Farkas-Jahnke, M. L. Senechal and W. Steurer. This Commission substituted as a new start the earlier *ad interim* Commission on Modulated Structures, Polytypes and Quasicrystals. The Commission first elaborated its terms of reference, which were published in *Acta Cryst.* (1992), A48, 928.

During these years, the Commission has actively supported the organization of two meetings: an International Workshop on Methods of Structural Analysis of Modulated Structures and Quasicrystals (Lekeitio, Spain, 1991), which focused on structure determination of both incommensurate structures and quasicrystals, and an International Conference on Modulated Structures, Polytypes and Quasicrystals (MOSPOQ 91) which took place in Balatonszékplak, Hungary, also in 1991. In 1992, the 4th International Conference on Quasicrystals, celebrated in St Louis, USA, was also sponsored by the IUCr, under the recommendation of this Commission. For the Beijing Congress in August 1993, the Commission devised the programme of the session on Quasicrystals and Incommensurate Crystal Structures.

After consulting other experts, the Commission has elaborated a set of guidelines for the contents to be included in structural reports of incommensurately modulated structures. This checklist has been presented to the IUCr Executive Committee for its approval and publication in *Acta Crystallographica*. The list is a set of recommendations to be considered by journal editors and authors as a substitute for the usual checklist considered in the case of normal crystals. The elaboration of a similar list for incommensurate composite structures has been postponed until, within this subfield, some standards become commonly accepted.

At the ACA meeting in Pittsburgh in 1992, some members of the Commission ascertained the feeling of many people involved

in the field that, at present, the adoption by the IUCr of a standard nomenclature for higher-dimensional space groups is premature. Sharing this opinion, the Commission sent a formal letter in this sense to the Sub-committee on the Nomenclature of *N*-Dimensional Crystallography of the IUCr Commission on Crystallographic Nomenclature.

Finally, according to its terms of reference, the Commission is organizing the next International Conference on Aperiodic Crystals for 18–22 September 1994, at Les Diablerets, close to Lausanne, Switzerland. Its first announcement has already been distributed. This type of conference will continue on a triennial basis and substitutes the former MOSPOQ meetings.

5 May 1993

J. M. PÉREZ-MATO, Chairman

### Appendix E: Report of Director of Archiving and Crystallographic Information

#### *Submission of CIF manuscripts to Acta Crystallographica Section C*

The recommendations from the report of the 1987–90 Working Party on Crystallographic Information for submitting structural papers in CIF format were implemented early in the triennium. The CIF format was adopted as standard for data input to crystallographic checking procedures undertaken at the Chester office. Checking software kindly provided *gratis* by the authors was implemented in a manuscript processing system in which structural data are checked before a paper is sent for consideration by a Co-editor. That system, developed by Brian McMahon, provides feedback to authors and reduces the loading on the Co-editors. What is more desirable, of course, is for authors to implement checking procedures on CIF manuscripts before submission.

Manuscripts in CIF format are flowing to *Acta Cryst. Section C* at a satisfactory rate. The intention now is to increase that flow towards the ultimate objective of having all *Section C* manuscripts submitted in that format. Perhaps the most serious obstacle is handling of structural diagrams. New high-capacity communication networks have the potential to handle the large data volumes required for graphics files in PostScript format, but other options will also be considered.

#### *CIF submission and data checking by other journals*

Possible implementation of CIF submission and standardized checking for other journals published by learned societies is being investigated. The desirability of achieving standards comparable with those in the IUCr journals is generally accepted, but there are practical difficulties related to the cost of achieving the standards desired. Access to personnel capable of monitoring the standard checks is a problem for some societies. Negotiations are continuing, with a view to finding practical methods of achieving higher accuracy in published crystallographic results.

#### *STAR/CIF development*

Extension of the STAR file concept from small-molecule structures to other crystallographic applications is continuing. The powder diffraction equivalent is essentially complete, and the protein structure version is at an advanced stage of development.

Potentially, the STAR file concept has many scientific and technological applications, and it would help crystallographers if the STAR structure were adopted as a standard or *de facto*

standard in areas close to crystallography. The histories of computer languages such as Fortran, and the Unix operating system, show how difficult it is to retain standardization in protocols that are widely utilized.

The approach taken with STAR is to encourage applications related to crystallography, under conditions that ensure that the benefits of standardization are retained.

#### *World Directory of Crystallographers*

The editor of the Ninth Edition of the *Directory*, Y. Epelboin, is directing compilation of data in a form that provides the option to assemble the directory as a database in STAR format. This would permit the *Directory* information to be updated dynamically. The technical requirements are not unduly onerous. Matters to be resolved relate to providing the desired degree of privacy to those listed in the database. One possibility is to provide potential users with access to the database at priority levels appropriate to the application. The policy questions involved will be referred to the IUCr Executive Committee.

#### *Future developments*

As electronic publication of research results and standards information gathers momentum, its impact on IUCr publishing operations will increase. For the time being, the costs are a minor perturbation to the IUCr budget, but that situation may change rapidly.

Many developments in electronic publishing, such as the preparation of CIF dictionaries, are labour intensive. Adapting to electronic publishing is taxing the capacity of those currently working on this task. That effort should be expanded to cope with:

- (i) CIF/STAR extensions;
- (ii) submission of structural diagrams by e-mail;
- (iii) improved input of general articles submitted in electronic form;
- (iv) providing access to stored CIF files in Chester;
- (v) providing access to IUCr journals in electronic form;
- (vi) relating crystallographic data storage to that of other scientific information.

In addition to the technical aspects of these developments, the financial and geopolitical implications for the IUCr must be assessed. This is complicated by the legal framework within which the IUCr operates in Switzerland and in the UK. Coordination to ensure that groups concerned with different types of publication within the IUCr are not working at cross purposes is necessary. The IUCr will require assistance from a group of people with a wide range of expertise in the coming decade.

7 April 1993

E. N. Maslen, Director of Archiving and Crystallographic Information

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

#### *American Crystallographic Association (ACA)*

In its first triennium as a Regional Associate, the ACA revised the By-Laws of the organization to formally recognize its new responsibility for representing crystallographers from the United States and from Canada. During the triennium, the ACA held three annual meetings. These meetings were characterized by large attendance and innovative new sessions and Schools. The

1991 meeting was held in Toledo, Ohio, with 800 participants and over 450 abstracts. The Martin Buerger Award was presented to J. Dunitz of the ETH-Zentrum, Zürich, Switzerland, and the B. E. Warren Diffraction Award was presented to J. Jorgensen of Argonne National Laboratory, Illinois. A protein crystallization Workshop attracted over 220 attendees prior to the start of the meeting. The 1992 meeting was held in Pittsburgh, Pennsylvania, in conjunction with the 50th Pittsburgh Diffraction Conference. The ACA's Fankuchen Memorial Award was presented to D. Caspar of Brandeis University, Massachusetts, and the Pittsburgh Diffraction Society's Sidhu Award was presented to R. Stevens of Harvard University. The 1993 ACA meeting was held in May in Albuquerque, New Mexico. The Patterson Award was presented to G. Sheldrick, University of Göttingen, Germany.

The ACA has developed two initiatives to promote the field of crystallography: a Summer School and a special programme at conferences for young scientists. The Pittsburgh ACA meeting was preceded by a Summer School for Crystallography which provided formal and practical training for 32 students over a 10-day period; during the School, data were collected for 24 structures, 20 of which were solved and refined during the School. This Summer School was so successful it was repeated in 1993. To welcome young crystallographers at their annual meetings, the ACA has a programme for young scientists with a faculty advisor. Programme highlights include special pre-meeting mixers and a formal mentoring programme. The ACA also presents the Pauling Award to the best student work presented at each meeting.

Serving on the ACA Council for the period were: J. Flippen-Anderson (1991–1992, President 1991), K. Watenpaugh (1991–1993, President 1992), R. E. Marsh (1992–1993, President 1993), E. T. Adman (Vice-President 1993), D. Duchamp (Past-President 1991), V. Cody (Secretary 1991–1993), S. N. Rao (Treasurer 1991–1993), I. D. Brown (Canadian Representative 1991–1993).

10 May 1993

P. W. CODDING, Representative

#### *Asian Crystallographic Association (AsCA)*

The AsCA Executive for the 1990–93 triennium is as follows: President: N. Kasai (Japan); Vice-President: Fang-ming Miao (China); Secretary–Treasurer: Yu Wang (Taiwan). The main event of AsCA activities in 1992 was the Inaugural Conference of the Asian Crystallographic Association, AsCA '92, which was held at the Regional English Language Centre (RELC), Singapore, 14–16 November 1992. A. Authier, President of the IUCr, and H. H. Huang, Deputy Vice-Chancellor, National University of Singapore, accepted an invitation and attended the opening ceremony of AsCA '92. The total registration was 320 with 260 full participants and 60 students, excluding 30 accompanied persons. This was 60% more participants than initially estimated. Several difficulties which were encountered due to the unexpectedly large attendance (the ideal capacity of the venue was 250–275) were solved by the kind cooperation of the executive members of the Organizing Committee with the staff at the RELC. The scientific programme consisted of 16 oral sessions with 73 papers and 22 poster topics with 190 papers.

A Committee of the Crystallographic Society of Japan, CrSJ, distributed the Japanese Young Scientists Funds, contributed from 29 enterprises, to 26 young scientists and an independent Committee in Australia also distributed funds from the Society of Crystallographers in Australia, SCA, to 15 applicants, so that no Japanese or Australian applications were considered for the IUCr grant of US \$7500 towards assistance for young scientists.

The success of AsCA '92 was a tribute to the organizers, to the sponsors and to the participants, but it is noted that the success is partly due to the fact that the SCA and CrSJ decided to hold their joint annual meetings under the auspices of the AsCA in order to promote the Inaugural Conference of the AsCA.

Several newsletters of the AsCA have been published in the triennium.

14 May 1993

J. HARADA, Representative

#### *European Crystallographic Committee (ECC)*

The IUCr Representative attended the meetings of the ECC held in July 1990 during the Bordeaux Congress, in August 1991 during ECM-13 in Trieste, Italy (moved from Ljubljana as a consequence of the civil war in the former Yugoslavia) and in August 1992 during ECM-14 in Enschede, The Netherlands. During these meetings he participated in the discussions of various topics giving, in particular, information about the work and decisions of the Executive Committee concerning the European Crystallographic Committee. In both Trieste and Enschede, he represented the President and the Executive Committee, who had been unable to attend these ECMs.

During the Trieste meeting, Albania and Turkey obtained observer status. The united Germany was already represented by one delegate from the united German National Committee. The proposal of the Swedish National Committee to form a European Crystallographic Association brought a lively discussion. The lengthy debate upon this important question was finally adjourned until the next meeting. The meeting received reports on the next European Crystallographic Meetings: ECM-14, Enschede, The Netherlands, 1992; ECM-15, Dresden (instead of Leipzig), 1994; and accepted an invitation from the University of Lund, Sweden, concerning ECM-16, 1995.

In Enschede, first the membership status of the new independent European countries was reviewed. Prior to this, the membership of ex-USSR and ex-Yugoslavia in the ECC was cancelled. After the presentation of their accreditations, Latvia, Croatia, Slovenia and Ukraine were admitted by voting as members of the ECC. During this meeting, the membership of Russia, Moldavia and Estonia, for various reasons, could not be approved. Reports were received on the organization of ECM-15 (28 August–2 September 1994) and ECM-16 (1995) and oral invitations were received from Egypt (Cairo) and Portugal (Lisbon) for 1997. The written invitation from Prague (now the Czech Republic) did not specify the date of the proposed meeting. The formation of an ECA, owing to the unstable political situation in Europe, was adjourned again to the next ECM in 1994.

The ECC officers for 1990–1993 are: Chairman: K. Huml (Czechoslovakia); Vice-Chairman: H. Fuess (Germany); Secretary: H. Flack (Switzerland). According to an unusual but joint decision of the ECC officers, no ECC meeting will be held in Beijing during the IUCr Congress and General Assembly in 1993. Consequently, the new officers will be elected only in Dresden in 1994.

5 May 1993

A. KÁLMÁN

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

The main activities of the IOCG during the triennium have been in the organization of the 10th International Conference on Crystal Growth (ICCG-10) and the 8th International Summer School on Crystal Growth (ISSCG-8) held, respectively, in San

Diego and Palm Springs, California, USA. Both events were hosted by the American Association of Crystal Growth (AACG), who provided a Conference and a Summer School of the highest quality.

ICCG-10 was held 16–21 August 1992 and was attended by 641 delegates, less than in the previous meeting in Japan in 1989. The delegates were from 33 countries and, for the statistics, 264 delegates were from the USA, 138 from Japan, 41 from Germany and more than 20 delegates only from China, CIS and the UK. As to topics, out of 32 sections, nine were devoted to semiconductors (80 communications), three to superconductors (26 communications), three to non-linear-optics materials (25 communications) and the others concerned various materials including biomaterials and solution-grown industrial crystals. The proceedings of ICCG-10 will be published as a special edition of the *Journal of Crystal Growth*.

ISSCG-8, held 9–15 August 1992, was well attended by about 150 participants, with an increase of about 20% with respect to the previous meeting in Japan. The School provided a high-level programme of lectures that covered a wide range of topics. The proceedings of the School will be published.

During ICCG-10 in San Diego, the IOCG dealt with its major business matters in meetings of the Executive Committee, Council and General Assembly. The IOCG Executive Council has been renovated for the coming triennium 1992–95. The slate of officials elected by the Council and formally approved by the General Assembly is the following: President: B. Cockayne (UK); Vice-Presidents: T. Nishinaga (Japan) and R. F. Sekerka (USA); Secretary: M. Schieber (Israel); Treasurer: E. Kaldis (Switzerland); Past President: R. Kern (France). Executive Committee: K. W. Benz (Germany), A. A. Chernov (CIS), R. Feigelson (USA), D. T. J. Hurle (UK), P. Ramasamy (India), R. Rodriguez-Clemente (Spain), G. M. van Rosmalen (The Netherlands), I. Sunagawa (Japan). *Ex officio* members: W. Bonner (USA), J. F. Wenkus (USA), C. F. Woensdregt (The Netherlands), P. Dauday (The Netherlands), R. A. Laudise (USA), V. V. Osiko (CIS), Representative to the IUCr, C. Paorici (Italy), Representative of the IUCr.

During the General Assembly in San Diego, it was decided that ICCG-11 and ISSCG-9 will be sequentially held in The Netherlands, the former in The Hague 18–23 June 1995 whilst the venue of the latter (to be held 11–16 June) has yet to be confirmed. The National Associations to be responsible for ICCG-12 and ISSCG-10, scheduled for 1998, have also been approved. ICCG-12 will be organized in Israel by the Israeli Association for Crystal Growth (IsACG) and ISSCG-10 by the Italian Association for Crystal Growth (IACG). Precise venues and dates will be a matter for future decision. During ICCG-10, the IOCG Frank and Laudise Prizes were also awarded. The Frank Prize was awarded to R. F. Sekerka (USA) for seminal contributions to the theory of crystal growth, whilst the Laudise Prize was awarded jointly to V. V. Osiko (CIS) and J. F. Wenkus (USA) for the understanding and development of techniques for growing large quantities of high-quality refractory crystals.

A last point worth mentioning is that for the first time the IOCG has made a compilation of the current membership numbers within the constituent national organizations. They are, for each country, as follows: CIS (CISSCG, 700), France (GFCC, 285), Germany (DGKK, 514), Hungary (HNCCG, 40), India (IACG, 200), Israel (IsACG, 180), Italy (IACG, 107), Japan (JACG, 680), Korea (KACG, 330), The Netherlands (KKN, 160), Poland (PSCG, 40), Spain (SGCC, 70), Switzerland (SKM, 250), UK (BACG, 350), USA (AACG, 750).

6 May 1993

C. PAORICI, Representative

### *International Centre for Diffraction Data (ICDD)*

The ICDD is the new name for what used to be known as the JCPDS. In my capacity as IUCr Representative to the ICDD, during the triennium I attended several of their semi-annual meetings and two special meetings of ICDD with IUCr representatives.

The ICDD is chartered as a not-for-profit organization. Its purpose can be described as to gather, cull, edit, and disseminate useful diffraction data, mostly powder data useful for crystalline phase identification, in the international arena. It is a substantial organization with a paid staff of more than 25 persons under the direction of General Manager J. Messick, its own building in Swarthmore (now Newton Square) in Pennsylvania, and 124 volunteer members in more than 10 countries. It is governed by a non-staff Board of Directors chaired, during this triennium, by D. Smith followed by L. Frevel and now by G. G. Johnson. A great amount of the work of acquiring new or improved powder diffraction patterns, of setting policy and new directions, of generating new ideas for services, and of testing out new products and ideas is carried out by volunteers organized into Committees, Sub-committees and Task Groups.

The international aspect of the ICDD character continues to grow. Currently, about 60% of the ICDD's income is from overseas sources and 63% of the Grant-in-Aid recipients are outside the USA. Two of the full members of the Board of Directors and several consultants are European. Many of the ordinary members are Asian, Australian or other non-US persons. ICDD operates a very substantial Grants-in-Aid programme which directly generates powder diffraction patterns deemed wanted but which are not otherwise available. The annual funding for the programme is in excess of US \$300 000.

The ICDD also gives grants in support of selected meetings and Workshops. It gave some financial support and ran a Workshop at the 1990 Satellite Meeting on Powder Diffraction in Toulouse, contributed US \$15 000 to the CPD-organized meeting Accuracy in Powder Diffraction II at NIST in May 1992 (which was used to pay travel for invited lecturers, who would provide sound and timely manuscripts for the Proceedings, which were actually issued about six months after the meeting), paid the travel of one invited teacher/lecturer at the International School of Crystallography: Computational Methods in X-ray Powder Diffraction Methods in Aswan, Egypt, 16–26 January 1993 (co-organized by the CPD), and will contribute US \$5000 to the 1993 Satellite Meeting on Powder Diffraction. The ICDD also makes cash contributions to and runs Workshops at various other meetings and Schools all over the world.

The ICDD operates a Crystallography Scholarship Awards programme, which provides two awards per year. The two awards in 1992 went to graduate students in the UK.

The ICDD has now adopted the CIF/STAR format as standard for the archiving and interchanging of PDF-3 (consisting of digitized whole patterns) data and future databases. PDF-3 is to be based on fully digitized patterns. A few hundred are now on hand and they are coming in at a rate of about 500–600 per year. There is a growing and spreading recognition that a great many analyses formerly undertaken with the '*d & I*' type of database can be performed much better with digitized full patterns. Included are quantitative phase analysis, phase identification in complex mixtures and extracting useful information from the 'pathologies' of the patterns, such as various effects characteristic of different clays. Such patterns might also be used for *ab initio* structure determinations.

The ICDD has dozens of projects in progress simultaneously, including several round robins:

- (i) Instrument parameters (Jenkins, ICDD);
- (ii) Automated peak finding (Ryba, Penn State University);
- (iii) Statistical process control (Blanton, Eastman Kodak);
- (iv) Profile fitting (Cline, NIST);
- (v) Preferred orientation (Diffraction Problems Subcommittee).

An ICDD Task Group was set up, with R. Snyder as Chair, to conduct a project jointly with the CPD on Crystallite Size and Microstrain. One aspect of the work is expected to be a Round Robin on Crystallite Size and Microstrain. (Dr Fiala chairs the CPD's Task Group on this.)

In accord with the adage that in science and technology nothing stands still, the process of phase identification by 'search-match' is also becoming more sophisticated, powerful and broadly applicable. Now, it is being shown that even electron powder diffraction data without recorded intensities can be used very successfully. (In fact, the new electron diffraction database is a current best seller among the ICDD offerings.) A large part of the key to this new success is a search method that simultaneously uses the electron powder diffraction database, the database formed from the 150 000 cell constants recorded in *Crystal Data* (the NIST publication assisted by the ICDD) and the X-ray powder diffraction database (PDF). The electron diffraction database may be used to develop several guesses about what the material might be and the other databases then are used in consistency tests to narrow down the range of possible candidates. Remarkable success rates were reported by the speakers and by two or three members of the audience at the October 1991 ICDD technical meeting.

In 1991 and 1992, the ICDD operated the 'clinics' on X-ray fluorescence and X-ray diffraction in 1992 at Swarthmore College. These are the 'clinics' that were established and operated by Henry Chessin at SUNY, Albany for more than 20 years.

The ICDD publishes the journal *Powder Diffraction*. The Editors of this and the Editors of the *Journal of Applied Crystallography* attempt to exchange or transfer manuscripts submitted to one journal which might better belong in the other. In so far as this Representative has determined, this cooperation is working well.

In early 1993, the ICDD moved from their Swarthmore address into their new 25 000 square foot building located at the Newton Square Corporate Campus, 12 Campus Blvd, Newton Square, PA 19073-3273, USA. They can now carry out all of their operations at a single location, which had not been possible for years in the Swarthmore building.

23 April 1993

R. A. YOUNG, Representative

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

#### *Condensed Matter Division of the European Physical Society (EPS CMD)*

Until 1989, the IUCr Representative actively took part in the annual work of the Action Committee on Conferences. Since the Committee had been reorganized in 1989, the Executive Committee decided in Bordeaux that the IUCr representation on this Committee should also be terminated. Of course, *Europhysics News* continues to report regularly on the conferences and other events related to the European community of crystallographers.

The IUCr Representative continued to attend the meetings of the Board of the Condensed Matter Division. In 1991, the Board met first on 8 April in Exeter, England, then on 11 November in Pisa, Italy. Both meetings were attended by the

IUCr Representative, who received reports on the activities of several sections of the CMD and he reported on the IUCr activities as well as the 1991 European Crystallographic Meeting, transferred from Ljubljana to Trieste.

On 7 April 1992 in Prague, Czechoslovakia, the Board elected its new Chairman, P. Wyder (Grenoble, France), and attended an evening talk given by Dr Metakides (EEC XIII Division) entitled 'On Science in a Changing Europe', which aimed to help eastern European scientists find their future in a new world around them. The Annual Meeting was held again in Geneva, Switzerland (14 November), where first a new Vice-Chairman (G. Martinez, Grenoble) and new full members of the Board were elected. To analyse the future of European Conferences on Condensed Matter, a Task Force was nominated and then elected. The EPS President, M. Jacob, presented the general philosophy that governs the contacts of EPS with the EEC representatives. It is of primary importance to convince the people in the EEC that EPS is the natural scientific entity that should be recognized as an independent community, providing the possibilities of expertise on various subjects.

In 1993, the Board met on 29 March in Regensburg, Germany, on the first day of the 13th General Conference of CMD. It had more than 3500 participants, overwhelmingly from Germany (ca 2800 active participants), presenting more than 3000 contributions (including 170 invited papers). It is worth noting that several topics of the GCs of CMD are strongly supported by crystallography. During the Board meeting, a report was received on the future meeting (Madrid, 1994) with the conclusion that after 1994 the EPS CMD should try to organize the annual conferences jointly with the European Material Research Society. Of course, an adequate reviewing of such joint meetings should be guaranteed. Progress on this plan will be reported at the next full Board meeting, which will be held again in Geneva at the end of 1993.

5 May 1993

A. KÁLMÁN, Representative

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

IDCNS is responsible for reviewing all recommendations concerning matters of nomenclature and symbols that originate within IUPAC Commissions and Divisions. Following revision and acceptance, these recommendations are published in *Pure and Applied Chemistry* and become binding on all IUPAC-related publications. The IUCr Representative and his Alternate (A. J. C. Wilson) evaluate each document and provide critical comment as appropriate from the crystallographic point of view. IDCNS met in September 1990 in Cambridge, England, August 1991 in Hamburg, Germany, and September 1992 in Oxford, England. Each meeting was attended by the Alternate rather than the Representative in order to reduce travel costs for the IUCr. These meetings provide the IUCr with a valuable insight into the complex interactions that exist between the major international bodies charged with standardizing the names, values and symbols of important quantities. They also provide direct IUCr input into IUPAC decisions of crystallographic importance. IDCNS became a member of the Comité Consultatif des Unités du Conférence Générales des Poids et Mesures (CCU) during the triennium. CCU is the body ultimately responsible for SI units, among other critical nomenclature standards; although IUPAC membership makes CCU more accessible to crystallographic concerns, it may be advisable for the IUCr to seek direct membership in CCU.

23 February 1993

S. C. ABRAHAMS, Representative  
A. J. C. WILSON, Alternate

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

The ICSTI Council meetings in the triennium have been held at Nancy, France, in May 1991, Berlin, Germany, in May 1992, and Williamsburg, USA, in May 1993. I attended the Berlin Meeting, at which A. J. C. Wilson, a former IUCr Representative on ICSTI, was the guest of honour. As is evident from the 1991 Symposium, on Squaring the Information Circle, and from the draft strategic plan to be considered at Williamsburg, ICSTI's objectives are closely attuned to the IUCr's requirements. Those objectives focus on providing scientific and technical information efficiently to all those who require access to that information. The role of standards in expediting the flow of scientific information is generally recognized. If those objectives were achieved it would help the IUCr to cope with the requirements for publishing the rapidly increasing volume of crystallographic information, and to make optimal use of improved communication technology as it becomes available. It would assist crystallographers generally by facilitating their access to the wide range of scientific information that is relevant to crystallography.

ICSTI does not have the financial and organizational strength necessary to achieve its laudable objectives. That reflects in part the failure, in the commercial sense, of most ICSTI publications. A contributing factor is its limited 'Class A' membership, which encompasses international and national scientific bodies. This situation is exacerbated by that membership being restricted, in a geographical sense, almost exclusively to western Europe and North America. ICSTI is aware of all these weaknesses, but its efforts to rectify them have not yet succeeded. Because its membership is dominated by commercial publishers, many of its activities reflect their management's concern to steer those organizations through the upheaval in publishing generated by new technology. It is, of course, easy to criticize. It is more difficult to identify how an alternative organization could do better, or to make practical improvements in ICSTI's performance. The main players in the publishing industry are members of ICSTI, and many of those members are keen to make improvements if suitable opportunities are available.

While recognizing its shortcomings, I recommend that the IUCr persist with its membership of ICSTI. As a matter of policy, the IUCr should foster links between ICSTI and CODATA, with the ultimate objective that those two organizations merge.

7 April 1993

E. N. MASLEN, Representative

*International Council of Scientific Unions (ICSU)*

ICSU is an international non-governmental and non-profit-making scientific organization whose principal objectives are:

- (1) to encourage and promote international scientific and technological activity for the benefit and well being of humanity;
- (2) to facilitate coordination of the activities of the International Scientific Unions;
- (3) to facilitate coordination of the international scientific activities of its National Members;
- (4) to stimulate, design, coordinate or participate in the implementation of international interdisciplinary scientific programmes;
- (5) to act as a consultative body on scientific issues that have an international dimension.

In respect of objectives (2) and (3), ICSU never attempts to interfere in any way with the activities of the Unions any more

than with those of its National Members (Scientific Research Councils or Science Academies). In pursuit of objective (1), it does make grants to the Unions from its own funds and other sources of funding to which it has access. Objectives (4) and to some extent (1) give rise to ICSU's global programmes such as the International Geophysical Year. In addition to the 20 International Scientific Unions and 75 multidisciplinary National Members, ICSU has 29 Scientific Associates, which are mainly international or regional federations and some of them are, in fact, International Scientific Unions not representing a single scientific discipline.

The decision-making bodies are: the General Assembly which meets every three years, the General Committee which looks after ICSU's affairs between General Assemblies and meets every year, and the Executive Board which looks after matters between the General Committee meetings. The IUCr Representative, who traditionally is the IUCr Immediate Past President, is an *ex officio* member of the General Committee. Within ICSU, the Unions and National Members conduct their interdisciplinary affairs largely in three working groups: (a) Biological Sciences; (b) Chemical, Mathematical, Physical, Earth and Space Sciences; (c) National Members. The Standing Committees of ICSU include the Committees on: Admissions, Finance, Structure and Statute, Free Circulation of Scientists, ICSU Press.

Because of objectives (4) and (5), there are a number of special Committees dealing with many general problems of science and technology in the world, like the Committees on: Agriculture, Forestry and Aquaculture; Biotechnology; Data for Science and Technology; Genetic Experimentation; Space Research; Science and Technology in Developing Countries; Water Research; Teaching of Science; Astronomical and Geophysical Data Analysis; Bioscience Networks; Natural Disasters; Radio Astronomy and Space Science; Geosphere-Biosphere Programme; Antarctic Research; Environment; Oceanic Research; Solar-Terrestrial Physics; World Climate Research; World Data Centres. These committees are becoming increasingly important in overall ICSU thought and planning.

ICSU occupies a unique role on the international scientific scene combining, as it were, the roles of the national academies of science and the supra-national characteristics of bodies such as UNESCO, but without political influences. It also acts as an interdisciplinary coordinator between the Scientific Unions and to a certain extent as the social conscience of science, a role that is not duplicated elsewhere.

In the last triennium, during the 28th General Assembly, held in Sofia, Bulgaria (1-5 October 1990), *inter alia*, it was decided that the General Assembly should meet every three years, rather than every two years as previously, and an *ad hoc* Committee was established to look into the problems of scientific research in central and eastern Europe.

At the 29th General Committee meeting, held in Oslo, Norway (25-27 September 1991), many problems concerning the organization of ICSU and the major programmes in which the Council is involved were examined and discussed. Also, the importance of ICSU's close cooperation with the scientific communities in central and eastern Europe, the availability of scientific literature for developing countries and the intellectual property aspects of the new generation of machine-readable text were considered.

Many general topics were discussed at the 30th General Committee held in Jerusalem, Israel (5-7 November 1992), among them it was found that: concerning free circulation of scientists, the number of cases of visa difficulties is decreasing, while other types of human rights issues involving the freedom of the pursuit of science is increasing; ICSU might contribute

to the general problem of ethics in science; more cooperation with scientists in developing countries should be promoted; cooperation with scientists in central and eastern Europe needs more effective coordination. Some amendments of Statutes have been proposed to ensure equality of votes for the two categories of membership, and financial aspects concerning annual dues of the members were considered to be submitted for approval to the 24th General Assembly which will be held in Santiago, Chile (October, 1993). Plans for the organization of this meeting were also discussed.

During these meetings, the IUCr Representative had the opportunity of illustrating: the policy of the IUCr for helping young scientists, particularly from countries with financial difficulties, to attend international scientific meetings and Schools on crystallography; the IUCr Visiting Professorship Programme organized by the IUCr Teaching Commission; the developments in automation of the publishing activity at the Chester Office; the new *Section D of Acta Crystallographica* on biological crystallography.

An interesting aspect of the General Committee meetings concerns the reports the Union Representatives give to illustrate the new scientific developments in the fields covered by their Unions. These reports were found very interesting and it is useful to have a picture of what is going on at the frontiers of modern science in the world.

30 March 1993

M. NARDELLI, Representative

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

CODATA is an interdisciplinary scientific Committee of ICSU which seeks to improve the quality, reliability, management and accessibility of data in all fields of science and technology. Two major international CODATA conferences were held in this triennium. The 1990 meeting in Columbus, USA, was coincidental with the Bordeaux Congress and was not attended. The 1992 meeting in Beijing, China, was entitled *New Data Challenges in our Information Age* and comprised 21 sessions covering materials science, the geosciences, biology, chemistry, industrial physics and environmental issues. Joint sessions were held with the ICSU Panel on World Data Centres. CODATA also organized 11 other specialist meetings and produced nine publications during the period of this report.

CODATA membership is currently made up of 21 National Members, 16 Scientific Unions, five Co-opted Members, one Affiliate and 27 Supporting Organizations. There are 14 Commissions and Task Groups addressing a wide variety of topics and issues, including biological macromolecules, artificial intelligence and computer graphics, and electronic publishing. Particular attention is paid to data activities, needs and accessibility; CODATA publications and data sources are freely applied to support these initiatives.

CODATA continues to be a valuable forum for the exchange of information on data activities across a broad scientific spectrum. In a period of global economic restraint and of geographical fragmentation, one of CODATA's most important tasks is to raise significant funding to respond to challenges and support developments in this increasingly important area of scientific activity.

24 May 1993

F. H. ALLEN, Representative  
J. R. RODGERS, Alternate

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

The purpose of this Committee is to promote science and technology in developing countries. Its organizational structure comprises an Executive Committee and a Plenary formed by National Members and some ICSU Bodies. The Central Secretariat of COSTED is located in Madras, India, and is headed by a Scientific Secretary. Regional Secretaries are located in Asia (Madras) and Latin America (Caracas). Efforts are under way to locate suitable centres in other regions of the developing world.

The major plans of COSTED are:

(1) Identifying a few high priority areas such as the environment, biotechnology and its applications, global change studies.

(2) Recognizing the importance and impact of scientific manpower generation in national development. In this respect, emphasis is placed on the ICSU-UNDP project on Strengthening Scientific Training and Research in the Third World.

(3) Curriculum development activities in selected scientific areas such as the environment, biotechnology, sustainable energy sources *etc.*

At its Annual Meeting in February 1992, the COSTED Executive Committee decided to collect information for a booklet describing the activities of the various ICSU bodies for developing countries. In this context, information has been given about the substantial financial support the IUCr gives to organizers of crystallographic meetings, specifically to assist young scientists (often from developing countries) to attend these meetings, Schools and Workshops. The IUCr Visiting Professorship Programme has been introduced, under the responsibility of the Teaching Commission, to enable developing countries to develop crystallography. Information was also given about journals, tables, books and teaching pamphlets published by the IUCr, crystallographic databases and International Congresses of Crystallography.

30 March 1993

M. NARDELLI, Representative

#### *ICSU Committee on Space Research (COSPAR)*

The main activity of COSPAR in the triennium was in the organization of the World Space Congress-I, held in Washington, DC, USA, 28 August-5 September. The Congress was jointly organized by COSPAR and IAF by merging the Plenary Meeting of COSPAR and the IAF Congress and was intended to celebrate the International Space Year, a concept first originated in the US and finally endorsed by the United Nations Assembly in 1990. The principal objective of World Space Congress-I was that of gathering a wide representation of the world space community at every level (universities, research centers, industry, governments, project and marketing managers), with the purpose of creating a meeting with such a critical mass of specialists that significant statements could be made in view of future preparation and planning of space research worldwide. The success of the Congress is given by numbers: it was attended by more than 4000 paying delegates from 65 countries, 1100 exhibitor personnel from 135 exhibiting companies, 284 print media representatives and 45 radio and TV crews. It was estimated that in total more than 10 000 persons participated in one way or another in the Congress. The next World Space Congress-II is scheduled in the year 2000, very probably in the same location in Washington.

A number of awards were made during the Congress. As relevant to crystallography, the following must be reported:

COSPAR International Cooperation Medal (1992) to Hubert Curien, for his untiring efforts to encourage international co-operation in many different areas, including crystallography, to which he made significant contributions (study of elastic waves in crystals, study of the Compton effect through the analysis of crystals by intense X-rays and others). Professor Curien is a former member of the IUCr Executive Committee. He has also been President of the European Physical Society and President (1981–84) of the Council of ESA.

Zel'dovich Award for Commission G (Materials Science in Space) to Stefan van Vaerenbergh, in recognition of his contributions to non-equilibrium thermodynamics, in particular with respect to the role of the Soret effect in directional solidification.

During the triennium, the *COSPAR Information Bulletin* (three issues per annum) has undergone several changes since 1991, including a section for Guest Articles. Contributed articles giving an overview of the relevance of crystallography and materials science in space research would be welcome

6 May 1993

C. PAORICI, Representative

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

A meeting of the ICSU Committee on the Teaching of Science (CTS) was held at the ICSU Headquarters in Paris, France, 1–2 May 1991, chaired by D. Waddington, University of York, Chairman of the CTS. The Secretary is J. P. Stoltman. Representatives from the constituent Unions of ICSU were present. The stated aims of this Commission are:

(1) To further on an international scale progress in the teaching of science at all levels.

(2) To cooperate with other organizations in order to further any aspects of the teaching of science.

(3) To facilitate cooperation between the Teaching Commissions of the International Scientific Unions.

It was very useful to find out how Teaching Commissions of other Unions disseminate information.

The International Geosphere–Biosphere Program has inspired CTS to initiate a curriculum development programme entitled Education in Global Change for 16- to 19-year-old science students. In this project, current global change issues are used to introduce and illustrate scientific principles. Teaching material is being prepared in a form that is readily available to all who need it. The four initial units of the project, drafted at a meeting of science educators in May 1990, involve the changing atmosphere, remote sensing (a window on global change), the global carbon cycle, and clues from the past and glimpses of our future. Material prepared on these subjects is currently under review. Additional subjects under consideration are land and ocean surface effects on global change, the stratosphere and energy cycles.

The Harare Generator Project was designed to bring African teachers together with experts in curriculum design and materials production in order to provide materials appropriate for teaching science in African Schools. Video and printed materials will be used as a pre-service teacher-training module. A meeting on the subject of this project, held at the University of Zimbabwe in January 1991, was described. A follow-up study of this project will be made in the near future.

A Project on Informatics and Microcomputers is in progress and a manuscript, nine chapters long with an appendix listing software reviews, lists of books and software listings, has been prepared and three volunteers for the CTS (representing IUPAP, ICASE and IUPS) will read and comment on this. A project in University Science Teaching is progressing. The biology project

is complete, printed and distributed. The chemistry component is almost complete. Interest continues on the production of inexpensive computing equipment, especially for laboratory instruction in the developing countries. A compilation of existing low-cost and locally produced laboratory equipment available worldwide and adapted to science teaching in a developing world is being prepared with input from the various Unions. The Subcommittee for Elementary Science and Mathematics Education for Future Elementary School Teachers.

In a report on Teaching about Ethical Issues, it was pointed out that the way that different cultures view science is an important issue and affects the development of and attention to ethics in science education.

New initiatives include:

(1) Leadership Workshops for implementing the Education in Global Change classroom materials in South Asia, Francophone Africa and Latin America.

(2) The Education in Natural Disasters Reduction Project will provide a handbook on natural disaster reduction through science education.

(3) CTS has participated in the Conference on Environment and Development (1992) and co-sponsored the Space Science Project for Teachers of Science (1992) and the UNESCO Conference on Science Education for All (1993).

The next meeting will be held 4 July 1993. At this time the restructuring of CTS within ICSU (new name, new charge *etc.*) will be discussed.

6 April 1993

J. P. GLUSKER, Representative

#### **Appendix H: Sponsorship of meetings: 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 Bordeaux 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. The Executive Committee's policy, 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, financial support for young scientists and, often, additional finance for general organizational expenses. The IUCr also provided substantial financial support to the Bordeaux Congress and the Beijing Congress. The financial support given to assist young scientists totalled SwFr 76 000 in 1990, SwFr 54 000 in 1991 and SwFr 90 000 in 1992. The support for 1993 is even larger. Hence, this support has helped several hundred young scientists attend scientific meetings during the triennium.

Symposium on Short Range Order in Ill-Ordered Materials, Orsay, near Paris, France, 16–18 July 1990 (Satellite Meeting of Bordeaux Congress)

Symposium on Powder Diffraction, Toulouse, France, 16–19 July 1990 (Satellite Meeting of Bordeaux Congress)

Symposium on Complementary Applications of Diffraction by Neutrons and by X-ray Synchrotron Radiation, Alpe d'Huez, near Grenoble, France, 29–31 July 1990 (Satellite Meeting of Bordeaux Congress)

Symposium on Symmetry in Physical Space and in Super-spaces. Physical Applications: Quasicrystals, Incommensurate Phases, Châtenay-Malabry, near Paris, France, 29–31 July 1990 (Satellite Meeting of Bordeaux Congress)

International School on Crystallographic Computing, Strasbourg, France, 29 July–5 August 1990 (Satellite Meeting of Bordeaux Congress)

Summer School for Beginners with the Rietveld Method, Cieszyn, Poland, 9–11 August 1990

XI Iberoamerican Congress on Crystallography (and associated Iberoamerican School on Crystallography), Mérida-Mérida, Venezuela, 9–14 September (and 2–8 September) 1990

Symposium on Computational Methods in Chemical Design. Molecular Modeling – Theory and Experiment, Schloss Elmau, near Garmisch-Partenkirchen, Germany, 15–20 October 1990

International Symposium on Crystallography and Molecular Biology, São Paulo, Brazil, 5–9 November 1990

First European Powder Diffraction Conference, München, Germany, 14–16 March 1991

Intensive Course in X-ray Structure Analysis, Aston, England, 18–24 March 1991

International Workshop on Methods of Structure Analysis of Modulated Structures and Quasicrystals, Bilbao-Lekeitio, Spain, 29 April–4 May 1991

Third European Conference on Crystal Growth, Budapest, Hungary, 5–11 May 1991

Second European Workshop on Crystallography of Biological Macromolecules, Como, Italy, 13–16 May 1991

International Workshop on Magnetism, Magnetic Materials and Their Applications, La Habana, Cuba, 21–29 May 1991

18th Course 'Static, Kinematic and Dynamic Aspects of Crystal and Molecular Structure', Erice, Italy, 30 May–9 June 1991

International Conference on Polytypes, Modulated Structures and Quasicrystals, Balatonszékplak, Hungary, 20–24 August 1991

Thirteenth European Crystallographic Meeting, Trieste, Italy, 25–30 August 1991

Conference on Charge, Spin and Momentum Densities, Konstanz, Germany, 1–7 September 1991

Summer School on Neutron Scattering, Oxford, England, 17–27 September 1991

International School on Materials for Electronics: Growth, Properties and Applications, Trieste, Italy, 18 November–6 December 1991

Direct Methods of Phasing in Macromolecular Crystallography, Panama City Beach, Florida, USA, 24–27 April 1992

Accuracy in Powder Diffraction II, Gaithersburg, Maryland, USA, 26–29 May 1992

Diffraction at High Pressure, Washington, DC, USA, 29–31 May 1992

4th International Conference on Quasicrystals, St Louis, Missouri, USA, 31 May–5 June 1992

School on Crystallographic Computing, Balatonfüred, Hungary, 31 May–6 June 1992

Gordon Research Conference on Electron Distribution and Chemical Bonding, Plymouth, New Hampshire, USA, 20–24 July 1992

Symposium on Organic Crystal Chemistry, Poznan, Poland, 26–30 July 1992

European Powder Diffraction Conference, Enschede, The Netherlands, 30 July–1 August 1992

Fourteenth European Crystallographic Meeting, Enschede, The Netherlands, 2–7 August 1992

American Crystallographic Association Meeting, Pittsburgh, Pennsylvania, USA, 9–14 August 1992

Eighth International Summer School on Crystal Growth and Tenth International Conference on Crystal Growth, Palm Springs and San Diego, California, USA, 9–14 August 1992 and 16–21 August 1992

Rietveld Summer School, Cieszyn, Poland, 13–15 August 1992

International Conference on Anomalous Scattering of X-rays and Neutrons, Hamburg, Germany, 17–21 August 1992

XII Congreso Iberoamericano de Cristalografía and II Escuela Iberoamericana de Cristalografía, Toledo and Madrid, Spain, 7–11 September 1992 and 14–18 September 1992

Inaugural Conference of the Asian Crystallographic Association, Singapore, 13–16 November 1992

Fourth International School of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis, Aswan, Egypt, 16–26 January 1993

Workshop on Optoelectronic Materials and their Applications, La Habana, Cuba, 18–25 February 1993

Fourth Intensive Course in X-ray Structure Analysis of Small and Medium Sized Molecules, Birmingham, England, 22–28 March 1993

Third European Workshop on Crystallography of Biological Macromolecules, Como, Italy, 24–28 May 1993

The organizers of all IUCr-sponsored meetings are requested to recommend the journals of the IUCr as a suitable channel of publication for the original papers presented at the meeting. 68 papers presented at the International Conference on Small Angle Scattering, held at Leuven, Belgium, 6–9 August 1990, were published in *J. Appl. Cryst.* (1991), **24**, 413–877.

Organizers of meetings wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the date of the meeting, writing to the Chairman of the Sub-committee. The present Chairman is P. Coppens. A new Chairman will be appointed at Beijing. Applications for sponsorship of Satellite Meetings must be submitted through the Chairman of the Organizing Committee of the main meeting.

#### Appendix I: IUCr/Oxford University Press Book Series

The launching of this Series was reported to the General Assembly at Perth (1987). The agreement between the IUCr and the OUP was finalized soon afterwards. The Series consists of three sub-series:

*IUCr Crystallographic Symposia* (IUCr CS)

*IUCr Monographs on Crystallography* (IUCr MC)

*IUCr Texts on Crystallography* (IUCr TC)

The Book Series Committee membership currently is J. H. Robertson (UK; Chairman), A. M. Glazer (UK), J. P. Glusker (USA), K. Kuchitsu (Japan) and V. I. Simonov (Russia), with H. J. Stanbury as the *ex officio* representative of the OUP and the President and the General Secretary of the IUCr as *ex officio* members. This Committee considers proposals for new publications, whether proceedings of Schools or Symposia, monographs or textbooks on crystallography, and makes recommendations to the IUCr Executive Committee and to the Delegates of the Press (the body responsible for approving all publications handled by the OUP).

*Books published since the Bordeaux General Assembly*

IUCr CS-4. Garbarczyk, J. B. & Jones, D. W. (Eds.) 1991. *Organic Crystal Chemistry*. (Proceedings of the symposium of that title held in Poznan, Poland, in August 1989.)

IUCr CS-5. Moras, D., Podjarny, A. D. & Thierry, J. C. (Eds.) 1991. *Crystallographic Computing 5. From Chemistry to Biology*. (Proceedings of the International School held in Bischenberg, France, in July/August 1990.)

IUCr MC-1. Domenicano, A. & Hargittai, I. (Eds.) 1992. *Accurate Molecular Structures*.

IUCr MC-2. Cruickshank, D. W. J., Juretschke, H. J. & Kato, N. (Eds.) 1992. *P. P. Ewald and his Dynamical Theory of X-ray Diffraction*. (This Monograph grew out of the commemorative Microsymposium held during the Perth Congress in 1987.)

IUCr MC-3. Cowley, J. M. (Ed.) 1992. *Electron Diffraction Techniques*, Volume 1.

IUCr MC-4. Cowley, J. M. (Ed.) 1993. *Electron Diffraction Techniques*, Volume 2.

IUCr MC-5. Young, R. A. (Ed.) 1992. *The Rietveld Method*. (Monograph based on invited papers at the International Workshop held in Petten, The Netherlands, in June 1989.)

IUCr TC-2. Giacovazzo, C. (Ed.) 1992. *Fundamentals of Crystallography*.

*Books expected to be published soon*

IUCr CS-6. Flack, H. D. (Ed.). *Crystallographic Computing 6*. (Proceedings of the International School held in Veszprém, Hungary, in June 1992.)

IUCr CS-7. Jones, D. W. & Katrusiak, A. (Eds.). *Organic Crystal Chemistry: Correlations, Transformations and Interactions*. (Proceedings of the Symposium of that title held in Poznan, Poland, in July 1992.)

IUCr TC-3. Paufler, P. *Physical Crystallography*. (This will be an up-dated and extended version of Paufler's original *Physikalische Kristallographie*.)

*Other topics under active consideration*

*Life's Molecular Machinery*. This topic, which has been on the table since the birth of the Book Series Committee, has recently found a prospective author.

*Instrumental Methods of X-ray Analysis*. A quite recent proposal, which looks very promising.

*Crystals*. A book (in English) to mark the 50th Anniversary of the Institute of Crystallography of the Academy of Sciences of Russia, in Moscow.

*Molecules and Crystals*. A possible book to bring together the important and related areas of molecular recognition and crystal engineering.

*Future membership of the Book Series Committee*

The current membership is willing to continue for a further three-year period.

24 May 1993

J. H. ROBERTSON, Chairman

**Appendix J: Budget estimates for period to Seventeenth General Assembly: determination of unit contribution***(a) Budget estimates*

The estimated budget for the General Fund (GF) is set out below, for the period until the next General Assembly. 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. 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 1993–31 December 1995.

<i>General Fund</i>	SwFr	SwFr
<b>INCOME</b>		
Subscriptions from Adhering Bodies*	404 820	
Yield from investments and banking accounts	960 000	
Subventions from Unesco through ICSU	58 000	1 422 820
<b>EXPENDITURE</b>		
Administration	645 400	
Subscriptions to ICSU and bodies of ICSU	19 300	
Administrative meetings	228 500	
Scientific meetings	295 000	
Transfers to other accounts	230 000	1 418 200
<b>ESTIMATED PROFIT</b>		<b>4 620</b>

\* This budget assumes an increase in the unit contribution for 1994 and 1995 (and 1996) from SwFr 890 to SwFr 1 000.

*(b) Unit Contribution*

According to Statute 5-10(k), the General Assembly has to determine the Unit Contribution to be paid by the Adhering Bodies for the period to the next General Assembly. The Executive Committee recommends to the General Assembly that the Unit Contribution should be increased from its present level of SwFr 890 to SwFr 1 000 for the years 1994–1996. It was last increased at the Ottawa General Assembly in 1981.

## 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 Committees 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 of 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 Officers 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

## INTERNATIONAL UNION OF CRYSTALLOGRAPHY

*Timetable during General Assembly*

		Statute	By-Law
'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

## Memberships of bodies belonging to the Union

## EXECUTIVE COMMITTEE

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† Until the close of the Eighteenth  
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Argentina	I	Consejo Nacional de Investigaciones Científicas y Técnicas	M. A. R. DE BENYACAR, División Física de Sólidos, Comisión Nacional de Energía Atómica, Av. del Libertador 8250, 1429 Buenos Aires
Australia	III	Australian Academy of Science	National Relations Officer, Australian Academy of Science, GPO Box 783, Canberra, 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	J.-P. DECLERCQ, Laboratoire de Cristallographie, Unité CPMC, UCL, Place Louis Pasteur 1, B-1348 Louvain-la-Neuve
Brazil	III	Conselho Nacional de Desenvolvimento Científico e Tecnológico	S. CATICHA ELLIS, DESCM, Instituto de Física, Universidade Estadual de Campinas, Campinas, São Paulo 13083-970
Bulgaria	I	Bulgarian Academy of Sciences	J. MACÍČEK, Bulgarian Academy of Sciences, Institute of Applied Mineralogy, Rakovsky str. 92, 1000 Sofia
Canada	III	National Research Council	C. P. HUBER, Institute for Biological Sciences, National Research Council, Building M-54, 1200 Montreal Road, Ottawa, Ontario K1A 0R6
Chile	I	Comisión Nacional de Investigación Científica y Tecnología	D. BOYS, Departamento de Física, Universidad de Chile, Casilla 487-3, Santiago
China, People's Republic of	IV	Academia Sinica	X.-J. XU, Department of Chemistry, Peking University, Beijing 100871
Croatia	I	Croatian Crystallographic Association (under the auspices of the Croatian Academy of Science and Arts)	S. POPOVIĆ, Ruđer Bošković Institute, PO Box 1016, 41001 Zagreb
Czech and Slovak Republics	I	Regional Committee of Czech and Slovak Crystallographers	M. KOMAN, Department of Inorganic Chemistry, Faculty of Chemical Technology, Slovak Technical University, Radlinského 9, SK-812 37 Bratislava, Slovakia
Denmark	I	Royal Danish Academy of Sciences and Letters	R. FEIDENHANS'L, Physics Department, Risø National Laboratory, PO Box 49, DK-4000 Roskilde
Egypt, Arab Republic of	I	Academy of Scientific Research and Technology	S. A. ABDEL-HADY, Physics Department, Faculty of Science, Cairo Higher Institute of Technology, Helwan, Cairo
Finland	I	Suomen Tiedeakatemiain Valtuuskunta	A. M. VAHVASELKÄ, Department of Physics, PO Box 9, (Siltavuorenpenger 20 D, Helsinki) FIN-00014 University of Helsinki
France	IV	Académie des Sciences (Institut de France)	B. CAPELLE, Association Française de Cristallographie, Tour 16, 4 place Jussieu, F-75252 Paris Cedex 05
Germany	IV	Deutsche Gesellschaft für Kristallographie	P. PAUFLER, Institut für Kristallographie und Festkörperphysik, TU Dresden, D-01069 Dresden
Hungary	I	Magyar Tudományos Akadémia	M. CZUGLER, Central Research Institute for Chemistry, Hungarian Academy of Sciences, POB 17, H-1525 Budapest
India	II	Indian National Science Academy	D. PANDEY, School of Material Science & Technology, Banaras Hindu University, Varanasi-221 005
Israel	III	Israel Academy of Sciences and Humanities	M. HAREL, Department of Structural Biology, The Weizmann Institute of Science, Rehovot 76100
Italy	III	Consiglio Nazionale delle Ricerche	G. FILIPPINI, CS per le Relazioni tra Struttura e Reattività Chimica, CNR, c/o Dip. Chimica Fisica Elettrochimica, Università, Via Golgi 19, I-20133 Milano
Japan	IV	Science Council of Japan	Y. OHASHI, Department of Chemistry, Tokyo Institute of Technology, O-okayama, Meguro-ku, Tokyo 152
Mexico	I	Consejo Nacional de Ciencia y Tecnología	A. E. CORDERO-BORBOA, Instituto de Física, UNAM, Apartado Postal 20-364, Del. Alvaro Obregón, 01000 México, DF

\* 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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New Zealand	I	The Royal Society of New Zealand	C. E. F. RICKARD, Department of Chemistry, University of Auckland, Private Bag 92019, Auckland
Norway	I	Det Norske Videnskaps-Akademi	B. FJAERTOFT, Institute of Pharmacy, University of Oslo, PO Box 1068, Blindern, 0316 Oslo
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Portugal	I	Sociedade Portuguesa de Física	M. M. R. R. COSTA, Departamento de Física, Universidade de Coimbra, 3000 Coimbra
Russia	IV	Russian Academy of Sciences	N. I. SOROKINA, Institute of Crystallography, Academy of Sciences of Russia, Leninsky prospekt 59, Moscow 117333
Serbia	I	Serbian Ministry for Science and Technology	LJ. KARANOVIĆ, Faculty of Mining and Geology, Džušina 7, 11000 Belgrade
Slovenia	I	Slovenian Ministry of Science and Technology	I. LEBAN, Department of Chemistry, University of Ljubljana, PO Box 537, SLO-61001 Ljubljana
South Africa	II	Foundation for Research Development	M. PILLAY, FRD, South African ICSU Secretariat, PO Box 2600, Pretoria 0001
Spain	III	Comisión Interministerial de Ciencia y Tecnología	M. MARTÍNEZ RIPOLL, Instituto Rocasolano, CSIC, Serrano 119, E-28006 Madrid
Sweden	II	Kungliga Vetenskapsakademien	R. NORRESTAM, Department of Structural Chemistry, Arrhenius Laboratory, University of Stockholm, S-106 91 Stockholm
Switzerland	II	Schweizerische Gesellschaft für Kristallographie	G. C. CHAPUIS, Institut de Cristallographie, Bâtiment des Sciences Physiques, CH-1015 Lausanne
Ukraine	I	Ukrainian Crystallographic Committee	B. YA. KOTUR, Department of Inorganic Chemistry, Lviv State University, Kyryla i Mefodiya Str. 6, 290005 Lviv
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	A. CLEARFIELD, Department of Chemistry, Texas A & M University, College Station, TX 77843
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\* See footnote on preceding page.

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