

International Union of Crystallography

Report of the Executive Committee for 1993

Sixteenth International Congress and General Assembly

The Sixteenth General Assembly and International Congress of Crystallography were held at the Beijing International Convention Centre, China, 21–29 August 1993, by invitation of China's National Committee for Crystallography and the Chinese Association for Science and Technology (CAST). A report, including a detailed report of the General Assembly, will be published in *Acta Crystallographica Section A*.

The General Assembly and Congress were attended by 1167 scientists from 53 countries and there were 218 accompanying members. The Third Ewald Medal and Prize were presented to Professor N. Kato at the Opening Ceremony. There were 18 Main Lectures and 48 Microsymposia and Open Commission Meetings. 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. A commercial exhibition was organized jointly with the 34th IUPAC Congress (15–20 August 1993). The exhibition comprised 15 industrial companies, four book exhibitions and two databank and software demonstrations.

The General Assembly met on the evenings of Sunday 22 August, Monday 23 August and Thursday 26 August. Applications for membership of the IUCr from Croatia (Category I), the Regional Committee of Czech and Slovak Crystallographers (Category I), Germany (Category IV), Russia (Category IV), Serbia (Category I), Slovenia (Category I), Ukraine (Category I) and Venezuela (Category I) were accepted. The changes in names of the Adhering Bodies of South Africa and Spain were accepted. The minutes of the Fifteenth General Assembly in 1990 were approved. It received the triennial financial report and the reports of the Executive Committee, the Commissions, the Scientific Associates and Regional Associates and the Union Representatives on Other Bodies since the Fifteenth General Assembly in 1990. New Officers of the Union, Chairmen and members of Commissions and Union Representatives were elected; the full list of these people will be given as an Annex to the report of the Sixteenth General Assembly and Congress. A Commission on Aperiodic

Crystals was established. The title of the Commission on Neutron Diffraction was changed to Commission on Neutron Scattering. The report of the Director of Archiving and Crystallographic Information was accepted and this position was replaced by a Subcommittee on Electronic Publishing, Dissemination and Storage of Information. The good progress of the IUCr/Oxford University Press Book Series was noted. The General Assembly increased the unit contribution for the years 1993–1996 inclusive to SwFr 1000. It reaffirmed its decision to hold the Seventeenth General Assembly and Congress in Seattle, USA. It also provisionally accepted an invitation from the Royal Society to hold the Eighteenth General Assembly and Congress in Glasgow, Scotland, in 1999.

The Executive Committee met for several days before, and most days during, the Congress, mainly to deal with matters directly related to the business of the General Assembly and the work of the Commissions.

Other meetings

In conjunction with the Congress mentioned above, the Union sponsored several satellite meetings in China, namely:

1. Summer School on Electron Crystallography – Theory and Techniques, Beijing, China, 16–20 August.
2. Neutron Scattering Satellite Meeting, Beidaihe, China, 17–19 August.
3. Symposium on Molecular Structure, Fuzhou, China, 31 August – 3 September.
4. Application of Synchrotron Radiation in Crystallography, Beijing, China, 31 August – 3 September.
5. Satellite Meeting on Powder Diffraction, Hangzhou, China, 31 August – 3 September.

Other meetings held in 1993 and sponsored by the Union were:

1. Fourth International School of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis, Aswan, Egypt, 16–26 January.
2. Workshop on Optoelectronic Materials and their Applications, La Habana, Cuba, 18–25 February.
3. Fourth Intensive Course in X-ray Structure Analysis of Small and Medium Sized Molecules, Birmingham, England, 22–28 March.
4. Third European Workshop on Crystallography of Biological Macromolecules, Como, Italy, 24–28 May.
5. Crystallography in Molecular Biology, Madras, India, 9–14 December.

Executive Committee

The membership of the Executive Committee, including new members elected at the General Assembly in 1993, is as follows:

President: Professor P. Coppens (USA); Vice-President: Professor Yu. T. Struchkov (Russia); General Secretary and Treasurer: Professor A. I. Hordvik (Norway); Immediate Past President: Professor A. Authier (France); Ordinary members: Professor E. N. Baker (New Zealand), Dr R. Chidambaram (India), Professor P. W. Coddington (Canada), Professor J. Harada (Japan), Professor M. Hart (UK), Professor H. Schenk (The Netherlands).

Publications

Volume 49 of *Acta Crystallographica*, Volume 26 of the *Journal of Applied Crystallography*, the third, revised edition of the *Brief Teaching Edition* of Volume A and Volume B of *International Tables for Crystallography* and Volumes 47B, 50B, 52B and 58A of *Structure Reports* were published.

Adhering Bodies

A list of Adhering Bodies of the Union, with names and addresses of the Secretaries of the National Committees for Crystallography, was published as Annex IV to the Report of the Fifteenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (1992), A48, 402–403]. An updated list will be published in *Acta Crystallographica Section A* in due course, in the Report of the Beijing General Assembly.

Work of the Commissions

Commission on Journals

Volume 49 of *Acta Crystallographica (Acta)* was published in 1993, and included a total of 1228 papers (an increase from 1156 in 1992) received from 60 countries, with an overall total of 4766 pages. Manuscripts received by Co-editors in 1993 numbered 1457, a 15% increase over 1992. The increase in papers represents a recovery in the number of papers submitted to *Acta C* and an increased number of submissions for *Acta D*. A total of 19 Book Reviews was received.

The average lengths of Full Articles in 1993 remained constant at 7.9 pages in *Acta A*, decreased in *Acta B* to 7.1 pages (7.4 in 1992), and was 9.0 pages in *Acta D*. *Acta C*'s Full Articles and Regular Structural papers showed slight increases at 3.5 and 2.4 pages. Median publication times for Full Articles in *Acta A* (6.2 months) and *Acta B* (6.5 months) increased slightly, with *Acta D* achieving a publication time of 4.6 months. The median publication time for Full Articles and Regular Structural

Papers in *Acta C* decreased to 6.3 and 5.8 months, respectively.

A total of 78 inorganic, 19 organometallic, and 57 organic papers appeared in *Section B* in 1993, compared with 37, 14 and 62 in 1992. The distribution of papers in *Section C* was 77 inorganic, 320 organometallic, and 483 organic in 1993, compared with 90 inorganic, 267 organometallic, and 540 organic in 1992.

The number of Full Articles for Volume 26 of the *Journal of Applied Crystallography (JAC)* in 1993 was 99, compared with 94 in 1992. The number of pages published was 848 (812 in 1992) and the median publication time for Full Articles remained constant at 5.8 months.

The average length for Full Articles in *JAC* was 7.2 pages in 1993, compared to 7.0 pages in 1992. The average length for Short Communications and Computer Programs was 2.6 and 4.2 pages in 1993, compared to 1.5 and 4.6 pages in 1992. A total of 190 papers from 24 countries were received by Co-editors.

Following the Closed Meeting of the Commission on Journals in Beijing, A. Authier was appointed Editor of *Acta A*, F. H. Allen appointed Editor of *Acta B*, and S. R. Hall appointed Editor of *Acta C*, joining J. P. Glusker as Editor of *Acta D* and A. M. Glazer as Editor of *JAC*. C. E. Bugg will serve as Editor-in-Chief and Chairman of the Commission on Journals. Initiatives undertaken by this group include: the expansion of Lead Articles to include more subjects of current interest to the crystallographic community; the introduction of brief and focused review articles on timely topics; new procedures for rapid publishing of Short Communications; and redesign of the covers and tables of contents for the *Acta* Sections and for *JAC*. Two new sections in *JAC* have been initiated: one on CIF applications and the second on crystallographic teaching and education.

The proposal to establish the new *Journal of Synchrotron Radiation (JSR)* was approved for initial publication in early 1995. Editors J. R. Helliwell, S. S. Hasnain and H. Kamitsubo have assembled an editorial board whose members will also become members of the Commission on Journals: Y. Amemiya, M. Ando, D. Bilderback, M. Colapietro, P. Elleaume, R. Fourme, M. Hart, T. Ishii, G. Kulipanov, H. Kuroda, T. Matsushita, D. McWhan, D. Mills, S. Mobilio, K. Moffat, T. Morrison, I. H. Munro, A. R. D. Rodrigues, R. Rosei, V. Saile, M. Sauvage-Simkin and H. Stuhmann.

F. Herstein was approved as a new Co-editor for *Acta* and P. Weber and O. Nittono approved for *JAC*. E. Prince retired from the *JAC* editorial board, and P. W. Coddington, H. Steinfink and N. W. Alcock retired from *Acta*.

Commission on Structure Reports

Volumes 47B (The Multi-Year Index for the Organic Compounds to 1980), 50B (Organic Compounds for 1983), 52B (Organic Compounds for 1985) and 58A

Table 1. Survey of the contents of the Union Journals

<i>Acta Crystallographica</i>													
Vol.	Year	Number of Pages*	Number of Papers	Full Articles		Regular Structural Papers†		Short Communications		Fast Communications			
				Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length		
A45 } B45 } C45 }	1989	920 } 600 } 2030 }	143 } 94 } 806 }	122 } 90 } 550 }	212 } 6.6 } 6.6 } 2.8 }	6.6 } 6.6 } 2.8 }	— } — } 239 }	— } — } 1.9 }	14 } 4 } 17 }	35 } 0.9 } 0.5 } 0.8 }	7 } — } — }	3.4 } — } — }	
A46† } B46 } C46 }		1990	998 } 864 } 2500 }	150 } 123 } 980 }	126 } 120 } 693 }	246 } 6.7 } 2.6 }	6.9 } 6.7 } 2.6 }	— } — } 270 }	— } — } 1.8 }	19 } 3 } 17 }	39 } 0.8 } 0.6 }	5 } — } — }	2.4 } — } — }
A47 } B47 } C47 }			1991	860 } 1030 } 2740 }	123 } 137 } 1076 }	104 } 130 } 678 }	234 } 7.2 } 7.4 }	7.3 } 7.2 } 2.7 }	— } — } 391 }	— } — } 1.8 }	15 } 6 } 7 }	28 } 1.2 } 1.0 } 0.6 }	4 } 1 } — }
A48 } B48 } C48 }	1992			954 } 856 } 2280 }	117 } 125 } 914 }	106 } 113 } 499 }	219 } 7.9 } 7.4 }	7.7 } 7.9 } 2.9 }	— } — } 407 }	— } — } 2.0 }	10 } 10 } 8 }	28 } 2.2 } 1.8 } 0.6 }	1 } 2 } — }
A49‡ } B49 } C49 } D49 }		1993		901 } 1075 } 2186 } 604 }	121 } 155 } 880 } 72 }	108 } 149 } 211 } 62 }	319 } 7.9 } 7.1 } 3.5 } 9.0 }	7.7 } 7.9 } 7.1 } 3.5 } 9.0 }	— } — } 658 } — }	— } — } 2.3 } — }	7 } 6 } 11 } 6 }	30 } 1.6 } 2.0 } 0.9 } 2.7 }	6 } — } — } 4 }

Journal of Applied Crystallography

Vol.	Year	Number of Pages*	Number of Papers	Full Articles		Short Communications		Fast Communications		Computer Programs		Short Items§	
				Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length	Number	Average Length
22	1989	642	125	81	6.7	18	1.6	—	—	12	4.3	14	0.8
23	1990	560	105	72	5.6	13	1.7	1	2.0	11	2.3	9	0.8
24¶	1991	1102	176	138	5.7	20	1.7	5	2.6	13	2.9	13	0.8
25	1992	812	127	94	7.0	9	1.5	2	3.5	12	4.6	10	1.2
26	1993	848	144	99	7.2	18	2.6	—	—	14	4.2	13	1.0

* Excluding indexes.

† Including Short Format Papers.

‡ Volume A46 includes, in addition, 540 pages of abstracts communicated to the Bordeaux Congress, and Volume A49, 515 pages of abstracts communicated to the Beijing Congress.

§ Excluding Union Announcements, Crystallographers, New Commercial Products and Book Reviews.

¶ Volume 24 includes 464 pages of 68 papers presented at the International Congress of Small-Angle Scattering, Leuven, Belgium, 1990.

(1913–1990 Metals and Inorganic Indices) were published in 1993. Publication of these volumes concluded the work of the Commission which has therefore been disbanded.

Commission on International Tables

In July 1993, the Chairman of the Commission on *International Tables*, A. J. C. Wilson, was succeeded by T. Hahn. The entire Commission owes great appreciation to Arthur Wilson for his many years of devoted service and for the editing of Volume C.

During the Beijing Congress and General Assembly of the IUCr (August 1993), the new Chairman reported on the present status of and the future plans for the various Volumes of *International Tables for Crystallography*. He used the occasion to discuss this work with a number of interested scientists.

Volume A. Space-Group Symmetry; Editor T. Hahn

In December 1993, new diagrams for the triclinic, monoclinic and orthorhombic space groups were completed. With this, the entire space-group-diagram project is finished: New diagrams are now available for all 17 plane groups and 230 space groups, as well as for the explanatory diagrams. In 17 orthorhombic, tetragonal and cubic space-group diagrams, the new graphical symbol for the *e* glide planes, recently introduced by the IUCr [cf. *Acta Cryst.* (1992), A48, 727–732], was incorporated. The new diagrams, as well as modifications and corrections of the text, were submitted to the Technical Editor in January 1994 for the fourth, revised edition of Volume A. A list of errata to the third edition (1992) will appear in *Acta Cryst. Section A* shortly after the publication of the fourth edition.

The third, revised and enlarged edition of the *Brief Teaching Edition of Volume A* appeared in the summer of

1993. As a new item it contains the 17 plane groups, so useful for teaching purposes.

Volume B. Reciprocal Space; Editor U. Shmueli

The first edition of Volume B appeared in print in the early summer of 1993. The full reference to this edition is: *International Tables for Crystallography* (1993). *Volume B: Reciprocal Space*, edited by U. Shmueli, 506 + xxii pages, ISBN 0-7923-2189-8. Dordrecht: Kluwer Academic Publishers.

Soon after the appearance of Volume B, all its authors were consulted by correspondence with regard to their views on desirable modifications to be introduced in future printings or editions of the volume. As a result of this exchange of views, and the rather extensive correspondence between the Editor of Volume B and the Chairman of the Commission on *International Tables*, a tentative plan for the second edition of Volume B has emerged. Three kinds of modifications are envisaged:

(i) updating of published material due to recent developments;

(ii) introduction of explanatory material in the chapters that are deemed to be difficult;

(iii) addition of new chapters, either newly planned or such that could not be prepared for the present edition.

Correspondence with authors is in progress.

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

The first edition of Volume C, *Mathematical, Physical and Chemical Tables*, appeared early in 1992. By early 1993 it was clear that the first printing would be exhausted in 1994, and the greater part of the current year has been spent in correspondence with the authors and others concerned, collecting information about misprints and other errors. The corrections range from the insertion of a comma to the insertion of a complete line of figures in a table – an error going back to the old Volume IV.

Preliminary work has begun on a fully revised and augmented second edition, the target date for publication is 1996.

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

Volume D consists of three parts. Part 1 is devoted to *Tensorial Aspects of Physical Properties*: mathematical introduction and reduction of polar and axial tensors according to crystal symmetry, group theory and representations, mechanical properties including non-linear elasticity, thermal expansion, dielectric properties, magnetic properties, classical and non-linear optical properties, transport properties, anisotropic displacement parameters, tensors for quasiperiodic systems. Part 2 treats *Symmetry Aspects of Excitations* (photons,

electrons, Raman scattering, Brillouin scattering, magnons). Part 3 is devoted to *Symmetry Aspects of Structural Phase Transitions, Twinning and Domain Structures*.

Several chapters have already been completed, work is progressing on most of the others, but some uncertainty remains with respect to a few of them.

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

The symmetry diagrams and general-position diagrams of the subperiodic groups and the figures for the guide to the tables of the subperiodic groups have been computer generated and recently completed. With this, the guide to and the tables of the subperiodic groups, *i.e.* the frieze, rod and layer groups, are complete.

The remainder of the material for Volume E, dealing with relationships between the crystallographic space groups and subperiodic groups, is being completed.

Commission on Aperiodic Crystals

During the Beijing General Assembly, the proposition to confirm the *ad interim* Commission on Aperiodic Crystals established in 1991 was accepted. The Commission will pursue its work on the basis of its terms of reference [*Acta Cryst.* (1992), A48, 928].

The Commission prepared a checklist for the description of incommensurate modulated crystal (IC) structures and this was approved by the Executive Committee. This document specifies the relevant parameters and information which should be included in a database or publication for complete characterization of IC structures. It should also assist journal editors and referees in their activities.

Work has been started on the extension of the CIF (Crystallographic Information File) dictionary for the inclusion of incommensurate structures. The creation of a database containing the information on the IC structures published to date is under discussion.

The Commission participated in the preparation of many conference programmes in the field of quasi- and incommensurate crystals. In particular, the Commission established the programme of the Open Commission Meeting on Quasicrystals and Incommensurate Crystal Structures, which took place during the Beijing Congress. The Commission also agreed to participate in the preparation of the programme of the Seattle Congress in 1996, ECM-16 (Lund, 1995) and the Quasicrystals International School (Balatonfüred, 1995).

The Commission had the opportunity to meet in Beijing to discuss the preparation of the Aperiodic'94 meeting which will take place in Les Diablerets, Switzerland, 18–22 September. This meeting will continue the tradition of the former MOSPOQ conferences held on a triennial basis under the responsibility of

the Commission. The first circular was distributed at the Beijing meeting.

Commission on Biological Macromolecules

A major concern of the Commission during the year was related to the deposition, validation, retrieval and the effective use of macromolecular structural data. The matter was discussed at the Closed Meeting of the Commission during the Beijing Congress and also through correspondence among the members. The rapid growth of macromolecular crystallography and the insistence, on the basis of the guidelines formulated by IUCr, by most journals on deposition of structural data, have led to a phenomenal increase in deposition at the Brookhaven Protein Data Bank. This calls for new ways of dealing with macromolecular data. The Commission noted with interest the joint North American-European Community initiative in this regard, and the development and usage of the *Procheck* software package.

The Commission feels that the substantial macromolecular crystallography community that exists in regions outside North America and the European Community countries should also be involved in operations concerned with macromolecular structural data. The organization of an appropriate meeting for this purpose for the benefit of researchers in these regions is under the active consideration of the Commission. It was decided that concrete steps in this direction should be taken after the current efforts at new ways of dealing with data take a definitive shape.

At the request of Dr W. L. Duax, the Commission provided its recommendations on the membership of the Programme Committee of the 1996 Seattle Congress and its views on a possible satellite meeting. At the Commission's recommendation, the President of the IUCr approved the appointments of Dr Guy Dodson (UK) and Dr Wenrui Chang (China) as consultants to the Commission.

Commission on Charge, Spin and Momentum Densities

The Commission has been actively engaged in promoting the study of electron-density distributions in real and momentum space by bringing together physicists, chemists and crystallographers and by coordinating projects in the field.

Meetings of the Commission. The Commission met at the Beijing Congress of the IUCr in its old composition. The Chairman reported that his report was approved and that the Executive Committee expressed its satisfaction with its activities. The total budget proposed by the Commission was not accepted but the project on multipole refinement will be subsidized by the Union directly. Since the Organizing Committee of the Congress could not meet the wish for a Microsymposium, the Commission used the Open Commission

Meeting to organize a successful symposium on electron densities.

An extra Open Commission Meeting was introduced on 25 August to discuss Commission business – in particular, the next Sagamore meeting. The organizers of this meeting intend to apply the Gordon Formula, with no Proceedings. To have some permanency, extended abstracts will be requested. The meeting supported the idea.

At the General Assembly, the Commission membership was extended to ten.

The next meeting will be at the Sagamore conference in Brest, 7–12 August 1994.

Projects.

1. *The Fermiology of High- T_c Superconductors via High-Resolution Synchrotron-Based Compton Scattering Spectroscopy* has developed into a successful enterprise. In addition to informal discussions between members on various occasions, the project coordinators organized a workshop in Poland in July 1993, see below.

2. The development of a program package for analysing electron densities from diffraction data is progressing. The project team met on 30 June and 1 July in Berlin. The budget was approved by the Executive Committee. It is proposed to submit a project in which the multipole refinement of electron-density distributions is studied in a broader perspective. A full programme will be submitted at the Brest meeting.

3. The scientific programme of the Beijing meeting showed considerable interest for maximum-entropy methods. It might be useful to consider a comprehensive approach. A proposal for a project will be submitted in Brest.

4. Lack of progress resulted in the death of the perovskite project. Nevertheless, interest remains and the Brest meeting may well see a proposal to revive the project.

Conferences/Workshops. The First International Workshop on High Resolution Compton Scattering as a Probe of Fermiology, 3–5 July, Krakow, Poland, brought together scientists from 13 countries, who are interested in the topic of the new project on Fermiology of High- T_c Superconductors via High-Resolution Synchrotron-Based Compton Scattering Spectroscopy. The meeting was chaired by W. Schülke of the University of Dortmund, Germany, and co-chaired by A. Bansil, Northeastern University, USA. The meeting was organized locally by a Polish group, chaired by L. Dobrzynski, University of Warsaw (Bialystok). Another strong contribution to the formation of the programme stemmed from N. Shiotani, University of Tokyo. The meeting was sponsored by the IUCr and the German Ministry of Research and Technology. 31 invited lectures were given.

It was the aim of this meeting to provide a forum for a thorough dialogue between theorists, engaged in research on the electronic structure of novel materials, and

experimentalists in that field, in the presence of experts familiar with the Compton technique as well as synchrotron-radiation instrumentation, so that a realistic plan for achieving the goals of the Commission project could be chartered. The Workshop ended with a discussion on how to proceed in the near future with the Commission project.

The next workshop on High-Resolution Compton Scattering as a Probe of Fermiology will be organized by the Japanese group, chaired by N. Shiotani.

Commission on Crystal Growth and Characterization of Materials

The essential activity of the Commission during the year was the preparation and sponsorship of the following two International Schools, which are held mainly for the benefit of young scientists from developing countries.

International Summer School on Growth and Characterization of Crystals, to be held on 4–14 September 1994 in Cracow-Krynica, Poland. The programme comprises 21 lectures on the fundamentals of crystal growth, on various growth methods and classes of materials (e.g. superconductors, organics, proteins), and on various methods of characterizations (e.g. etching, X-ray diffraction, electron microscopy). The Commission is strongly engaged in the International Programme Committee (with six present or previous Commission members) and the lecturing programme (with five Commission members). The School is sponsored and financially supported by the IUCr.

International School on Advanced Electronic Materials, Crystal Growth Centre of the Anna University in Madras/India. The School was originally planned to be held in December 1993, but was abandoned after the International Centre for Theoretical Physics ICTP (sponsor of the preceding International Schools) had declined financial support because of budget problems. Now it is planned to run this School 6–15 February 1995 with financial support by Indian institutions (for local hospitality of lecturers) and by the IUCr (mainly for the participation of young scientists), and by recruiting lecturers who can raise travel funds from their home institutions.

In addition, the Commission has helped to organize the 2nd European Symposium on X-ray Topography and High-Resolution Diffraction, which is a satellite meeting to the Fifteenth European Crystallographic Meeting (ECM-15) in Dresden, Germany, and held on 5–8 September 1994 in Gosen near Berlin. This Symposium is co-sponsored and financially supported by the IUCr (mainly young scientist awards).

Commission on Crystallographic Apparatus

During 1993, the Commission on Crystallographic Apparatus has continued actively to pursue its charter. It

has contributed substantially to the understanding of the fundamental parameters of X-ray scattering (f' , f'' and m/r), and continued its activities in the fields of two-dimensional detector systems, lattice-parameter determination, XAFS, absolute structure determination for light atoms and high-pressure structure determinations.

In August, the structure of the Commission changed, with Professor H. Hashizume taking over the role of Chairman from Professor D. C. Creagh, and three new members joining the Commission. An accompanying change of emphasis in the activities of the Commission has of course occurred, mirroring necessarily the nature of the problems which beset the crystallographic community with respect to their instrumentation and their needs for data reduction. A brief report of projects that are being undertaken is given below.

1. The *X-ray Attenuation Project* (D. C. Creagh). The publication of tables of dispersion corrections (f' and f'' : in Section 4.2.6) and absorption corrections (in Section 4.2.4) of *International Tables for Crystallography* Volume C was the culmination of a decade of work to establish reliable, evaluated tables of these important parameters. Recent review articles have been published [Creagh (1990): *Nucl. Instrum. Methods*, **A295**, 417–434; Creagh (1993): *Indian J. Phys.* **67B**(6), 511–525]. Because a Second Edition of *International Tables for Crystallography* Volume C is scheduled for printing in 1996, revisions of the text to bring the sections up-to-date will be undertaken. Some minor errata (associated with the text, not the tables) will be published in a forthcoming volume of *Acta Crystallographic Section A*.

2. The *Single-Crystal Lattice Parameter Project* (G. DeTitta). The project has reached the stage when it can start to distribute properly characterized samples to laboratories participating in the project. Two kinds of sample were prepared (zeolite) and the mounting and packaging were tested for shipping the samples to the participating laboratories.

3. The *Accuracy in XAFS Project* (D. C. Creagh). A Committee of the International XAFS Society (IXS) is continuing the production of an International Short Course on XAFS with the aim of providing existing XAFS users, and those new to the field, with a standard reference work on 'Good Practice' in the field of XAFS. Some of this information will be incorporated in the revised Section 4.2.3 of *International Tables for Crystallography*, Volume C which is scheduled for printing in 1996.

It is hoped that some form of affiliation can be negotiated between the IUCr and the IXS before the next IUCr Congress.

4. *Evaluation of Two-Dimensional Detectors* (H. Hashizume *et al.*). The decision was taken at the Commission Meeting at the Beijing Congress to focus on this topic during this triennium. Considerable interest was shown by the crystallographic community in this matter, both at Bordeaux in 1990 and at Beijing. Draft

programs were worked out for publication of a series of articles reviewing recent integrating and nonintegrating two-dimensional detectors. Articles will be prepared from the users view point and provide information on available detectors. On preliminary contact, the Editor of *Journal of Applied Crystallography* (A. M. Glazer) welcomed such reviews to be published in his journal.

5. The *Absolute Structure Determination of Light Atom Compounds* (L. Malakhova). Professor Malakhova was awarded funding to pursue this project during the coming triennium.

6. The *High Pressure Group* (R. Nelmes). The high pressure group has continued its fostering of the study of the crystallography of materials subjected to extremes of pressure. It organized a highly successful Microsymposium at the recent Beijing Congress.

At the Beijing Congress, the Commission organized a meeting, which was very well attended, on Developments and Directions of Crystallographic Apparatus. Commission members were also involved in organizing and giving talks in other Microsymposia.

It is the wish of the Commission on Crystallographic Apparatus to be very sensitive to the requirements of crystallographers, and all members of the crystallographic community should feel free to communicate their needs to Commission members.

Commission on Crystallographic Computing

The main activities of the Commission during 1993 were:

(1) Refereeing of the section Computer Program Abstracts in *Journal of Applied Crystallography*: until August 1993, this was carried out by A. Olsen and G. Reck, currently by D. Watkin and M. Ramanadham.

(2) The experience with the CONCISE bulletin, as a computerized information system for crystallographers, was continued in conjunction with the European Crystallographic Committee. Connection details are given in the *IUCr Newsletter* (Vol. 1, No. 1).

(3) Organization of a Microsymposium on Crystallographic Computing as an Open Commission Meeting at the Beijing Congress: 7 communications on different modern aspects were presented.

(4) Two Commission meetings in Beijing: one of the old Commission and one of the newly elected Commission. Proposals for new activities were discussed.

(5) The volume of the notes of the Veszprim School (1992, Editors: H. D. Flack, L. Párkányi and K. Simon) has been published in the IUCr series of monographs by Oxford University Press.

(6) Negotiations are under way to find a site for a School in the Asian area in 1995. The school will be organized jointly by the Teaching and the Computing Commissions and will be connected to the Meeting of the Asian Crystallographic Association. It is intended to be a school on the most basic aspects of crystallography and

crystallographic algorithms. Demonstrations on personal computers are also planned.

(7) Planning of a Crystallographic Computing School/Workshop as a satellite meeting of the Seattle Congress was initiated. Dr P. Bourne and Dr K. Watenpaugh, acting as the local organizing committee, proposed the Evergreen State College, Olympia, Washington (USA) as the most likely location. Particular emphasis will be given to new developments in macromolecular crystallography. Lectures and tutorials/workshops will be given almost equal time, and software demonstrations are foreseen.

(8) Following a suggestion of Dr D. Watkin, plans for the organization of a small regional school, more oriented towards computational aspects, are under way. As a first trial the Commission has entrusted Dr Watkin to explore the possibility of running such a workshop in Europe within the next 12–15 months.

Commission on Crystallographic Data

The activities of the Commission for 1993 centred around future developments of various applications of the STAR syntax. These applications of the STAR syntax were

- (i) upgrading the CIF core;
- (ii) development of the Macromolecular CIF Dictionary;
- (iii) the CIF Powder Dictionary.

In consultation with the Executive Committee, it was decided to establish a separate IUCr Committee for this activity to be denoted as the Committee for the Maintenance of the CIF Standard (COMCIFS). This new Committee held its first meetings at the Beijing Congress and will report directly to the Executive Committee. Collaboration with the Chemical Structure Association concerning the implementation of their Standard Molecular Data (SMD) format as a STAR application have continued. This application, the Molecular Information File or MIF, is designed as a standard carrier of chemical structure (connectivity) information. Publication of the standard is scheduled for late 1994.

The Commission organized a joint Open Meeting with the Commission on Journals at the Beijing Congress. A closed meeting of available Commission members was also held.

Commission on Crystallographic Nomenclature

The work of the Commission in 1993 was accomplished partly internally and partly by the continuing efforts of its committees and sub-committees, with all communications conducted either by ordinary or by electronic mail. Membership of the Commission is entirely *ex officio*, as Editors of the IUCr journals and individual volumes of *International Tables for Crystallography* in addition to the chairs of the IUCr/OUP Book

Series Committee and the Commission on Crystallographic Teaching.

The Abstract of a Report entitled *Nomenclature, symbols and classification of the subperiodic groups. Report of a Working Group of the International Union of Crystallography Commission on Crystallographic Nomenclature* by V. Kopsky & D. B. Litvin was published in *Acta Cryst.* (1993), A49, 594. Preprints of the Report are available from the second author pending its publication in the forthcoming Volume E of *International Tables for Crystallography*.

A new Working Group, selected from the membership of the former Sub-committee on Statistical Descriptors in Crystallography, was appointed by the Commission and charged with examining the possible impact of the International Standardization Organization's *Guide to the Expression of Uncertainty in Measurement* on crystallographic statistical nomenclature, in light of the Commission's Sub-committee report *Statistical Descriptors in Crystallography* [*Acta Cryst.* A45, (1989), 63–75], and making recommendations for change as appropriate. The Working Group, consisting of D. Schwarzenbach (Chair), S. C. Abrahams, H. D. Flack, E. Prince and A. J. C. Wilson, has been very active in considering the optimum applications to crystallography of the new concepts concerning uncertainty in measurement. The Working Group's final recommendations are expected to affect the nomenclature used in all IUCr publications.

The resignation of Professor A. J. C. Wilson from the chairmanship of the Sub-committee on the Nomenclature of *N*-Dimensional Crystallography was accepted with deep regret. The Commission noted its great appreciation for his wise and generous service over a span of many decades. The Commission appointed Professor T. Janssen as Chair of the Sub-committee, all original members [see *Acta Cryst.* (1991), A47, 610–611] were invited to continue serving, together with one or more new members. The final composition of the Sub-committee was not fully determined at the time of writing.

Consideration is being given to establishing a new sub-committee charged with examining the merits of recommending a uniform approach to reporting atomic displacement factors, in view of the existing confusion apparent in the crystallographic literature. Also under consideration is the establishment of a working group charged with studying the multiple nomenclature in current use for naming the sequence of phases that a material may form as a function of temperature or pressure.

T. Hahn deputized for the Commission Chair at the Beijing General Assembly and related activities.

Commission on Crystallographic Teaching

Visiting Professorships. Dr Deane Smith gave a 15-hour course on *Geometrical Crystallography* at Ain

Shams University, Cairo, Egypt, from 27 January to 7 February, 1993. This course was given immediately after the Fourth International Workshop of Crystallography: Computational Methods in X-ray Powder Diffraction Analysis, which was held in Aswan, Egypt, from 16 to 26 January 1993. In his role as Visiting Professor, Dr Smith also visited students and crystallographers at Assut University (Aswan Branch), the Egyptian Geological Survey in Cairo, Cairo University, Military Technical College, Suez Canal University, Heiwan University and the Egyptian Antiquities Museum. In each case, he discussed techniques in powder diffraction.

In December 1993, Dr Ward Robinson and Professor Syd Hall were IUCr Visiting Professors in various Asian Universities (Kuala Lumpur, Mysore, Tiruchiappalli, Bombay etc.).

In addition, the Commission is considering a number of requests for Visiting Professorships in various parts of the world (Bulgaria, Russia, Vietnam, Thailand, Egypt etc.); these are planned for 1994 and 1995.

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 45401, USA). Future pamphlets include:

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

21. *Radiation Measurement and Protection in X-ray Laboratories.* By Henning von Philipsborn (under review).

22. *Crystal Packing.* By Angelo Gavezzotti (under review).

23. *γ -ray Diffraction Study of Single Crystals.* By Alexander Kurbakov (in preparation).

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

International Schools. An Asian-Region Seminar on Crystallography in Molecular Biology took place in Madras, India on 9–14 December 1993. Professor S. Parthasarathy was the Convener and some members of the Commission were on the Organizing Committee, with Dr Jenny Glusker as the Chairperson. All members of the Commission who were present (J. P. Glusker, C. M. Gramaccioli, P. Phavanantha, W. Robinson and H. Schenk) took an active part in teaching. This meeting was sponsored by the IUCr, which also provided funds for young scientists to attend. The meeting was well attended, with several speakers from various countries dealing with interesting subjects (among these were Dr T. Ashida from Nagoya, Japan, Dr B. C. Wang from

Pittsburg, PA, Dr M. Sundaralingam from Columbus, OH, and Dr D. Davies from Bethesda, MD). The contributions made by industrial companies and by the IUCr were appreciated.

During the time of this School, an informal meeting of the Commission members who were present took place: on that occasion, it was pointed out that the best teaching activity should include either Visiting Professorships and Schools or Seminars, since these activities do not exclude each other and perform different functions.

The possibility of holding a crystallography school in Asia on the occasion of the Asian Crystallography Meeting in 1995 is also being considered.

Other activities. At the Beijing meeting, a Microsymposium (OCM-19.1) was held on Crystallographic Teaching: Practical Hints and New Concepts. As usual, the room was full for the entire symposium and the quality of presentations was high. An informal meeting of the Commission took place at the beginning of the meeting.

Commission on Electron Diffraction

The second volume of the Commission's publication on *Electron Diffraction Techniques* was published in May 1993 by Oxford University Press as part of the *IUCr Monographs on Crystallography* series. At the Beijing General Assembly, there was a Microsymposium on Direct Phasing from Electron Diffraction Data for Crystal Structure Analysis that was well attended and gave a timely review of the exciting developments in this field. A Symposium on Fullerenes jointly proposed by the Commission included a lecture involving electron diffraction by S. Iijima, and K. Kuo, a member of the Commission, gave a main lecture on Quasicrystals.

The meeting of the Commission in Beijing heard a report on the first of its two Summer Schools on Electron Crystallography, Theory and Techniques. The School was held in Beijing and was attended by 43 participants from 17 countries. Chaired by Professors J. M. Cowley and J. C. H. Spence, it was judged a successful venture, well worth following up with a Second Summer School on the same topic planned for Bristol and Bath 11–15 July 1994, immediately prior to the 13th International Congress on Electron Microscopy in Paris. The Commission heard a report by Professor van Dyck of his survey of computer programs in use to calculate electron diffraction data. It was decided to explore the possibility of mounting a related exercise in connection with computer codes for electron diffraction from surfaces.

Commission on Neutron Scattering

A significant event for the former Neutron Diffraction Commission was its change of name to the above at the Beijing General Assembly. This change of name had been thoroughly canvassed by members of the Commis-

sion throughout the neutron scattering community and represents more accurately the comprehensive constituency of the Commission. Neutron diffraction from both single crystals and powders still constitutes the core of the Commission's structural interest but recent General Assemblies, Satellite Meetings and Microsymposia have reflected the growing interest in less well ordered materials (such as biological systems), mesocrystalline materials, crystalline disorder and dynamical phenomena. The emphasis in the recent letter by Philip Coppens [*IUCr Newsletter* (1994), Vol. 2, No. 1] is welcomed by the Commission.

The major event of 1993 was the Beijing meeting and its Satellites. John White was a member of the Programme Committee and a number of members of the Commission contributed not only to the programme development of the General Assembly and Microsymposia, but helped to make the Satellite Meeting at Beidaihe the resounding success that all who participated there felt it to be. At it and in the Open Commission Meeting, the future plans for the Commission were discussed with plans being outlined for an Asia-Pacific meeting in 1995 to complement the ICNS meeting being organised for Kyoto, Japan, October 1994.

The Commission will continue its work in the development of training courses with the IAEA, particularly intending to bring the latest developments in neutron scattering such as structure and dynamics in biology, in polymeric systems and catalytic materials to the attention of a wider audience and to cooperate with those countries where new neutron beam installations are being prepared. Members of the Commission are active also in the promotion of the complementarity of neutron radiation for structural problems and close links with the synchrotron-radiation community are being maintained. This is particularly appropriate because of the contiguity of major neutron scattering and synchrotron-radiation centres at Brookhaven National Laboratory, Grenoble, Argonne National Laboratory and at the KEK School, Ibaraki.

The Commission again recognizes the important work of *Neutron News* in bringing the latest scientific and other news to the whole community and again recognizes the work of Gerry Lander (with John Axe and Yasuo Endoh) in keeping this journal as a focus of interest.

With the change in membership in the Commission at the Beijing meeting, it is a pleasure for the new Chairman to thank Dr Sax Mason for his many contributions to the Commission's work and to welcome the new members in the expectation of their active contribution and frequent contacts with him by e-mail.

Commission on Powder Diffraction

1993 was a very busy year for the Commission on Powder Diffraction (CPD). Highlights of the year were: (i) the very successful Satellite Meeting on Powder

Diffraction held in Hangzhou immediately following the Beijing Congress; (ii) translation of the CPD Newsletter No. 10 into Chinese and its distribution to 300 powder diffractionists in that country; and (iii) publication of the book *The Rietveld Method* (Oxford University Press), edited by CPD Past Chairman Professor R. A. Young.

Two *Newsletters* were issued in 1993, the April one being edited by CPD member Dr Jaroslav Fiala of the Czech Republic and the November one by Dr Ludo Frevel of the USA, the ICDD Representative to the CPD. More than 800 copies of each of these issues were distributed to the current CPD mailing list, with a further 600 made available for pick-up at various conferences and in other mailings.

CPD Member Professor Lin Shao-Fan of Nankai University, China, arranged for *Newsletter* No. 10 to be translated into Chinese and for it to be distributed, along with a translation of the journal *Powder Diffraction*, to 300 powder diffractionists in China. This process will be continued for the foreseeable future and will significantly expand the number of people exposed to the CPD by more than 500 persons.

The CPD was co-organiser of the Fourth International Workshop on Crystallography. Computational Methods in X-ray Powder Diffraction Analysis (PDSE-93), held in Aswan, Egypt, 16–26 January 1993. The Programme Committee was chaired by the then CPD Chairman Professor R. A. Young, with two other CPD members Drs J. Ian Langford and Daniel Louër also serving on the Committee. The then CPD Consultant, Professor Deane Smith, was able to attend as a much-needed invited lecturer because he was in Egypt with travel funds from the IUCr's Visiting Professorship Programme to give an Intensive Course on Quantitative Phase Analysis at Ain Shams University in Cairo.

A multi-author book entitled *The Rietveld Method* was published by Oxford University Press in April 1993, representing No. 5 in the series of *IUCr Monographs on Crystallography*. This book was edited by the CPD Past Chairman, Professor R. A. Young. It is an outcome of the International Workshop on Rietveld Refinement organized by the CPD and held in Petten, The Netherlands, in June 1989, but is much more than a proceedings volume and captures the state of the Rietveld art as of about mid-1992.

The CPD organized the Satellite Meeting Advances in Powder Diffraction, SMP-93, in Hangzhou, China, 31 August – 3 September 1993, immediately after the Beijing Congress. The main aim was to present recent developments in powder diffraction theory and practice and to emphasize the power of modern diffraction methods in materials science. 140 delegates from 18 countries attended. The undoubted success of the meeting was due to the excellent efforts of Professor Ling Rong-Guo, Chairman of the Organizing Committee and to CPD member Dr J. Ian Langford, Chairman of the Scientific Programme Committee, with much appreciated

assistance from Professor Shen Shan-Hong, President of Hangzhou University, and Professor Lin Shao-Fan.

The CPD contributed, through the Task Group Chairmanship of Dr J. Ian Langford, to the development and acceptance of a powder diffraction dictionary for use in the CIF–STAR format for archiving and transferral of crystallographic data. This ongoing CPD project is undertaken in collaboration the ICDD through the leadership of now CPD consultant Dr J. Ian Langford and, representing the ICDD, Dr Brian Toby. The CPD was also involved in extended negotiations with the ICDD prior to acceptance of the CIF format for ICDD databases.

CPD members have been invited to serve on the Programme Committees for powder diffraction meetings to be held in Russia and Slovakia in 1994 and 1995, respectively. Both of these Committees are being chaired by CPD member Dr Jaroslav Fiala. The meeting in Slovakia will focus on the determination of crystallite size and microstrain from powder diffraction data; a Task Group has been formed jointly with the ICDD, with Dr Fiala and Professor R. L. Snyder as Co-chairmen. The meeting is likely to give rise to a round robin survey of the methods and models in common use.

I take this opportunity to express the gratitude and appreciation of the current and past CPD members to Professor Ray Young for his enthusiastic and very able chairmanship of the CPD during the first two triennia of the CPD's existence, from 1987 to 1993. The past six years have been extremely active for the CPD and we welcome his continued activity and influence as a CPD consultant for the next three years.

Commission on Small Molecules

This report refers both to activities organized by the 1990–1993 Committee (Chair Bill Duax) and by the 1993–1996 Committee (Chair Frank Herbststein) during the calendar year 1993. The principal achievements for this year under Duax's leadership were the Open Session under the title New Viewpoints in Structure Analysis, held at the Beijing Congress and the Fuzhou post-Congress Satellite Symposium on Molecular Structure, held immediately thereafter. The three-hour Microsymposium included five lectures (Boese, Harding, Lenstra, Maslen, Feil) and four shorter contributions (Niu, Kakuma, Wang, Viterbo) and attracted an audience of more than 100. The almost week-long Fuzhou Symposium, which was organized in close cooperation with Chinese crystallographers, especially those from Fuzhou and vicinity, was a very special occasion because of its scientific content and its intimate social atmosphere, which allowed for much closer contact between Chinese crystallographers and those from abroad than had been possible during the very large Beijing meeting. The Symposium was highlighted in the fall edition of the *IUCr Newsletter* [(1993), Vol. 1, No. 4].

Both Committees were represented at a meeting in Beijing, at which forthcoming activities were charted. These include the joint CSM-ACA Symposium on New Trends in Small Molecule Crystallography, with more than 20 speakers from a wide range of countries and extending over three days at the Atlanta ACA Meeting in June-July 1994. This material will be published, after normal review, in a special issue of *Acta Crystallographica Section B* to appear early in 1995. Other activities concerned recommendation of IUCr sponsorship for CMCD-4 (Computational Methods in Chemical Design) at Kloster Irsee in May 1994 (the organizer is John Stezowski, first Chair of the CSM) and the Organic Crystal Chemistry Symposium to be held near Poznan, 23-29 August 1994, which is a Satellite Meeting to be held just before ECM-15 in Dresden. A similar recommendation is being considered for a proposed workshop on the fundamental principles of molecular modelling to be held in South Africa during 1995.

The CSM data-collection programme is being continued under the supervision of Maureen Mackay; this programme makes contact between crystallographers who lack adequate facilities for data collection and those with up-to-date equipment who are willing to collect at least one data set per year. Finally, the question of whether the current name satisfactorily represents the activities of the Commission is under discussion. One suggestion is to change the name to Commission on Chemical Crystallography; comments and alternative proposals are welcomed. A decision here is one of the prerogatives of the General Assembly.

Commission on Synchrotron Radiation

In this period, the main activities involved the Beijing Congress, a detector workshop held in Rome and development of the *Journal of Synchrotron Radiation*.

At the Beijing Congress, synchrotron radiation (SR) figured prominently. In addition, the Commission organized the Satellite Meeting on Synchrotron Radiation in Crystallography held at the Institute of High Energy Physics, Beijing. A detailed report of the Congress and the Satellite Meeting was published in *Synchrotron Radiation News*, *The Bulletin of the Association of Asian Pacific Physical Societies* and the *IUCr Newsletter*.

In May 1993, a Workshop was held in Rome University on CCD Detectors in Macromolecular Crystallography. This brought participants in this field together and so will help facilitate the growth of detector development to match that of source development. A detailed report was published in *Synchrotron Radiation News*, written by N. Allinson, York University.

The *Journal of Synchrotron Radiation*, having been proposed in 1991, was actively pursued. Detailed discussions continued with the Executive and Finance Committees of the IUCr following the consultative

exercise with the SR community and representative organizations. The final details were agreed in Beijing with the Executive Committee and at the General Assembly. An Editorial Board was appointed by the IUCr. It was decided that publication is to be bimonthly from 1 January 1995, with an introductory issue to be circulated in September 1994. The Editors were confirmed by the Executive Committee in Beijing as S. S. Hasnain, J. R. Helliwell and H. Kamitsubo.

The Commission members have been active in planning meetings for the coming years, most notably a request and approval for a Satellite Meeting in Argonne, Illinois, prior to the Seattle Congress in 1996. Other meetings actively supported include the European Crystallography Meetings in Dresden (1994) and in Lund (1995) and the International School and Symposium on Synchrotron Radiation in Natural Sciences, Jaszowiec, Poland, 1994.

Sub-Committee on the Union Calendar

The Sub-Committee receives and considers requests for IUCr sponsorship and nominal financial support and makes recommendations to the Executive Committee. Acting on the recommendations made by the Sub-Committee, during 1993 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1993 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1994, but approved in 1993, are listed below:

1. Gordon Research Conference on Structural Phase Transitions in Non-Metallic Solids, Volterra, Italy, 8-13 May 1994.
2. Symposium on Computational Methods in Chemical Design, Molecular Modelling - Theory and Experiment, Kloster Irsee near Kaufbeuren, Germany, 16-20 May 1994.
3. 21st Crystallographic Course on Crystallography of Molecular Biology, Erice, Italy, 27 May - 5 June 1994.
4. 1994 American Crystallographic Association Annual Meeting, Atlanta, GA, USA, 26 June - 1 July.
5. Symposium on New Trends in Small Molecule Crystallography, Atlanta, GA, USA, 26 June - 1 July 1994.
6. Summer School on Electron Crystallography Theory and Practice, Bristol and Bath, England, 11-15 July 1994.
7. Sagamore XI Conference, Brest, France, 7-12 August 1994.
8. Pre-ECM-15 Symposium on Organic Crystal Chemistry, Poznan-Rydzyna, Poland, 23-27 August 1994.
9. International Summer School on Growth and Characterization of Materials, Cracow, Poland, 4-14 September 1994.

10. 2nd European Symposium on X-ray Topography and High-Resolution Diffraction, Berlin, Germany, 5–7 September 1994.

11. International Conference on Aperiodic Crystals, Lausanne/Les Diablerets, Switzerland, 18–22 September 1994.

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. If organizers intend to publish proceedings, they should consider either a special issue of one of the journals of the IUCr or, for computing schools, the IUCr Crystallographic Symposia Series, which is published jointly by the IUCr and Oxford University Press.

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 Chairperson of the Sub-Committee. The present Chairperson is Professor P. W. Coddington, Department of Chemistry, The University of Calgary, 2500 University Drive NW, Calgary, Alberta, Canada T2N 1N4 (email: pcoddington@acs.ucalgary.ca).

Applications for sponsorship of satellite meetings require the approval of the Chairperson of 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 will be sent to the Chairperson of the Congress Programme Committee for his approval or otherwise.

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.

Sub-Committee on Electronic Publishing, Dissemination and Storage of Information

In the first half of 1993 considerable effort was directed to consolidating existing crystallographic applications of the CIF and STAR files. As the progress made on CIF submission of manuscripts describing structure analyses, on powder diffraction, on protein structure information and on the World Directory of Crystallographers is described in the abstracts of the Beijing Congress, it is unnecessary to repeat that information here. Significant progress has been made on developing new software tools for using STAR files, and on the extension of the CIF concept to chemical information generally.

The Sub-committee, formed at the Beijing Congress, recognizes the importance of determining how the rapid improvements in hardware and software technologies can be used to benefit crystallography in the coming triennium. That task is complicated by the need to achieve a smooth transition from current practices based on older technologies. It requires careful assessment of the power and the longevity of emerging technologies. It involves choosing from many possible strategies one that is likely to serve crystallographers well in these times of uncertainty for publishers of scientific information. Its work will involve liaison with the Commissions of the Union that have direct responsibility for its publishing activities. It may require liaison with other Commissions, such as Computing, Data and Teaching, on matters that relate to the effective use of electronic publishing. The Sub-committee is currently reviewing the alternatives and will make recommendations to the Executive Committee on the options available early in the coming year.

Regional Associates and Scientific Associates

American Crystallographic Association (ACA)

The ACA continues to experience rapid growth in the size of its annual meetings. The 1993 meeting was held in Albuquerque, New Mexico, and was attended by over 830 scientists. The meeting was preceded by a two-day workshop sponsored jointly by the ACA Continuing Education Committee and the Molecular Graphics Society of the Americas. The workshop on Biomolecular Interactions: a Practical Workshop on Computational Approaches was attended by 160 scientists. The Patterson Award was presented to Professor George Sheldrick of Göttingen, Germany, at the annual meeting. The ACA has been very successful in attracting young scientists to the annual meeting by providing 17 student travel awards funded in part by the IUCr, five Pauling prizes for best student posters, and special social functions for the young scientists. The 1994 annual meeting is planned for late June in Atlanta, Georgia, and the 1995 meeting will be held in Montreal, Quebec, Canada. The officers for 1993 are Richard Marsh, President; Elinor Adman, Vice-President; Keith Watenpugh, Past-President; David Brown, Canadian Representative; Vivian Cody, Secretary; S. N. Rao, Treasurer.

The ACA has been particularly successful in raising funds to support crystallographic colleagues in the former Soviet Union. In 1993, the ACA provided 39 crystallographers with awards totalling \$18,000. The funds were raised through donations from the membership and a matching grant from the Sloan Foundation in the USA.

The ACA continues to offer a Summer School for Crystallography in Pittsburgh, which provides practical education in crystal structure determination. The 1993

school was attended by 23 students from the USA and Canada.

Asian Crystallographic Association (AsCA)

The council meeting was held at the International Convention Center, Beijing, China, 25 August 1993 during the Beijing Congress. The Councillors for 1993–1996 were recorded as: Dudley Creagh and John W. White (Australia); Altaf Hussain (Bangladesh); Z. Zhang (China); Thomas C. W. Mak (Hong Kong); G. R. Desiraju, S. P. Sen Gupta and K. K. Kannan (India); Waloejo Loeksmanto (Indonesia); Tamaichi Ashida and Tatsuyuki Uragami (Japan); Young-Ja Park (Korea); Hoong-Kun Fun (Malaysia); W. T. Robinson (New Zealand); Anwar ul Haq (Pakistan); Wyona C. Patalinghug (Philippines); Lip Lin Koh (Singapore); Richard P. Gunawardane (Sri Lanka); Yu Wang (Taiwan); Phathana Phavanantha (Thailand); Nguyen Van Tri (Vietnam).

The elected Executives for 1993–1996 are Professor W. T. Robinson (President); Professor Yu Wang (Vice-President); Professor Z. Zhang (Secretary and Treasurer). In addition to the regular issue of *AsCA Newsletters*, it was confirmed that the second AsCA science meeting should be held in 1995. Three places (Kuala Lumpur, Bangkok and Hong Kong) were suggested as the possible site for AsCA'95.

European Crystallographic Committee (ECC)

No formal ECC meeting was held in 1993. New officers will be elected at ECM-15, Dresden, 28 August – 2 September 1994.

International Centre for Diffraction Data (ICDD)

Background. The International Centre for Diffraction Data (ICDD) is a non-profit scientific organization, which collects, edits, publishes and distributes powder diffraction data for the identification of crystalline materials. The very wide range of activities of the ICDD can be appreciated from the titles of the various Sub-committees, namely, New Product Research and Development, Data Collection and Analysis, Search/Match Methods, Pattern Calculations, Crystal Data, Minerals, Organic and Forensic, Ceramics, Metals and Alloys, Electron Diffraction, Education, and Database.

The ICDD operates with a staff of 29 full-time employees and about 100 elected volunteer members and many volunteer non-members. The volunteers are organized into the Sub-committees listed above, which further divide into Task Groups. There is also a Technical Committee (TC) that consists of all Sub-committee Chairs plus other *ex officio* members. ICDD meetings are held twice a year, during which the Sub-committees receive and discuss reports from the Task Groups, and pass on recommendations through the TC to the ICDD Board of Directors and its Committees for action.

Involvement with the IUCr Commission on Powder Diffraction (CPD). CPD Secretary, Dr Daniel Louër (France), is Chairman of the ICDD Data Collection and Analysis Sub-committee and Consultant to the Board of Directors. CPD members Dr Jaroslav Fiala (Yugoslavia) and Dr Hideo Toraya (Japan) were elected members of the ICDD during 1993. The CPD Chairman, Dr Rod Hill (Australia), is *ex officio* IUCr Representative to the ICDD, and Dr Ludo Frevel (USA), Distinguished Fellow of the ICDD, is their Representative to the CPD. Dr Fiala jointly Chairs, with Professor Robert Snyder of the ICDD, a Task Group on Crystallite Size and Microstrain, which will be the main focus of a forthcoming CPD-sponsored meeting in Slovakia in August 1995, and which may evolve into a round robin study. The ICDD contributed \$5000 to the IUCr Satellite Meeting on Powder Diffraction in Hangzhou in August 1993 and a further \$3000 to assist the attendance of young Chinese scientists.

ICDD activities. The highlight of the year was the dedication of the new ICDD Headquarters in Newtown Square, Pennsylvania, USA, in October, 1993. The building represents a \$4 200 000 investment for the ICDD and offers excellent facilities for conferences, with modern and well equipped lecture rooms. On this occasion, talks were presented by the Director of the Board, Professor G. G. Johnson, the General Manager, Julian Messick, the Treasurer, Gerhard Fischer, and special recognition was given to the Distinguished Fellows of the ICDD, J. W. Caum, W. L. Fink, L. K. Frevel, J. D. Hanawalt, H. F. McMurdie, M. E. Mrose, B. Post, S. Weissmann and A. J. C. Wilson. Special awards were also made to Ben Post and Sig Weissmann for 40 years of editing of the Powder Diffraction File.

During the year, Dr Ron Jenkins of the ICDD was presented with the Barrett Award in August for his outstanding work on diffraction techniques and instrumentation and for his untiring global activities in educating a generation of powder diffractionists. Member Helen Hitchcock was given an award by the Director of the Kennedy Space Centre (NASA) as a Manned Flight Awareness Honoree for her contribution to the manned space program. Dr Larry Calvert and Professor Yoshio Takeuchi were elected to join the other members who have been recognized as Distinguished Fellows by the Board of Directors for their sustained outstanding contributions to the ICDD. Larry Calvert is the first such member to be honoured posthumously.

A report by T. Blanton (Eastman Kodak) on silver behenate as a possible candidate for a low-angle standard sample [d spacing (001) = 58.38 Å] was published in *J. Appl. Cryst.* (1993), **26**, 180–184.

A round robin on Profile Fitting is being organized by J. Kline of the NIST. Search manuals and software for the analysis of organic functional group functionality are now available on CDROM and will operate under Windows.

The Grants-in-Aid Program for the synthesis, collection and analysis of powder diffraction data at laboratories around the world continued at an annual rate of \$300 000. Two Crystallographic Scholarships (\$2000 each) were awarded to students in Canada and the UK; the interest in these scholarships has been so strong that in 1994 the number will be increased to three. Grants were also made during the year to the Denver X-ray Conference (\$5000), the European Powder Diffraction Conference EPDIC-III (\$5000 for the conference and \$5000 to assist Eastern European scientists), and additional Grants-in-Aid to nine scientists in the Former Soviet Union, including one-year free subscriptions to *Powder Diffraction* and discounts on Powder Diffraction File products.

The ICDD continues to be a dynamic and growing organization.

International Organization for Crystal Growth (IOCG)

Following the 10th International Conference on Crystal Growth (ICCG-10) and the 8th International Summer School on Crystal Growth (ISSCG-8) in San Diego and Palm Springs, CA, USA, in June 1992, there was no formal activity of the IOCG in 1993. The following forthcoming IOCG-sponsored meetings are in preparation by the Dutch Organization for Crystal Growth (KKN):

Eleventh International Conference on Crystal Growth (ICCG-11), The Hague, The Netherlands, 18–23 June 1995. Chairman: C. F. Woensdregt, Utrecht University, The Netherlands.

Ninth International Summer School on Crystal Growth (ISSCG-9), Papendal/Arnhem, The Netherlands, 11–16 June 1995. Director: J. P. van der Eerden, Utrecht University, The Netherlands.

Representatives on Other Bodies

Interdivisional Committee on Nomenclature and Symbols (IDCNS)

The annual meeting of IDCNS, held 9–10 August 1993 in Lisbon, could be attended neither by the IUCr representative nor his alternate. IDCNS acts on all nomenclature proposals originating in the various divisions and commissions of IUPAC before their publication in *Pure Appl. Chem.* Over 40 such proposals were received in 1993 for review by the representative. Among the documents of potential interest to the IUCr are nomenclature standards relating to molecular spectroscopy, chemical thermodynamics, inorganic chain and monocyclic compounds, inorganic branched chain and polycyclic compounds, stereochemistry, fullerenes, and terms relating to phase transitions of the solid state. The latter document, which is of particular interest to crystallographers, has been considerably revised and

improved. The IUCr makes every effort to maintain consistency with the nomenclature recommendations of IUPAC and its other sister international organizations. It was reported in Lisbon that the new edition of the ISO Handbook *Quantities and Units* was due to be published later in the year and would be obtainable from National Standards Institutions. It was also reported that panel ISO/TC 12 was preparing a proposal for the Comité Consultatif des Unités du Conférence Générales des Poids et Mesures to deprecate units in temporary use with the SI, including Å. In order to improve the accessibility of IUPAC recommendations, the possibility of making documents generally available in electronic form by file transfer over Internet will be investigated.

International Council for Scientific and Technical Information (ICSTI)

The 1993 ICSTI Council meeting was held in Williamsburg, Virginia, USA. Other commitments prevented the representative from attending that meeting, and involvement with ICSTI during the year was by correspondence. Ongoing activities, such as updating information on numeric databases and assisting users to access desired information more efficiently, continue. A majority of the bodies adhering to ICSTI expresses concern about electronic publishing for reasons similar to those that affect the IUCr's thrust towards adopting that technology. Satisfactory means for recovering the cost of information provided in electronic form are not yet in place. Finding an acceptable solution is complicated by the speed at which communication and information technologies are evolving, and by the international character of the electronic network communications, for which existing procedures for making commercial transactions are cumbersome. There is strong pressure to rationalize such matters sooner rather than later, and it is likely that some members of ICSTI will be able to influence the relevant decisions. It is prudent for the IUCr to retain its membership, because of the likelihood that action by ICSTI will have a significant impact on future IUCr operations and on other crystallographic publications.

International Council of Scientific Unions (ICSU)

The International Council of Scientific Unions (ICSU) was established to facilitate the coordination between the activities of the Scientific Union Members and of the National Scientific Members. It acts as the non-governmental adviser to the UN, Unesco and like organizations on all major scientific issues of international dimensions such as global change, the prevention of natural disasters, biodiversity *etc.* It plays a major role in the development of interdisciplinary research programmes and its action has been decisive in enforcing free circulation of scientists.

ICSU consists of Scientific Union Members (the Scientific Unions), the number of which has just increased from 20 to 23, National Scientific Members, the number of which is now 74, observers and associates (scientific, national and regional). It has established 18 Interdisciplinary Bodies and is also involved in a number of joint initiatives with other organizations.

It is run by an Executive Board which follows its activities on a day-to-day basis and meets several times a year, a General Committee where every Scientific Union Member has a representative and which meets every year, and a General Assembly which meets every three years. It is assisted in its work by a number of Standing Committees and *Ad Hoc* Committees.

The 31st meeting of the ICSU General Committee (1–3 October 1993) and the 24th ICSU General Assembly (4–8 October 1993) were held in Santiago, Chile. The most important features of the meetings are given below.

I. Administrative decisions

(a) *Finances*. The scientific activities of ICSU are ever increasing and the finances are in a difficult situation. It has therefore been decided to raise the dues in 1994 by 5%. The Unions are invited to pay the expenses of the travel of their representative at one of the two General Committee Meetings which take place between two successive General Assemblies. This had already been suggested during the past triennium.

(b) *Statutes*. A certain number of changes have been made to the statutes, the most important ones being to ensure parity between the Scientific Union Members and the National Scientific Members: equality of voting power at the General Assembly, equal numbers of elected representatives of the National Scientific Members and of representatives designated by the Scientific Union Members (one for each Union) on the General Committee, single scale of dues for both types of Member, with Categories ranging from 1 to 50. The Standing Committees on Admissions and on Structure and Statutes have been merged. At the preceding General Assembly, the position of President-elect had been suppressed.

(c) *Admissions*. Three new Unions have been admitted to ICSU: International Union of Anthropological and Ethnological Sciences (IUAES); International Society of Soil Sciences (ISSS); International Brain Research Organization (IBRO); and eight National Scientific Members.

(d) *Elections*. Dr J. C. I. Dooge, Ireland, was elected President of ICSU and Dr L. J. Cohen, UK, was elected Secretary General. M. Petit, France, remained Treasurer.

II. Report on and discussions of the scientific activities of ICSU and of its Interdisciplinary Bodies.

The following bodies were discussed:

Committee on Space Research (COSPAR).

Scientific Committee on Solar–Terrestrial Physics (SOCOSTEP).

Committee on Water Research (COWAR).

International Council on Laboratory Animal Science (ICLAS).

Committee on Science and Technology in Developing Countries (COSTED).

Committee on Science in Central, Eastern Europe and the Former Soviet Union (COMSCEE). The role of this Committee is to promote the role of science in rebuilding Central and Eastern Europe and to help scientists and scientific research in these countries. It has been considered that the action of this Committee is a long-range one and it was decided to transform it from an *ad hoc* Committee to a special Committee. The representative of the IUCr has been elected a member of that Committee.

Standing Committee on the Free Circulation of Scientists (SCFCS). This committee has been very successful. Recently, it ensured that *bona fide* scientists from all parts of the former Republic of Yugoslavia were able to publish personal scientific papers in internationally distributed scientific journals. The General Assembly, considering that this action should be amplified in order to help avoid possible violations of free collaboration among scientists and free exchange of scientific information, decided to widen the mandate of the Committee and to change its name to Standing Committee on Freedom in Conduct of Science, with the same acronym. The General Assembly also encourages its members to consider the impact of increasing charges for scientific meetings and of page charges applied by some journals on science and developing countries and to bear in mind the position of scientists in developing countries when setting these fees or prices.

Scientific Committee on the Application of Science to Agriculture (CASAF). It was decided to terminate this committee in its present form; the establishment of a new committee related to agriculture and forests will be investigated.

Committee on Genetic Experimentation (COGENE).

Scientific Committee on Biotechnology (COBIO-TECH). The possibility of merging this committee and COGENE was discussed at great length, but it was finally decided to postpone this idea.

Committee on the Teaching of Science (CTS). In view of strengthening the action in this direction and to widen its scope, it was decided to transform this committee into a Committee on Capacity Building in Science with a small number of members (ten). A meeting of the Chairpersons of the Teaching Commissions of the various Unions will precede that of the new committee.

ICSU Press. This committee gives advice to the Unions in all matters related to publishing. ICSU has established an International Network for the Availability of Scientific Publications (INASP). A new activity of

ICSU Press is related to the emphasis now given to electronic publishing. Strong ties have been established between ICSU Press and the IUCr, which is at the forefront of developments in this field.

III. Reports on scientific issues of major interest and on international programmes where ICSU is involved

The following problems were reported on and discussed: population issues; World energy supplies; nuclear waste; adverse environmental impacts on astronomy; water quality; technological advances in the biosciences; Earth system research; natural disasters; biodiversity; follow up on ASCEND (ICSU Conference on an Agenda of Science for Environment and Development into the 21st Century) and UNCED (UN Conference on Environment and Development).

IV. Scientific programme

The following seminars took place, in cooperation with scientists from Chile and other Latin American countries: To the Biodiversity Convention and Beyond; El Niño and Related Phenomena; Ozone Depletion; Megatelescopes for the Southern Sky; Scientific Aspects of Natural Disasters; Science and Food Security in the 21st Century; Population and Human Reproduction.

Scientific contacts took place between participants to the ICSU General Assembly and Chilean scientists. The IUCr delegates took this opportunity of visiting the Chilean crystallographers and the Executive Secretary demonstrated the use of the CIF at the University of Chile.

V. ICSU Press Exhibition

ICSU Press had organized an exhibition of scientific books and publications where the IUCr was very well represented. An ongoing series of demonstrations of software took place in this framework and the IUCr Executive Secretary made daily demonstrations of the possibilities of CIF and of the advances of the IUCr in the matters of checking and electronic publishing.

VI. Resolutions

The General Assembly adopted resolutions on the following topics: the danger of outer space advertizing; electromagnetic pollution from the earth and extraterrestrial objects; biodiversity and taxonomy; brain research; animal research; patenting of partial human DNA sequences.

VII. Next meeting

The next meeting of the ICSU General Committee will take place in October 1994 in Morocco.

ICSU Committee on Data for Science and Technology (CODATA)

The major CODATA activities for 1993 were the following meetings. In February, the Commission on Industrial Data and the CEC held a joint Workshop on Materials Data for Computer Aided Engineering in Germany. Also in Germany, in March, the Task Group on Biological Macromolecules organized a colloquium on Why and How to Sequence a Genome, featuring lectures from the major international genome initiatives. Immediately following, the Task Group held a joint meeting with the Commission on Standardized Terminology for Access to Biological Data Banks to exchange information and ensure linkage of their activities. In September, the Task Group on Biological Macromolecules convened a symposium entitled CODATA International Workshop of Epitope Data in Japan and the Task Group on World Data Depository for Experimental Data on Thermophysical Properties sponsored a workshop on Thermophysical Property Data Banks and Process Simulators in Poland. Finally, in November, the Task Group on Artificial Intelligence and Computer Graphics arranged an international workshop on Decision Making in Science and Technology: Design Needs in Materials Science in France. In addition, six meetings of other Task Groups and Commissions took place. The *ad hoc* Committee on Data Issues, convened by ICSU, with representatives from CODATA, the Federation of Astronomical and Geographical Data Analysis Services (FAGS), the Panel on the World Data Centre (WDC) and the International Geosphere-Biosphere Programme (IGBP) Data Information Service (DIS), prepared and presented an interim report entitled *Report on ICSU Activities in Data and Information* to the ICSU General Assembly in October. CODATA provided secretariat to the Committee. For the same General Assembly, at the request of ICSU, CODATA prepared and submitted a report on data activities in the Scientific Unions. Continued attention was paid to data needs, accessibility and activities in developing countries.

ICSU Committee on Science and Technology in Developing Countries – International Biosciences Network (COSTED-IBN)

A certain lack of communication of COSTED has been noted in the past. Its President has promised an improvement in this direction. Guidelines for applicants of grants will be prepared. The Visiting Professorship Programme (similar to that of the IUCr) is working well, and could be used by the IUCr as a complement to its own programme. A very important decision was taken at the 24th ICSU General Assembly in Santiago, Chile, 4–8 October 1993, to merge COSTED with the International Biosciences Network (IBN), which is a joint ICSU–Unesco undertaking established to assist developing

countries build up their capacities in the biosciences. The Physics, Chemistry and Mathematics working group concluded that it was not realistic to establish such a network in these disciplines.

ICSU Committee on Space Research (COSPAR)

The 50th COSPAR Bureau Meeting was held 11–12 May 1993 under the Chair of its President, Professor W. I. Axford, in Paris, France. Among the 20 items on the Agenda, the following two topics are of general interest.

(i) The 30th COSPAR Scientific Assembly and Associated Activities, to be held in the Congress Centrum, Hamburg, Germany, 11–21 July 1994. The preparation of this large Congress of 1700 expected participants was the main COSPAR activity of 1993.

(ii) In 1994, the new COSPAR President and Vice-President and new Bureau and Finance Committee Officers had to be elected. The elections were performed during the 30th COSPAR Scientific Assembly in Hamburg. For this purpose, a Nomination Committee under the Chair of Professor D. J. Southwood was established.

COSPAR has sponsored or co-sponsored eight scientific meetings in various countries. The following National Institutions became new COSPAR Members in 1993: Chinese Academy of Sciences, Czech Academy of Sciences and Slovak Academy of Sciences (successors to Czechoslovakia), Iranian Remote Sensing Center.

ICSU Committee on Capacity Building in Science (CCBS)

At the ICSU General Assembly in Santiago, Chile, in October 1993, it was decided to transform the Committee on the Teaching of Science (CTS) into a Committee on Capacity Building in Science with a small number of members (ten). A meeting of the Chairpersons of the Teaching Commissions of the various Unions will precede that of the new committee.

Finances

The audited accounts of the year 1993 are given at the end of this Report. For comparison, the figures for 1992 are provided in italics. The accounts are presented in Swiss Francs.

The Unesco rates of exchange, as issued by the ICSU Secretariat, have been used in the preparation of these accounts. As a consequence of the many fluctuations in exchange rates during the year, the following procedure has been adopted for the accounts. Assets and liabilities in currencies other than Swiss Francs at 31 December 1993 have been translated into Swiss Francs in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into Swiss Francs by applying the rates of

exchange appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, an apparent gain has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 73 291. This gain has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1993. It should be noted that this gain in Swiss Francs is not a real gain of money, but rather a gain on paper resulting from the accounts being expressed in Swiss Francs.

Investments are noted in the balance sheet at their market value at 31 December 1993. The difference between revalued cost and market value has been shown as an adjustment in order that the investments can be stated at cost. This prevents the fluctuations in value from influencing the General Fund. The revalued cost is obtained by converting the cost of investments in the currencies of purchase into Swiss Francs using the exchange rates operative on the balance sheet date.

The total of SwFr 790 391 with the banks at the end of the year was represented by US \$94 175 with Merrill Lynch, £285 097 with National Westminster Bank and SwFr 7 157 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, excluding stocks of unsold publications but including the gain of SwFr 73 291 resulting from fluctuations in rates of exchange, have increased during the year, from SwFr 5 325 909 to SwFr 5 685 546.

Transfers of SwFr 60 000 and SwFr 40 000 were made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund and the *International Tables* Fund, respectively. A transfer of SwFr 40 000 was made to the Research and Education Fund from the *Acta Crystallographica* Fund and a transfer of SwFr 15 000 was made to the Ewald Fund from the General Fund. A transfer of SwFr 25 000 was made to the President's Fund from the General Fund to provide additional funds for cases of special need.

Beneath the detailed figures of the expenditure and income for each fund account, the balance at 1 January, the difference between income and expenditure for the year and the fluctuations in rates of exchange during the year are given, showing how the balance at 31 December is obtained.

The General Fund account shows a deficit of SwFr 96 228, before the transfers totalling SwFr 40 000 to the President's Fund and the Ewald Fund, as compared with a deficit of SwFr 8 989 in 1992, before transfers totalling SwFr 195 000 to the Research and Education Fund, the President's Fund and the Ewald Fund. The administrative expenses were SwFr 263 472 in 1993 as compared with SwFr 304 323 in 1992. Of this amount, SwFr 79 041 was charged to the publications of the Union.

SwFr 9 956 was given for general support of scientific meetings, in addition to SwFr 48 763 for financial support to young scientists attending meetings, which

appears in the expenses of the Research and Education Fund, and SwFr 9 610 in special grants from the President's Fund. SwFr 62 151 was spent on the Sixteenth General Assembly and Congress and SwFr 41 050 in assisting the work of the non-publishing Commissions. The cost of the *IUCr Newsletter* was SwFr 47 561. The expenses of the Union representatives on other bodies were SwFr 3 605. The cost of the two Finance Committee meetings held in 1993 was SwFr 12 220, while the Executive Committee meeting cost SwFr 68 131. The Union received SwFr 18 522 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 131 720. Interest on bank accounts and investments credited to the General Fund was SwFr 173 820.

The President's Fund, the Publications and Journals Development Fund, the Research and Education Fund and the Ewald Fund received interest, at a nominal rate of 8% per annum, on the balances in the funds.

The President's Fund therefore received interest of SwFr 2 120, in addition to the already mentioned transfer of SwFr 25 000 from the General Fund. Grants totalling SwFr 9 610 were paid from the fund.

The *Acta Crystallographica* account for 1993 shows a surplus of SwFr 286 923 before the transfer of SwFr 100 000 to other fund accounts, as compared with a surplus of SwFr 275 139 in 1992 before transfers of SwFr 150 000.

The subscription rates were increased for 1993. In its first year of publication, the new *Section D* of *Acta Crystallographica* was distributed free of charge to subscribers to *Sections A* and *B*. The number of paid subscriptions to all sections of *Acta*, including 92 personal subscriptions in 1992 and 89 in 1993, decreased from 1005 in 1992 to 962. For the number of paid subscriptions to the separate sections of the journal, those to *Section A* increased from 276 in 1992 to 294, those to *Section B* increased from 208 to 218 and those to *Section C* increased from 144 to 147. As usual, the cost of the technical editing office has been divided between the *Acta Crystallographica* and the *Journal of Applied Crystallography* accounts in percentages based on the number of text pages published during the year. The technical editing costs for *Acta Crystallographica* were SwFr 614 311 as compared with SwFr 593 862 in 1992. The journal's accounts have also been charged

with administration expenses as in previous years and as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a surplus of SwFr 57 026, as compared with a surplus of SwFr 52 221 before a transfer of SwFr 50 000 to the Publications and Journals Development Fund in 1992. The number of subscriptions, including 108 personal subscriptions in both 1992 and 1993, decreased from 1006 in 1992 to 971 in 1993.

The *Structure Reports* account shows a surplus of SwFr 61 777 in 1993 as compared with a deficit of SwFr 9 357 in 1992. One A Series volume and three B Series volumes were published in 1993 (one A Series Volume and one B Series volume in 1992). Editorial expenses were SwFr 46 972 as compared with SwFr 90 188 in 1992. The net income from sales was SwFr 241 560 in 1993 as compared with SwFr 143 172 in 1992.

The *International Tables* account shows a surplus of SwFr 113 426 before a transfer of SwFr 40 000 to the Publications and Journals Development Fund as compared with a surplus of SwFr 46 637 in 1992. Volume B and the third, revised edition of the *Brief Teaching Edition of Volume A* were published in 1993. The net sales income of SwFr 227 883 derived mostly (and fairly equally) from Volumes A, B and C.

The Book Fund is credited with the sales of the remaining publications of the Union including those of *Molecular Structures and Dimensions*, for which until 1991 there had been a separate fund account. The main sales income was from the *Historical Atlas of Crystallography*, edited by J. Lima de Faria.

As mentioned earlier, the income for the President's Fund account, the Publications and Journals Development Fund account, the Research and Education Fund account and the Ewald Fund account includes interest as well as transfers from other fund accounts. In the Publications and Journals Development Fund account, the expenses of SwFr 159 872 for computer expenses, including the purchase of computing equipment for the Chester office, relate to the technical editing of the journals, software development and the provision of on-line services. SwFr 48 763 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union, was charged to the Research and Education Fund account.

International Union of Crystallography Balance Sheet as at 31 December 1993

	Swiss Francs		Swiss Francs	
	1993	1992	1993	1992
FUND ACCOUNTS				
General Fund	1,053,301	1,053,301	27,803	40,935
President's Fund	36,114	36,114	762,588	452,834
<i>Acta Crystallographica</i>	1,783,370	1,783,370		493,769
<i>Journal of Applied Crystallography</i>	435,705	435,705		17,405
<i>Structure Reports</i>	2,557	134,055		356,679
<i>International Tables</i>	3,107	164,550		30,260
Book Fund	11,435	11,435	13,350	898,113
Publications and Journals	9,562	741,785	1,057,673	171,776
Development Fund	745,264	745,264		726,337
Research and Education Fund	700,989	700,989	291,874	4,583,625
Ewald Fund	261,126	261,126	765,799	321,028
	5,325,909	5,325,909	4,905,970	4,904,653
			13,777	15,947
			5,685,546	5,325,909
			5,685,546	5,325,909
			5,696,748	4,904,653
			4,905,970	4,583,625
			790,778	321,028
			5,696,748	4,904,653
			13,777	15,947
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			13,777	15,947
			5,685,546	5,325,909
			5,685,546	5,325,909
			5,696,748	4,904,653
			4,905,970	4,583,625
			790,778	321,028
			5,696,748	4,904,653
			13,777	15,947

President's Fund Account for the year ended 31 December 1993

	Swiss Francs		Swiss Francs	
	1993	1992	1993	1992
Grants	9,610	13,818	2,120	1,005
<i>Excess of income over expenditure carried to balance sheet</i>	17,510	12,187	25,000	25,000
	27,120	26,005	27,120	26,005
Balance at 1 January	36,114	26,377		
Difference between income and expenditure	17,510	12,187		
Fluctuations in rates of exchange	700	-2,450		
Balance at 31 December	54,324	36,114		
			Interest (Note 6)	
			Transfers from other Funds:	
			General Fund	

Acta Crystallographica Account for the year ended 31 December 1993

	1993		1992		1993		1992	
	Swiss Francs		Swiss Francs		Swiss Francs		Swiss Francs	
Publication expenses:								
Printing and binding Volume 49 (1992 Volume 48)	633,342		565,172		1,970,340		1,850,963	
Distribution and postage	120,286		121,224		28,432		23,308	
Airfreight costs	25,364		41,747		62,127		52,636	
	<u>778,992</u>		<u>728,143</u>		<u>-1,393</u>		<u>4,855</u>	
					684		964	
Biological crystallography section Index to Volume 48 (1992 Volume 47)	14,259		22,558		2,060,190		1,932,726	
Documenter	31,440		17,024		139,914		131,199	
Supplement to Volume A49	89		-					
Microfiche costs		824,780		776,635		1,920,276		1,801,527
						1,850		1,433
Editorial expenses:								
Editorial honoraria	53,268		40,761					
Secretarial assistance	19,537		23,554					
Postage, travel and sundries	64,026		24,536					
Technical Editing:								
Salaries and expenses	570,997		567,173					
Computer expenses	37,796		20,713					
Depreciation of office equipment	5,518		5,976					
		751,142		682,713				
Administration expenses		59,281		68,473				
Transfers to other Funds:								
Publications and Journals	60,000		150,000					
Development Fund	40,000		-					
Research and Education Fund		100,000		150,000				
		186,923		125,139				
		<u>1,922,126</u>		<u>1,802,960</u>		<u>1,922,126</u>		<u>1,802,960</u>
<i>Excess of income over expenditure carried to balance sheet</i>								
Balance at 1 January	1,783,370		1,779,195					
Difference between income and expenditure	186,923		125,139					
Fluctuations in rates of exchange	25,730		-120,964					
Balance at 31 December	<u>1,996,023</u>		<u>1,783,370</u>					

Journal of Applied Crystallography Account for the year ended 31 December 1993

	1993		1992		1993		1992	
	Swiss Francs		Swiss Francs		Swiss Francs		Swiss Francs	
Publication expenses:								
Printing and binding Volume 26 (1992 Volume 25)	87,190		85,991		351,586		335,730	
Distribution and postage	20,433		24,373		7,148		5,128	
Airfreight costs	7,595		7,865		7,714		7,753	
Net loss on reprints	115,218	118,359	118,229	119,660	1,038		1,300	
	3,141		1,431		367,486		349,911	
Editorial expenses:								
Editorial honoraria	7,078		4,952		25,111		23,860	
Secretarial assistance	2,510		2,797					
Postage, travel and sundries	11,897		1,963					
Technical Editing:								
Salaries and expenses	118,101		116,168					
Computer expenses	6,670		4,242					
Depreciation of office equipment	974	147,230	1,224	131,346				
Administration expenses		19,760		22,824				
Transfers to other Funds:								
Publications and Journals				50,000				
Development Fund		57,026		2,221				
Excess of income over expenditure carried to balance sheet		342,375		326,051		342,375		326,051
Balance at 1 January		435,705		463,037				
Difference between income and expenditure		57,026		2,221				
Fluctuations in rates of exchange		6,435		-29,553				
Balance at 31 December		499,166		435,705				

International Tables Account for the year ended 31 December 1993

	1993	Swiss Francs	1992	Swiss Francs	1993	Swiss Francs	1992
Publication expenses:							
Reprinting Volume A	—						
Printing and Typesetting Volume B	47,820		40,471		90,192		87,410
Printing and Typesetting Volume C	29,302		48,364		102,160		—
		77,122	88,835		5,229		5,939
					11,902		17,032
					98,467		121,674
Editorial expenses:							
Editorial honoraria	6,725		8,465		307,950		232,055
Secretarial assistance, postage and office equipment	28,169		12,354		80,067		60,334
Technical Editing	2,441		15,430				
		37,335	36,249				
Transfer to other funds:							
Publications and Journals Development Fund		40,000	—				
		73,426	46,637				
		227,883	171,721		227,883		171,721
<i>Excess of income over expenditure carried to balance sheet</i>							
Balance at 1 January	164,550		129,062				
Difference between income and expenditure	73,426		46,637				
Fluctuations in rates of exchange	3,107		-11,149				
		241,083	164,550				
Balance at 31 December							

Research and Education Fund Account for the year ended 31 December 1993

	1993	Swiss Francs 1992		1993	Swiss Francs 1992
Expenses:			Transfers from other funds:		
Young Scientists' Support	48,763	90,850	Acta Crystallographica	40,000	150,000
1989 ECM Fund creditor	6,399	2,697	General Fund	—	44,336
Visiting Professorship Programme	-4,714	9,665	Interest (Note 6)	52,043	—
<i>Excess of income over expenditure carried to balance sheet</i>	<u>41,595</u>	<u>91,124</u>		<u>92,043</u>	<u>194,336</u>
Balance at 1 January	700,989	657,412			
Difference between income and expenditure	41,595	91,124			
Fluctuation in rates of exchange	9,697	-47,547			
	<u>752,281</u>	<u>700,989</u>			
Balance at 31 December	<u>752,281</u>	<u>700,989</u>			

Ewald Fund Account for the year ended 31 December 1993

	1993	Swiss Francs 1992		1993	Swiss Francs 1992
Selection Committee and expenses	—	1,692	Transfers from other funds:	15,000	20,000
Ewald prize	37,250	—	General Fund	17,910	19,173
			Interest (Note 6)	—	—
<i>Excess of income over expenditure carried to balance sheet</i>	<u>—</u>	<u>37,544</u>	<i>Excess of expenditure over income carried to balance sheet</i>	<u>4,340</u>	<u>—</u>
				<u>37,250</u>	<u>39,173</u>
Balance at 1 January	261,126	241,294			
Difference between income and expenditure	-4,340	37,544			
Fluctuations in rates of exchange	3,355	-17,712			
	<u>260,141</u>	<u>261,126</u>			
Balance at 31 December	<u>260,141</u>	<u>261,126</u>			

Cash Flow Statement for the year ended 31 December 1993

	1993	Swiss Francs	1992
Net cash inflow/outflow from operating activities	217,166		-388,986
Returns on investments			
Interest received	47,482	62,520	
Investment income	245,242	312,396	
Net cash inflow from returns on investments	292,724		374,916
Investing activities			
Purchase of office equipment	-6,454	-5,680	
Purchase of investments	-1,854,509	-1,568,914	
Disposal of investments	1,672,322	1,717,825	
Net cash outflow/inflow from investing activities	-188,641		143,231
Increase in cash and cash equivalents before and after financing	321,249		129,161

Notes to the Financial Statements

1. Accounting Policies

(a) Accounting convention

The financial statements are prepared under the historical cost convention and in accordance with applicable accounting standards. The particular accounting policies adopted are described below.

(b) Rates of exchange

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

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

The revalued cost of fixed assets and investments referred to in the balance sheet and Note 4 to the accounts arises by applying this method.

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

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

(c) Publication costs

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

(d) Stocks of unsold copies of Union publications

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

(e) Expenditure on premises

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

(f) Depreciation

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

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

(g) Investment income

Notional dividend income re-invested in accumulation investment funds is treated as income when declared and added to the accumulated cost of investments. Other dividends are recognized when received.

2. Rates of exchange

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

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

	1993	1992
Netherland Guilders	1.2887	1.2500
Danish Crowns	4.5662	4.2918
Pounds Sterling	0.4496	0.4583
US Dollars	0.6711	0.6944

The net assets of the Union at 1 January 1993 (SwFr 5,325,909) would have had the value of US \$3,698,311 or £2,440,864 if expressed in those currencies.

At 31 December 1993, these assets (SwFr 5,685,546) would have had the value of US \$3,815,569 or £2,556,221 respectively, being an increase of

US \$117,258 or an increase of £115,357 from the previous year.

3. Taxation

As an association incorporated in Switzerland, the Union is exempt from Swiss Federal and Geneva Cantonal tax. Under the terms of the United Kingdom/Switzerland Double Taxation Agreement dated 8 December 1977, investment income arising within the United Kingdom under present circumstances will not be subject to United Kingdom tax.

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

4. Investments

	Holding at revalued cost 1 January 1993	Additions during the year	Revalued cost of disposals/ redemptions during the year	Swiss Francs Fluctuations in rates of exchange	Holding at revalued cost 31 December 1993	Market value 31 December 1993
Held by Merrill Lynch						
(Corporate Government Securities)						
US \$20,692 GNM P146535-2016	23,615	—	-7,921	766	16,460	18,221
US \$58,544 GNM P169332-2016	70,278	—	-20,480	2,302	52,100	57,687
(Mutual Funds/Unit Investment Trusts)						
2,231 Units ML Capital Fund/CLB (US \$)	129,680	—	—	4,503	134,183	153,446
US \$4,750 Temple Worldwide Fund G	72,162	—	-75,670	3,508	—	—
US \$4,750 Temple Worldwide Fund I	72,162	—	-74,668	2,506	—	—
US \$785 Haussman Holdings	438,032	—	—	15,209	453,241	918,623
US \$60,139 Global Allocation Portfolio Class A	—	90,804	—	-1,203	89,601	88,667
US \$101,000 Meridian Funds Global Government Fund	—	150,490	—	—	150,490	153,753
US \$101,675 Permal Investment Holdings NV	—	153,530	—	-2,034	151,496	158,140
10,568 Units Meridian Charter Income Fund	—	167,860	—	-1,172	166,688	169,586
(Certificates of deposit)						
US \$50,000 FHLMC 8.5% Sep. 15 20RG	42,447	—	-43,115	668	—	—
US \$50,000 CITI CDT Cards 8.25% Nov. 15 1993	72,113	—	-74,617	2,504	—	—
US \$75,000 British Gas Finance	111,046	—	—	3,856	114,902	124,999
US \$75,000 GEC	108,990	—	—	3,784	112,774	119,388
US \$8,000 MLST World income portfolio	115,574	—	-121,192	5,618	—	—
Held by Foreign & Colonial						
34,298 Units Reserve Asset Fund Class D (US \$)	476,635	32,780	—	16,549	525,964	572,168
11,964 Units Reserve Asset Fund Class L (£)	422,855	20,016	—	6,904	449,775	577,298
43,064 Units Reserve Asset Fund Class X (£)	469,521	28,245	—	6,595	504,361	491,804
17,617 Units Reserve Asset Fund Class H (ECU)	347,332	—	-343,816	-3,516	—	—
20,929 Units Reserve Asset Fund Class C (US \$)	468,219	136,695	—	14,753	619,667	646,049
11,080 Units Reserve Asset Fund Class M (US \$)	270,164	8,493	—	9,381	288,038	309,454
5,028 Units Reserve Asset Fund Class E (£)	—	194,058	—	-1,283	192,775	199,737
375,000 Units UK Treasury 7.75% 22/9/2006	—	871,538	—	11,917	883,455	937,728
Held by National Westminster Bank						
£Nil (1992 £400,000) cash on one year deposit	872,800	—	-877,600	4,800	—	—
	<u>4,583,625</u>	<u>1,854,509</u>	<u>-1,639,079</u>	<u>106,915</u>	<u>4,905,970</u>	<u>5,696,748</u>

Investments are noted in the balance sheet at their market value at 31 December 1993. The difference between revalued cost and market value has been shown as an adjustment in order that the investments can be stated at revalued cost. This prevents the fluctuation in

market value from influencing the General Fund.

The revalued cost is obtained by converting the cost of investments in the currencies of purchase into Swiss Francs using the exchange rates operative on the balance sheet date.

5. Bank interest

	Swiss Francs	
	1993	1992
National Westminster Bank PLC		
Manchester SMMO Account	–	10,545
Manchester Business Reserve Account	4,065	7,600
Manchester Capital Reserve Account	19,778	10,111
Amsterdam–Rotterdam Bank NV		
Current Guilder Account	3	4
Guilder Savings Account	–	35
US \$ Accounts	–	6
Union Bank of Switzerland		
Current Swiss Francs Account	–	28
Merrill Lynch		
CMA Account	4,801	3,558
Foreign & Colonial		
Cash balances	152	149
Petty cash accounts	5	–
Interest from Munksgaard	18,678	30,484
	<u>47,482</u>	<u>62,520</u>

6. Investment income

	Swiss Francs			Swiss Francs	
	1993	1992		1993	1992
Meridian Charter	2,635	–	Allocated to President's Fund	2,120	1,005
GEC	8,859	8,121	Allocated to Ewald Fund	17,910	19,173
British Gas	9,647	9,220	Allocated to Publications and		
ML Capital fund	8,327	8,437	Journals Development Fund	46,831	44,134
P146535–2016	1,949	2,429	Allocated to Research and		
P169332–2016	6,105	6,994	Education Fund	52,043	44,336
Temple Worldwide Fund G	698	5,942	Balance left in General Fund	126,338	203,748
Temple Worldwide Fund I	6,454	4,583			
Foreign and Colonial Fund M	8,493	7,872			
Foreign and Colonial Fund H	–	31,407			
Foreign and Colonial Fund X	28,244	54,004			
Foreign and Colonial Fund D	32,780	31,578			
Foreign and Colonial Fund L	20,016	16,985			
Foreign and Colonial Fund C	23,095	–			
Foreign and Colonial Fund E	14,456	–			
FHLMC	2,560	5,738			
MLST World income portfolio	3,241	7,080			
CITI CDT Cards	5,548	5,827			
National Westminster Bank deposit account	62,135	106,179			
	<u>245,242</u>	<u>312,396</u>		<u>245,242</u>	<u>312,396</u>

7. Profit/loss on disposal/redemption of investments

	Swiss Francs	
	1993	1992
Proceeds	1,672,322	1,717,825
Revalued cost	1,639,079	1,784,451
Profit/loss allocated to General Fund	<u>33,243</u>	<u>–66,626</u>