

## International Union of Crystallography

### Report of the Executive Committee for 1994

#### Meetings

The IUCr sponsored the following Meetings held during 1994:

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 Modeling – Theory and Experiment, Kloster Irsee near Kaufbeuren, Germany, 16–20 May 1994.
3. 21st Crystallographic Course ‘Crystallography of Molecular Biology’, Erice, Italy, 27 May–5 June 1994.
4. 1994 American Crystallographic Association Annual Meeting, Atlanta, USA, 26 June–1 July 1994.
5. Symposium on New Trends in Small Molecule Crystallography, Atlanta, USA, 26 June –1 July 1994.
6. Summer School on Electron Crystallography – Theory and Practice, Bristol and Bath, England, 11–15 July 1994.
7. Third ACA Summer Course on Crystallography, Pittsburgh, USA, 1–12 August 1994.
8. Sagamore XI Conference, Brest, France, 7–12 August 1994.
9. Pre-ECM-15 Symposium on Organic Crystal Chemistry, Poznan-Rydzyna, Poland, 23–27 August 1994.
10. Fifteenth European Crystallographic Meeting (ECM-15), Dresden, Germany, 28 August–2 September 1994.
11. International Summer School on Growth and Characterization of Materials, Cracow, Poland, 4–14 September 1994.
12. Second European Symposium on X-ray Topography and High Resolution Diffraction, Berlin, Germany, 5–7 September 1994.
13. International Conference on Aperiodic Crystals, Lausanne/Les Diablerets, Switzerland, 18–22 September 1994.
14. Meeting on Neutrons in Biology, Santa Fe/Los Alamos, USA, 24–28 October 1994.
15. Southern Africa Powder Diffraction Workshop, Pretoria, South Africa, 24–27 October 1994.
16. XIII Iberoamerican Congress of Crystallography and III Iberoamerican School of Crystallography, Montevideo, Uruguay, 4–9 December and 12–16 December 1994.

The Executive Committee met in Chester, England, in June. The Finance Committee met in Chester, England, in March, to prepare its advice and recommendations on finances, establishment and staff matters. The most important items dealt with by the Executive Committee at its Meeting, and in postal ballots, were:

- (1) editorial policy, pricing policy and subscription rates, approval of appointments of Co-editors, separate editorial boards for *Acta Crystallographica* and other matters concerning the IUCr journals;
- (2) publication of the new *Journal of Synchrotron Radiation*;
- (3) staffing requirements in the IUCr office in Chester;
- (4) upgrading of office technology in the IUCr office in Chester;
- (5) cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and Fachinformationszentrum Karlsruhe;
- (6) the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* papers and other uses of

CIF, patent application and adoption of the STAR file and CIF by other bodies;

- (7) progress with Volumes A, B, C, D and E of *International Tables for Crystallography* and consideration of possible further volumes;
- (8) the IUCr *Newsletter*;
- (9) the Ninth Edition of the *World Directory of Crystallographers*;
- (10) approval of publications, jointly with the Oxford University Press, in the IUCr/OUP Book Series;
- (11) approval of the audited accounts for the previous year;
- (12) the General Fund estimates and the level of the unit contribution;
- (13) investment policy;
- (14) funding and uses of the Publications and Journals Development Fund and the Research and Education Fund;
- (15) appointment of the Selection Committee for the fourth Ewald Prize;
- (16) report of the Sub-committee on Statutes and By-Laws;
- (17) applications for membership of the IUCr;
- (18) free circulation of scientists;
- (19) discussion of the arrangements for the Seattle General Assembly and Congress;
- (20) sponsorship and financial support for Meetings, including young scientists’ support;
- (21) review of the activities of the Commissions.

#### Publications

Volume 50 of *Acta Crystallographica*, Volume 27 of the *Journal of Applied Crystallography* and the Inaugural Issue of the *Journal of Synchrotron Radiation* 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 Sixteenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (1995), A51, 596–648].

#### Work of the Commissions

##### *Commission on Journals*

##### *Acta Crystallographica*

A number of significant changes were made to the Golden Jubilee volume of *Acta Crystallographica (Acta)* in 1994. The appointment of separate editors allowed each section to benefit from having the full energies of an editor devoted strictly to the development of the individual section. The journal covers were redesigned in distinctive colors with space allocated for graphics, the contents pages revamped to include a short synopsis of each paper, and a single presentation format was adopted. New *Notes for Authors* were published that mapped out the criteria for submitting manuscripts for the next decade. Topical Reviews, brief and focused review articles on

Table 1. Survey of the contents of the Union Journals

*Acta Crystallographica*

Vol.	Year	Number of pages*	Number of papers	Full Articles†		Short Communications‡	
				Number	Average length	Number	Average length
A46§	1990	998	150	126	7.0	24	1.5
B46		864	123	120	6.7	3	0.8
C46		2500	980	963	2.6	17	0.6
A47	1991	860	123	104	7.2	19	1.4
B47		1030	137	130	7.4	7	1.7
C47		2740	1076	1069	2.6	7	0.6
A48	1992	954	117	106	7.9	11	2.2
B48		856	125	113	7.4	12	1.9
C48		2280	914	906	2.5	8	0.6
A49§	1993	901	121	108	7.9	13	2.1
B49		1075	155	149	7.1	6	2.0
C49		2186	880	869	2.5	11	0.9
D49		604	72	62	9.0	10	3.0
A50	1994	798	103	91	8.1	12	1.4
B50		782	99	94	8.1	5	2.4
C50		2102	852	847	2.5	5	0.6
D50		920	135	121	7.2	14	3.0

*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
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
27	1994	1078	171	116	8.1	11	2.2	3	4.2	15	4.0	26	1.4

*Journal of Synchrotron Radiation*

Vol.	Year	Number of pages*	Number of papers	Full Articles		Short Communications		Computer Programs		Short Items¶	
				Number	Average length	Number	Average length	Number	Average length	Number	Average length
1	1994	106	15	15	6.7	-	-	-	-	-	-

\* Numbered pages excluding indexes.

† Including Lead Articles and Topical Reviews for Sections A, B and D, and Short Format Papers (now discontinued) for Section C.

‡ Including Fast Communications (now discontinued in *Acta*).

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

¶ Laboratory Notes, Letters to the Editor, Meeting Reports and Computer Program Abstracts.

timely topics, were introduced. These changes were designed to modernize the image of the journal, make it more visible in libraries, and make it easier to locate papers of importance to individual readers.

Volume 50 of *Acta* included 1189 papers with an overall total of 4602 pages. 1556 manuscripts were received by Co-

editors during 1994, a 7% increase over 1993. The number of papers submitted to the Managing Editor slightly increased to 1295. Median publication times for Full Articles in *Acta A* (6.3 months), *Acta B* (6.5 months), and *Acta D* (5.2 months) increased slightly, and in *Section C* the median publication time for Regular Structural Papers increased to 6.5 months. These

increases are linked to a high editing backlog during 1993 and early 1994 that has been significantly reduced.

New *Acta* Co-editors appointed during the year were G. Ferguson, J. Harada, T. Janssen, P. G. Jones, L. L. Koh, R. E. Marsh, R. Parthasarathy, J. J. Stezowski, M. R. Taylor and Z. Zhang. M. Hursthouse retired from his Co-editorial duties at the end of the year.

#### *Section A (A. Authier, Editor)*

Being more traditional in nature, the changes in *Section A (Foundations of Crystallography)* affected only the format and not the content. The total number of papers published in *Section A* has decreased slightly over the past few years, but the actual number of papers received by Co-editors increased in 1994. To increase submissions, a more active policy of commissioning Lead Articles was instituted. Two were published during the year, and eight more are being written, with the aim to have one per issue. Likewise, the first five Topical Reviews were commissioned and it is expected that once readers become familiar with these papers, successive reviews will be submitted by potential authors. Efforts are on-going to attract more Lead Articles and Reviews to *Section A*.

#### *Section B (F. H. Allen, Editor)*

*Section B (Structural Science)* continued to receive a constant flow of high-quality papers describing research across a broad range of topics in structural science. Increasingly, crystallographic results are being correlated with physical, chemical and biological properties, and we are receiving more papers describing crystallographic studies carried out in conjunction with other experimental or computational techniques. Discussions with other Editors about subject borderline papers were minimal and *Section B* now appears to have a clear niche in both the local (*Acta*) and the global publication activities in this area. High-quality Lead Articles were published on an occasional basis, and a number of invitations to write Topical Reviews were issued.

#### *Section C (S. R. Hall, Editor)*

The new *Notes for Authors* published for *Section C (Crystal Structure Communications)* placed particular emphasis on the use of electronic submissions using the CIF format. By the end of the year, over half of the *Acta C* submissions were being received in CIF format. During 1994, a number of adjustments were made to the editorial processing of *Acta C* manuscripts designed to reduce the workload for the Chester staff and improve the *Acta C* publication times. These included the introduction of fast-track processing for electronically submitted manuscripts devoid of checking errors; stricter criteria for the initial processing of submitted material; and the rewriting of *Review Guidelines* to promote consistent final acceptance standards across the review process. Finally, through the considerable efforts of the Chester staff, and some changes to handling procedures, the backlog of *Section C* manuscripts in the checking and editing streams was reduced from numbers of about 250 in mid-1994 to less than one hundred at the end of the year. The goal is to maintain these backlogs at below 50 from now on.

#### *Section D (J. P. Glusker, Editor)*

Six issues of *Section D (Biological Crystallography)* were published in 1994, one of which covered papers presented at the Fifth International Conference on Crystallization of Biological Macromolecules in August 1993. This issue was devoted to various aspects of the crystallization of biological macro-

molecules and contained 52 articles. The other issues covered a wide range of macromolecular crystallography, including reports of protein crystallizations, structure determinations of new macromolecules, from the points of view of methods development and reports of the actual structure determination, details and pitfalls of macromolecular structure refinement, features of macromolecular database access and management, and analyses of structural results in terms of, for example, enzyme mechanisms and drug-receptor binding.

#### *Journal of Applied Crystallography (A. M. Glazer, Editor)*

Volume 27 of the *Journal of Applied Crystallography (JAC)* was published during 1994, containing 116 Full Articles. The total number of pages was 1078, a 27% increase over 1993. Co-editors received 177 manuscripts for review during the year and submitted 160 papers to the Managing Editor. The median publication time for Full Articles was 7.3 months. J. S. Pedersen was appointed as a new *JAC* Co-editor during the year. *JAC* also began the year with a redesigned cover and contents page. The range of topics in the six volumes published covered equipment, theory, powder diffraction, single-crystal diffraction and synchrotron radiation. There was also an increase in contributions from the more biologically oriented researchers, especially in the areas of protein crystallization and flash-cooling techniques. An excellent Lead Article was published in the June issue on interpretation of diffuse X-ray scattering, and one of the diagrams from this paper has been selected for the journal's 1995 cover. Other important papers included one on Laue image analysis and a large paper on the Rietveld round robin (analysis of monoclinic  $ZrO_2$ ), undertaken by the IUCr Commission on Powder Diffraction.

#### *Journal of Synchrotron Radiation (J. R. Helliwell, S. S. Hasnain, H. Kamitsubo, Editors)*

During 1994, the *Journal of Synchrotron Radiation (JSR)* came into being with the publication of the Inaugural Issue in October. 15 Full Articles were published in Volume 1, comprising 100 pages. The median publication time was 3.7 months. The aim of the journal is to cover the full range of activity in the differing regions of the electromagnetic spectrum, from hard X-ray to VUV, and was borne out in the papers presented. In particular, there were papers covering synchrotron-radiation sources, beamlines and optics, detectors, electronics and data acquisition, sample chambers and environment, diffraction and spectroscopy. Unfortunately, there were no papers on imaging. Through the year, *JSR* had to compete in particular with the *Rev. Sci. Instrum.* Special Issue associated with the Triennial Synchrotron Radiation Instrumentation Congress held at SUNY, Stonybrook, in July 1994. The Inaugural Issue of *JSR* was well received in terms of its balanced representation of the field as well as the high standard of the papers and the production quality.

#### *Commission on International Tables*

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

The material for the fourth, revised edition of Volume A was submitted to the Technical Editor in January 1994; first proofs were read in September, second proofs in December 1994. The new edition is scheduled for publication in the spring of 1995. It will contain a complete set of new diagrams for the plane groups and the space groups, as well as new explanatory diagrams in Section 2.6. Furthermore, this edition will contain the new graphical and printed symbols for the 'double glide plane  $e$ ', introduced by the IUCr in 1992. This has necessitated

major changes in Section 1. A list of errata to the third edition of Volume A (1992) will appear in *Acta Cryst.* (1995), A51, 592–595.

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

The first edition of Volume B [full reference *International Tables for Crystallography* (1993). Volume B: *Reciprocal Space*, edited by U. Shmueli, 506 + xxii pp. ISBN 0-7923-2189-8. Dordrecht: Kluwer Academic Publishers] was the basis of the activities during 1994, which were mainly aimed at the preparation of the second edition of Volume B. This edition was decided upon in the previous year, 1993, following the appearance of Volume B. The editorial work dealt with several topics: (i) discussion of modifications of existing chapters with their authors, (ii) preliminary exchange of letters and e-mail messages with potential authors of new contributions and, subsequently, their formal invitation, and (iii) completion of a significant revision of Chapter 2.1, co-authored by the Editor.

As of now, the new contributions to the second edition deal with (i) application of direct methods to electron crystallography, (ii) X-ray and electron diffraction by polymers, and (iii) dynamical theory of neutron diffraction. Also, several existing chapters will have undergone more or less extensive revision, all aiming at a proper updating of the first edition.

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

The first edition of Volume C was published in March 1992. Early in 1993, it became evident that the first printing would become exhausted within a few months and it was decided to publish a reprint with corrections and additions rather than a simple reprint. Material for the amended reprint was solicited from all authors, consolidated, and sent to the Technical Editor in December 1993. There have been numerous delays at the printers, and publication of the reprint has been delayed to 1995. A list of the corrections will appear in *Acta Cryst.* (1995), A51, 441–444.

During the work on the reprint, all the authors were informed that a fully revised second edition was likely, and formal invitations to submit revisions, or entirely rewritten contributions, were issued in January 1994, with an official deadline of 31 December 1994. Few authors met that date, but most of the expected contributions arrived in January 1995, and reminder letters are being sent.

Those contributions that have arrived are being edited, and Part 1, most of Part 2, and some of Part 3 are already with the Technical Editor.

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

About one third of the manuscripts for Volume D have now been received by the Editor and work on coordinating them is progressing. Nearly all the others should be received by the end of 1995. The author of one chapter remains to be found.

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

Volume E consists of seven sections divided into two parts. Part 1: *Subperiodic Group Tables: Frieze Groups, Rod Groups and Layer Groups*, containing five sections, has been reviewed and sent to the Technical Editor. Part 2: *Space Group–Subperiodic Group Relationships* contains two sections. The first section, *Subperiodic Groups as Factor Groups of Reducible Space Groups, Plane Groups and Layer Groups*, is completed and under review. A first draft of the second section of Part 2, *Sectional Layer Groups*, has been written. It

is anticipated that a final version of Part 2 will be sent to the Technical Editor during the first half of 1995.

During 1994, preparations for two new volumes of *International Tables for Crystallography* were completed, and the appropriate proposals were submitted to the Executive Committee by the Commission Chairman (the designations and names of the two volumes below are still preliminary).

*Volume 'F'. N-Dimensional Space Groups; Editor T. Janssen (for the Nijmegen group): proposal submitted in May 1994*

This volume will consist of a printed volume and a diskette or CD-ROM with a computer program.

The program permits, dimension-independent, the generation of all  $n$ -dimensional space groups belonging to a given  $n$ -dimensional point group, in any desired orientation or setting. Input is a set of generators of the point group in  $(n \times n)$ -matrix form. For an  $n$ -dimensional space group, all data given in Volume A for the three-dimensional space groups can be calculated. This program would probably be the first 'electronic book' distributed and sold by the IUCr.

The accompanying printed volume will contain an introduction to  $n$ -dimensional crystallographic groups, a manual and a tutorial for the use of the software.

*Volume 'A1'. Maximal Subgroups of Space and Plane Groups; Editor H. Wondratschek (for a group of three authors): proposal submitted in December 1994*

This a companion to Volume A, in which the data on subgroups in Volume A are extended and completed as follows:

(i) All maximal subgroups of index 2, 3 or 4 are listed individually and not only by type.

(ii) All maximal subgroups of index  $> 4$  are listed implicitly as members of infinite series (these subgroups are always isomorphic).

(iii) All subgroups are listed either by their general positions or by a set of generators.

(iv) The matrix for the basis transformation and the column for the origin shift are added in short form.

(v) Conjugate subgroups are connected by a curly bracket.

The subgroup data for Volume A1 are essentially completed and will be transmitted to the Technical Editor in electronic form ( $\LaTeX$ ).

Both new proposed volumes are awaiting final approval by the Union's Executive Committee.

*Commission on Aperiodic Crystals*

Most of the efforts of this Commission were dedicated to organizing the Conference Aperiodic'94, which was held 18–22 September in Les Diablerets, Switzerland. According to its Terms of Reference, the Commission is to actively promote the organization of this series of Conferences on a triennial basis. All the members of the Commission acted as the Programme Committee and thus contributed to the success of the Conference by selecting a very high level of invited speakers and by a careful choice of abstracts. The Programme Committee took great care to ensure the interdisciplinary character of the Conference by maintaining a balance between quasicrystal, incommensurate and composite crystal, and polytype specialists. A full report of the Conference has been published elsewhere [IUCr Newsletter (1995), Vol. 3]. The Conference organizers took full advantage of the possibilities offered by the World Wide Web (WWW) by making the abstracts available first to the Programme Committee and

then to interested scientists. All the Conference information, including the programme, were available on Internet well in advance of the Conference. This was the first Meeting sponsored by the IUCr to operate within the frame of the WWW and the experiences gathered by the Committee could be transmitted to future Meeting organizers.

The next Meeting, Aperiodic'97, will be organized by our French colleagues and will take place in the Grenoble area. The Commission was also very active in coordinating other Meetings in the field of aperiodic crystals, namely the International School on Quasicrystals in Balatonfüred and the 5th International Conference on Quasicrystals in Avignon (both in May 1995). In particular, the Commission supported the organizers in their efforts to obtain financial help from the Executive Committee of the IUCr.

Following the establishment in 1993 of a checklist for the description of incommensurately modulated structures by the Commission, the *CIF Dictionary* for modulated structures is now being considered for approval by COMCIFS (the CIF Management Committee). In addition to the structure descriptors fulfilling the checklist, additional items concerning composite crystals have been considered. The Commission is further pursuing its work on this matter.

Contacts have been established with the IUCr Commission on *International Tables* regarding the possible inclusion of material concerning quasicrystals. This topic will continue to be studied by the two Commissions.

#### *Commission on Biological Macromolecules*

The Commission continued to be concerned with the deposition, validation, retrieval, dissemination and usage of macromolecular crystallographic data. The activities of the Brookhaven Protein Data Bank have received added momentum with the appointment of Joel Sussman as its Director. The PDB has also adopted new checking and classification procedures. The joint North American-European Community efforts in new ways of dealing with macromolecular data continue to make progress. The Commission has been keen that the available information pertaining to this area should be widely disseminated within the rest of the international macromolecular crystallographic community, who should also be encouraged to contribute to the on-going efforts. With this purpose in view, plans have been finalized to organize an International Seminar-cum-School on Macromolecular Crystallographic Data in Calcutta, India, 16–20 November 1995. The topics planned to be covered at the Meeting include protein data bank file structure and services available; validation tests and criteria for deposition of data; error and quality of crystallographic protein models; data-deposition procedure; comparison with NMR and other non-crystallographic models; dissemination of data; and use of structural data in knowledge-based molecular modelling, drug design, protein engineering, macromolecular structure analysis and elucidation of general principles of macromolecular architecture.

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

The Commission continued to promote the study of electron-density distributions in both real and momentum space by bringing together physicists, chemists and crystallographers, by coordinating projects and by organizing Conferences, Workshops and Schools.

#### *Meetings of the Commission*

The Commission met twice during the Sagamore XII Conference held in Brest, 7–12 August, and also held an Open Commission Meeting at which the Commission's projects were briefly reviewed and ideas for new projects canvassed. As a result of the latter activity, the Commission confirmed its wish to launch a project on the application of maximum-entropy methods to its field of interest. This project will have the active participation of M. Sakata, G. Bricogne and others. The next full Meeting of the Commission will take place during the General Assembly and Congress in Seattle, 8–17 August 1996, but a significant number of Commission members will also meet at the Gordon Conference on Electron Distributions and the Chemical Bond to be held in Plymouth, USA, 2–7 July 1995.

#### *Projects*

1. *Fermiology of High- $T_c$  Superconductors via High-Resolution Synchrotron-Based Compton Scattering.* Participants in this project were engaged in planning the Workshop to be held in Himeji, Japan, at the site of SPring-8 sometime during July 1995.

2. *Quantum-Chemical Description of Electronic Structure from Experimental Charge and Momentum Densities.* This density-matrix project comprises essentially four areas: theory, analysis, reconstruction and direct measurement. Ten groups are now active in the area and, after a relatively slow start, impressive progress has been made. Major achievements since 1991 have been the identification of the elements of matrices which are fixed by observables, the extension of the analysis to the Wigner and Husimi functions and to the pure momentum-density matrix and an exploration of the limits of reconstruction.

The first density matrices of solids (ionic and metallic) have been calculated and analysed (LiH, LiF, LiFHF, KFHF and Li). Reconstructions have been made of the density matrices of crystalline formamide and acetylene (from X-ray diffraction data), of gaseous neon and methane (from experimental Compton-profile data) and of the methane molecule from theoretical data for the position and momentum density with superimposed experimental noise. In addition, a model density matrix has been derived from directional Compton-profile data for LiH. Measurements have been made of some off-diagonal Compton profiles of Si with largely improved precision. In 1994, the project members organized a very successful Workshop which is described below.

3. *Multipole Refinement and Related Topics.* The group, which is receiving direct financial support from the IUCr for the development of a new multipole refinement package *XD*, is making good progress and a test version, including programs for the calculation of electrostatic and topological properties, has been released to participating groups. Discussions of the project as a whole were held during the Sagamore XI Conference (see below).

#### *Meetings, Workshops and Schools.*

1. A Workshop on Density Matrices was held in Brest at the Ecole Nationale Supérieure des Télécommunications de Bretagne (ENSTBF) overlooking the Rade, 5–6 August, just before the Sagamore XI Conference. There were 39 scientific participants, about half of them were from the field, the other half having less experience. 28 talks totalling almost 14 hours of presentation were given, and there were 3.5 hours of discussion in total. The structure of the Workshop was: I Theory of

Density Matrices (Introduction and Advances); II Relation of Density Matrices to Specific Experiments; III Measurement and Reconstruction of Density Matrices; and IV Density Matrices as an Interpretative Tool. The general view was that the talks were good throughout and presented with great enthusiasm and that substantial progress was reported. The vivid atmosphere led to a desire to discuss for even longer than the allotted 3.5 hours and there was an important exchange of information among the members of the project. A 'newcomer' was heard to remark, 'Now I understand much better what density matrices are and what they are good for!'

2. The triennial Sagamore XI Conference was also held at the ENSTBF near Brest. The Conference was admirably organized for the Commission by Geneviève Loupias of the Laboratoire de Minéralogie-Cristallographie, Université Pierre & Marie Curie, Paris, and Sohrab Rabii, visiting from the University of Pennsylvania. With a record of attendance of 180, the Conference demonstrated the continuing vitality of both the science and the scientists. Although at least six of the latter had attended Sagamore I, their effect on the average age of the attendees was adequately counterbalanced by the numbers of research students and young post-docs. The Conference was opened by Professor Hubert Curien, sometime Minister for Science in the French government, who spoke of the cooperation and financing required for large scientific instruments throughout the world and stressed the difficulty of obtaining long-term commitments to operational funding which would last beyond the life of a current administration.

Topics during the rest of the Meeting included the theory of X-ray and neutron scattering, X-ray dichroism and the terrain beyond the local density approximation; positron annihilation, the application of maximum-entropy methods to the reconstruction of charge and magnetization densities; magnetic scattering of neutrons and of synchrotron radiation; magnetic Compton scattering, molecular dynamics, pseudopotential calculations of ground-state charge densities, multipolar analysis, the potential of the ESRF for charge studies using hard X-rays and spin density waves in organic conductors.

Professor E. F. Bertaut, the most senior of the six who had attended Sagamore I, showed how electrostatic potentials at the surface of molecules and crystals could be calculated on the back of an envelope, or at least without a computer. We heard about charge densities and excitations, Compton scattering, including a contribution from high-energy neutron scattering, about extinction and thermal vibrations, about how to calculate charge densities and their total energies and about their topological properties and finally about fermiology and (*e, 2e*) spectroscopy.

During the Conference, the Commission held an Open Meeting for reports on two of its current projects: Quantum Chemical Description of Electronic Structure from Experimental Charge and Momentum Densities (leaders W. Weyrich and V. Smith Jr) and Fermiology of High- $T_c$  Superconductors via High-Resolution Synchrotron-Based Compton Scattering Spectroscopy (leader: A. Bansil). Discussions also took place on the Multipole Refinement and Properties Project (leader: C. Lecompte), which included a report from the group that is receiving financial support from the IUCr for the development of a new multipole refinement package.

The Commission was very gratified by the lively and extensive discussion that accompanied almost every contribution and received many favourable comments about the breadth and interdisciplinary nature of the programme.

3. The Commission took an active role in helping to plan a School on Charge Densities to be held in Argentina (organizer: G. Punte). It had been hoped to hold this School in November 1994, but this was not possible and it took place 18–24 May 1995 at the Universidad Nacional de La Plata.

4. The programme for the Gordon Conference on Electron Density and the Chemical Bond to be held in 1996 has been arranged after full consultation with the Commission.

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

During 1994, the Commission helped to organize the 2nd Symposium on X-ray Topography and High-Resolution Diffraction, which was held 5–8 September 1994 in Gosen, Germany (near Berlin), as a Satellite Meeting of the Fifteenth European Crystallographic Meeting (ECM-15) in Dresden, Germany. About 220 scientists attended the Symposium, 80 from Germany, 58 from other Western European countries, 62 from Eastern European countries and 16 from countries outside Europe (mainly from the USA and Japan). The scientific programme comprised 43 oral presentations (among them 3 reviews and 21 invited reports) and 149 poster contributions. This relatively high number of participants and of scientific contributions demonstrates clearly the great and worldwide interest in Symposia of this kind. The Symposium was financially supported by the IUCr. Eleven attendees received IUCr Young Scientist Awards. The Proceedings of the Symposium were published in *J. Phys. D*, (1995), **28**, A1–A300. The 3rd European Symposium on X-ray and High-Resolution Diffraction will be held 22–24 April 1996 in Palermo, Italy.

An essential activity of the Commission during 1994 was the organization of a School for young scientists mainly from East European countries. The International Summer School on Growth and Characterization of Crystals was held 4–14 September 1995 in Krynica, a famous health resort in Poland close to the border with Slovakia. The organization of the School was performed by Professor S. Hodorowicz (Cracow) and Professor K. Sangwal (Lublin). Four present and two previous members of the Commission were active on the International Programme Committee. Three present and two previous Commission members presented lectures. As a whole, 41 lectures (each 1 hour) were presented by 18 speakers from various countries. The content of the lectures covered practically all important growth and characterization techniques for bulk crystals and epitaxial layers, and a broad spectrum of materials (inorganic and organic including proteins, and semi-conducting and superconducting materials). The total number of participants was 29, most of them coming from East European countries. The School was financially supported by the IUCr. Ten attendees received IUCr Young Scientist Awards.

Another important Commission activity of the year was the preparation of the International School on Advanced Electronic Materials, which was held 6–15 February 1995 in the Crystal Growth Centre of the Anna University, Madras, India. The local organization was performed by Professor C. Subramanian and his staff. The Commission was strongly engaged in the International Programme Committee with six present and two previous Commission members. A serious problem was the small financial base of the School, which did not allow support to be granted to lecturers. Nevertheless, 16 non-Indian and 6 Indian speakers were recruited and a programme of 46 lectures (each 1 hour) was established. Three Commission members

were active as lecturers. The School was sponsored and financially supported by the IUCr, mainly for the subsistence of young scientists.

#### *Commission on Crystallographic Apparatus*

During 1994, the Commission continued its activities in the field of lattice-parameter determination, absolute structure determination for light atoms, two-dimensional radiation detectors and high-pressure crystallography. A brief report of the projects being undertaken is given below.

(1) *Precision and Accuracy of Lattice Parameter Determination* (G. DeTitta and L. Finger). The project aims at the determination of realistic limits on the precision and accuracy of lattice parameters as reported in the structural crystallography literature. It has in its scope to determine the strengths and weaknesses of various approaches, assess the important issues in an accurate and precise measurement, devise tools to aid in the measurement and to characterize the equipment used in these determinations. Two main thrusts of the project are (1) a round-robin experiment in which structural crystallographers are asked to determine the lattice parameters for an unknown sample and a known standard sample, and (2) to develop a standard reference material and associated instructional material to allow the structural crystallographer both to gauge the quality of lattice-parameter determination coming out of the laboratories and to improve that quality.

With support from the IUCr and NIST, kits containing properly characterized ruby crystals and five zeolite crystals, mounted and ready for lattice-parameter determination, have been prepared and nine kits have been shipped to participants in the round-robin project. Kits are in South Korea, Russia, the US, Canada, the UK and France. As yet we have not received any results but we expect them soon. With the money that NIST made available, 4000 ruby spheres were purchased; NIST plans to turn them into a SRM (standard reference material). The IUCr fund made it possible to hire a masters student for the summer to handle the details of the packaging and shipment of the kits.

The zeolite crystals are thin plates that have been mounted in such a manner that the plate normals are not exactly perpendicular to the  $\varphi$  axis, making their optical alignment non-trivial. On the other hand, alignment of the rubies is straightforward. What the results are expected to show is that problems with lattice-parameter determination have more to do with misalignment of the crystal and/or of the diffractometer than any other fundamental problem. Results with the ruby spheres should give us information about the alignment of the diffractometers, which we will be able to include in our analysis of the zeolite results. Since the actual cell constants for both samples are well known, we can interpret the reported cell constants as perturbations of the true constants owing to beam nonhomogeneities (spatial and spectral), misalignments of the crystal/diffractometer, misidentification of the wavelength operative for each reflection centered, centering methods *etc.* Participants are being asked to report the actual diffractometer angles used in the determination of the cell parameters.

(2) *The Absolute Structure Determination of Light Atom Compounds (ASDLA)* (L. Malakhova and E. F. Weckert). This project aims at a comparison of various methods used for the determination of the absolute structure of light-atom compounds and a generalization of the experimental and practical experience accumulated by scientific laboratories. Since the first determination by Bijvoet (1951), absolute structures have

been receiving increasing attention, in particular in the field of biological compounds and pharmacology. The anomalous-scattering technique is well established now but the technique is not applicable to biological and organic crystals including only light atoms (H, C, N, O) and no heavy atoms. This problem has led to the use of complicated apparatus (synchrotron radiation) or to long-lasting and careful experiments or to the appearance of novel experimental techniques for the determination of the absolute structure (direct measurements of triplet phases, use of three-beam interaction). The present project involves the determination of the absolute structure of a given series of crystals with different characteristics by all project participants with the use of techniques and apparatus available in respective laboratories. The data obtained should allow us to establish the numerical correlation between the sample characteristics, parameters of the experimental apparatus used and the results of the absolute-structure determination by different techniques.

According to the proposed time schedule encompassing 1994 to 1996, the key points of the ASDLA project, suggested for consideration for the project participants, were discussed, added and approved in essence in 1994. The crystal substances suitable for the project performance were chosen after discussion among the participants. Information about the variety of the absolute-structure-determination techniques as well as apparatuses available to the project participants shows good conditions to carry out the project. We are about to do the first experiments. Out of 11 laboratories originally planned, 7 have remained with the project. There were no financial expenses in 1994.

(3) *Review article of position-sensitive detectors* (H. Hashizume and G. McIntyre). In view of the continued development and interest in position-sensitive detectors (p.s.d.'s), the publication of a review article was discussed in the Commission to provide crystallographers with information on the advantages and limitations of various detectors, as well as to correct misunderstandings or confusions about some detector properties. Furthermore, detector development is so rapid that crystallographers are not always well informed about available detectors. The standpoint of the review would not be that of detector builders but of users. Our position is not that of a crystallographer who is given a detector and thinking about possible experiments. Rather, we will prepare articles that supply information on up-to-date p.s.d.'s and help crystallographers select the most appropriate detector for his experiment. Dr A. M. Glazer, Editor of *J. Appl. Cryst.*, was very much interested in our project, and agreed to publish any articles in the journal.

An agreement was reached that the review will cover up-to-date integrating and nonintegrating p.s.d.'s for X-rays, neutrons and other particles including electrons. Separate articles would be devoted to different radiations. In addition to 1D and 2D p.s.d.'s, we planned to cover high-count-rate point detectors, which are greatly required at synchrotron sources. Detectors based on different principles and technologies, commercially available or not, would be surveyed. Each article would briefly describe the detector principle (or physics) and construction, but details would be left to references. The properties on which the authors are advised to provide information were discussed. Critical comparisons of different types of detector will be most helpful. Descriptions of typical applications will be illustrated. Overlaps between the articles are inevitable and would not be minimized: evaluations from different viewpoints would be of interest. Exhaustive reference lists will be required in each

article. According to this plan, a list of possible contributors was drawn up by March 1994. Soon after, the inaugural issue of the *Journal of Synchrotron Radiation* was published, which included a review similar to that planned by the Commission. Discussion is under way to work out a new plan.

(4) *High Pressure Group* (R. J. Nelmes). The principal activities of the High Pressure Group (HPG) in 1993–94 have been the promotion, support and organization of specialist Meetings of various kinds. New experimental techniques on synchrotron and neutron sources, plus the advent of third-generation synchrotrons, are stimulating such an extraordinarily rapid growth in the range and quality of high-pressure crystallography that quite frequent Meetings are needed to keep the community in touch with the latest developments. The Group has been involved, at some level, in the following Meetings during the past year.

1. A Microsymposium on High Pressure Crystallography at the IUCr Congress in Beijing, in August 1993. The Organizing Chairman was Y. Fujii, a member of the HPG.

2. A one-day Workshop on Synchrotron Radiation at High Pressure, in Stony Brook, USA, organized as a Satellite to the Synchrotron Radiation Instrumentation '94 Conference, in July 1994.

3. A Microsymposium on High Pressure Crystallography at the European Crystallographic Meeting (ECM-15) in Dresden, in September 1994. The Organizing Chairman was R. J. Nelmes, Chairman of the HPG, with H. Schulz, Past Chairman of the HPG, acting as Co-chairman.

4. A one-day Workshop on Diffraction at High Pressure, in Dresden, immediately following ECM-15. The organizer was D. Hausermann, a member of the HPG.

5. An International Seminar on Neutron Scattering at High Pressure, held in Dubna, Russia, in October 1994.

Looking to the future, plans are currently well advanced for a three-day International Workshop to be held in Tsukuba, Japan, in March 1995. This is the fourth in a series of HPG Workshops, following previous ones in Munich (1989), Daresbury (1991) and Washington (1992). The organizing Chairman is O. Shimomura, a member of the HPG. Beyond that, it is intended to organize a Workshop in the USA in 1996, in association with the IUCr Congress in Seattle (possibly as an official Satellite Meeting). The HPG is requesting a Microsymposium and a Plenary Lecture at the Congress itself.

#### *Commission on Crystallographic Computing*

The main activities of the Commission during 1994 were:

(1) Refereeing of the section Computer Program Abstracts in *Journal of Applied Crystallography*, which has been carried out by D. Watkin and M. Ramanadham.

(2) Thanks to H. Flack, the experience with the CONCISE bulletin board, 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) The major activity of the Commission was the organization of a School in the Asian area in 1995. The School, organized jointly by the Teaching and the Computing Commissions, will be a Satellite of the Second Meeting of the Asian Crystallographic Association. After a long period spent trying to find a suitable site in a country willing to comply with ICSU rules for the circulation of *bona fide* scientists, the final choice was Bangkok, where Professor P. Phavanantha

offered his valuable cooperation and accepted the invitation to act as Chairman of the Local Organizing Committee for both the School and the AsCA Meeting. The School will take place immediately after the AsCA Meeting, 27–30 November 1995. The programme of the School includes the most basic aspects of crystallography and crystallographic algorithms, as well as some of the most recent developments. Demonstrations and practical sessions on personal computers are also foreseen.

(4) The organization of the Macromolecular Crystallography Computing School as a Satellite Meeting of the Seattle Congress is now at a more advanced stage. Dr Philip Bourne and Dr Keith Watenpaugh, acting as local organizing persons, proposed the Western Washington University, Olympia, Washington, USA, as the most likely location. The School will concentrate on the most recent aspects of macromolecular crystallography computing, both theoretical and practical. Lectures and Tutorials/Workshops with hands-on sessions will be given almost equal time. The main topics will be: data processing, phasing, model building, refinement and analysis of macromolecular data.

(5) Following a suggestion of Dr D. Watkin, plans for the organization of a small regional School, more oriented towards computational aspects, were continued. 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. Apart from a few enthusiastic replies, there was little response. Since the idea is viewed with favor by most Commission members, its feasibility is being reconsidered.

#### *Commission on Crystallographic Data*

No report has been received from the Chairman.

#### *Commission on Crystallographic Nomenclature*

The Commission's work in 1994, as in previous years, was continued partly through its internal efforts and in larger part through the important contributions made by its Subcommittees and Working Groups, with communications being conducted primarily by electronic means. Membership in the Commission is entirely *ex officio*, by virtue of being an Editor of an IUCr journal or of an individual volume of *International Tables for Crystallography*; the Chairpersons of the IUCr/OUP Book Series Committee and the Commission on Crystallographic Teaching are also *ex officio* members.

The Working Group on the Expression of Uncertainty in Measurement, with membership as given in *Acta Cryst.* (1995), A51, 211 and with D. Schwarzenbach as Chair, completed its Report entitled *Statistical Descriptors in Crystallography. II* during the year. The Report was accepted by the Commission in September and by the Executive Committee in December 1994 and is now in press [*Acta Cryst.* (1995), A51, 565–569]. Among the Report's major recommendations are replacement of the term estimated standard deviation by standard uncertainty or by combined standard uncertainty in statements of the statistical uncertainties of data and results. The report presents the concepts of standard uncertainty as developed by the International Organization for Standardization, and of Type A and Type B evaluations of standard uncertainties. The result of a measurement is only an estimate of the value of the measurand and is now considered complete only when accompanied by a quantitative statement of the uncertainty of that estimate.

Several membership changes have occurred in the Subcommittee on the Nomenclature of *N*-Dimensional Crystallography.

Its new Chair is Professor T. Janssen, with J. L. Birman, Th. Hahn, V. Kopstik, M. Senechal, D. Weigel, H. Wondratschek and A. Yamamoto as members and S. C. Abrahams as an *ex officio* member [see also *Acta Cryst.* (1995), A51, 211]. The Subcommittee is proceeding very systematically in its consideration of the concepts, definitions and terminology of crystallography in  $N$  dimensions, achieving concensus as it progresses. Definitions of higher-dimensional point groups, crystal classes, holohedry and space groups, for example, have been considered as have rules for ordering four-dimensional families and symbols for point groups and their transformations. The task is large and progress is expected to be slow but deliberate.

Two new Subcommittees were established by the Commission in 1994. Professor K. N. Trueblood was elected Chair of the new Subcommittee on Atomic Displacement Factor Nomenclature, with H.-B. Bürgi, H. Burzlaff, J. D. Dunitz, C. Gramaccioli, H. H. Schulz and U. Shumeli as members with S. C. Abrahams as an *ex officio* member. The Subcommittee's charge is to examine the merits of adopting a uniform approach to reporting atomic displacement factors in structural papers and with making such recommendations as may be appropriate. The motivation for establishing this Subcommittee sprang from the widespread confusion in the literature regarding the use of such terms as  $U$ ,  $B$  and  $\beta$  and the different ways in which they have sometimes been defined. A thorough treatment has been developed of the displacement parameters based on the Gaussian approximation, and also those needed when that approximation is not valid. A final report is expected in the first half of 1995.

A Working Group on Phase Transition Nomenclature was also formed in 1994. Professor P. Tolédano was elected Chair, with A. M. Glazer, E. Parthé, R. L. Snyder and Th. Hahn as members and S. C. Abrahams *ex officio*. The Working Group is 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 and with making whatever recommendations may be appropriate. In view of the interdisciplinary interest in phase transitions, the members were selected both for their expertise in the field and for their varied scientific backgrounds. In addition, at the Commission's invitation, Professor R. S. Berry was appointed by IUPAP and Professor R. Metselaar by IUPAC as liaisons to the Working Group. The Chair initiated discussions by providing a valuable and comprehensive overview of the primary kinds of phase transitions and transformations. Travel by members has slowed the rate of progress, but this is expected to increase in 1995.

#### *Commission on Crystallographic Teaching*

The main activities of the Commission in 1994 were:

1. *The IUCr Visiting Professorship Programme.* Professor N. Kasai, a member of this Commission, was granted a Visiting Professorship of three weeks in March–April 1994, in Hanoi, Vietnam, and in August 1994 he also visited the Chiang Mai University in Thailand. In June 1994, two Visiting Professorships were granted to Profesor Theo Hahn and Professor Hans Wondratschek for a School on crystal symmetry held in Sofia, Bulgaria, 3–10 June 1994, and two visiting Professorships were also granted to the same persons for the St Petersburg School (see below). A Visiting Professorship was granted to Dr P. Mallinson from the University of Glasgow in connection with

the School on charge density studies to be held at La Plata, Argentina, in May 1995.

2. *Teaching Schools.* Sponsorship and active participation in the organization of two Schools taking place in Bangkok in connection with the next AsCA Meeting have been considered. These Schools will focus on crystallography applied to precious materials and to computing; the latter is being developed jointly with the Commission on Crystallographic Computing. Sponsorship for another School taking place in Calcutta on Macromolecular Crystallographic Data has also been requested (by the main organizers Professor Vijayan and Professor Dattagupta). In Europe, Dr David Watkin started his work on organizing a course on Small-Molecule Structure Analysis (Aston, England, Easter 1995). Two courses in Russia (St Petersburg and Moscow) on Space-Group Symmetry and the Rietveld Method, which are taking place in summer 1995, were planned with the sponsorship of this Commission and the active work of Dr Aslanov. Dr I. D. Brown started the organizational work for a School on the Structural Chemistry of Solid-State Materials to be held in Canada in Summer 1995. Support for the School on Charge Density in La Plata, Argentina, was given by granting a Visiting Professorship (see above). In April 1994, Dr Karimat El-Sayed organized a Workshop on Fourier Series, Fourier Transforms and their Application in Physics and Crystallography: sponsorship of this Commission was requested, and two Visiting Professorships were granted for the purpose.

3. *Symposia on Crystallographic Teaching.* A Microsymposium on this subject has been organized in connection with the next European Congress (ECM-16) in Lund, Sweden, with the active collaboration of Dr A. Oskarsson, a member of this Commission.

#### *Commission on Electron Diffraction*

The Commission held a one-week Summer School on Electron Crystallography – Theory and Practice, at the Universities of Bath and Bristol immediately prior to the 13th International Congress on Electron Microscopy in Paris. The School, which was sponsored by the International Union of Crystallography as well as a number of companies, was attended by 50 students from 21 countries. It was widely regarded as effective in presenting the state of the art in electron crystallography. Further details about the School, which had no other published record, may be found in the article by Doug Dorset in the *IUCr Newsletter* (1994), No. 2, p. 19.

The Commission is now involved in planning a Winter Workshop on Electron Diffraction and Imaging at Surfaces to be held in Arizona, 2–5 January 1996. Professor M. A. Van Hove of UC Berkeley, California, is chairing the Organizing Committee. A related activity is the round-robin on RHEED computer codes being organized by Professor A. Ichimiya of the University of Nagoya.

The Commission is represented on the Programme Committee for the XVII International Congress of the IUCr in Seattle in 1996 by John Steeds and Doug Dorset.

#### *Commission on Neutron Scattering*

The major event of 1994 was the award of the Nobel Prize for Physics to Professors B. N. Brockhouse, FRS, and C. Shull for their pioneering work on neutron diffraction and neutron inelastic scattering. At the informal Meeting of the Commission at Sendai (Japan), messages of congratulation

were sent. The occasion was especially joyful as the news came during the course of the Meeting. With the change of name of the Commission on Neutron Diffraction agreed at the General Assembly of the International Union at its Meeting in Beijing, August 1993, the Commission now embraces both of the subject areas recognized in the awards.

The Commission, while still holding neutron diffraction from both single crystals and powders at the core of its work, has initiated and become involved with projects likely to be of long-term value to both structural and dynamical studies. A series of consultations by e-mail and by the Chairman in Europe and USA (June 1994) and in Japan, Europe and USA (November 1994) indicated that the Commission might be able to facilitate two projects: International Standards for Neutron Inelastic Scattering Cross Sections (NISC) and Internationally Agreed Exchange Format for Neutron and Synchrotron Data. These projects are at a very early stage but cooperation has been agreed for the first, which will involve the exchange of a standard sample of  $\text{PrAl}_3$  initially between eight major neutron scattering centres. This system has a well defined crystal-field excitation at about 4.3 meV whose cross section is precisely calculable and for which there is very little dispersion. Intercalibration of instruments between countries and the increase in accuracy of measurement that could follow and the growing power of pulsed neutron sources are all good reasons for starting this project now. It could allow neutron inelastic intensities to become of routine use. Members of the Commission and a number of leading scientists in several countries have suggested additional test samples and volunteered their help in carrying out this programme.

The Commission has offered to facilitate the work of the second programme, which was started by members of the European Network for Neutron Instrumentation (ENNI) and reported at the ISIS (Rutherford Appleton Laboratory, England) International Science Advisory Committee in December 1994. A Workshop on Neutron Scattering Software (SoftNEss) was organized by Dr Ray Osborn (Argonne National Laboratory) in October 1994 with the data exchange format as the main topic. A proposal for a world-wide neutron scattering data format was agreed and will be prepared by Przemek Klosowski, Jon Tischler and Mark Konnecke for 1995. Dr Osborne has agreed to keep the Commission informed.

In connection with these projects, the Commission may wish to appoint consultants and should be grateful for the agreement of the Executive Committee at the appropriate time.

The Commission held an informal Meeting at the ICNS Meeting in Sendai, Japan, in November 1994. Present at Sendai were: Endoh, Kulda, Lebech, Mason, Ye, White; absent: Prince, Powell, Forsyth, Albinati. In addition, Professor Keith McEwan (UK) was invited as a key person for item 4 of the agenda, which covered (1) Satellite Meeting for the Seattle Congress in 1996, (2) Main Programme for the Seattle Congress in 1996, possible Plenary Lecturers, (3) Regional International Meeting and Workshop (Asia/Pacific) in 1997, (4) Absolute Inelastic Cross Section Project, (5) any other business.

As concerns the Satellite Meeting, it was agreed that Ted Prince would design the programme in the first instance but he was asked to iterate this with the Commission through John White. It was agreed that, like the Beijing Congress, a mix of crystallography and other neutron scattering was desirable. It was agreed that Dr Prince, through the Commission, should seek money for student participation in the Satellite Meeting.

The impact of siting the Neutron Scattering Satellite at NIST in 1996 at the venue for the next ICNS Meeting was also discussed. There had been bids to Professor Endoh already from NIST, Oak Ridge, Zürich, Munich and Jülich.

The Commission will continue its work on 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.

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.

It is a pleasure for the Chairman to thank all members of the Commission for their contributions to the Commission's work.

#### *Commission on Powder Diffraction*

During 1994, the Commission on Powder Diffraction (CPD) was involved in the organization of two very successful powder diffraction Meetings in Russia and South Africa, and assisted with the preparation for three Meetings scheduled for 1995 in England and Slovakia. Planning also continued for the CPD's involvement in the IUCr Congress in Seattle in 1996, together with the associated Satellite Meeting on Powder Diffraction in Denver. The results of Part II of the Rietveld Refinement Round Robin were published, and a grant was provided in support of the continued development of the *World Directory of Powder Diffraction Programs*. Direct communication with powder diffractionists continued with the issuing of two further CPD *Newsletters* in April and October.

The International Workshop on Advanced Powder Diffraction Techniques in Mineral and Materials Processing was held in Pretoria, South Africa, in October 1994, and was co-organized by the Crystallographic Society and Mineralogical Association of South Africa. CPD member Dr Lynne McCusker was an invited speaker and served as Chairman of the Scientific Programme Committee, member Dr Ian Langford was also an invited speaker, while CPD Chairman Dr Rod Hill contributed to the Programme Committee. The Meeting was an outstanding success, with participants from many countries in Southern Africa gaining valuable experience from a series of carefully crafted lectures, tutorials and hands-on Workshop sessions on all aspects of powder diffraction analysis, including sessions presented by the ICDD.

The International Conference on Powder Diffraction and Crystal Chemistry was held in St Petersburg, Russia, in July 1994, co-organized by the Russian Association of Powder Crystallography, the Department of Crystallography of St Petersburg University and the CPD. Lectures and posters were presented to 165 participants from 20 countries, including a Workshop run by the ICDD, and a 211-page book of abstracts was produced. St Petersburg's strong past and current links with crystallography, dating from Federov's discovery of the 230 space groups in 1890, along with its geographic beauty, provided a very appropriate and delightful backdrop for a most successful Conference.

The CPD lent its support to the EPDIC IV Meeting in Chester in July 1995 and the International Conference on X-ray Powder Diffraction Analysis of Size/Strain, Macrostress and Texture in

Slovakia in August 1995; CPD member Dr Jaroslav Fiala and the CPD Chairman served on the Programme Committees for both of these Meetings, Dr Fiala as Chairman for the Slovakia Meeting. Preparations for a CPD-organized Microsymposium on powder diffraction at the Seattle Congress commenced, including nominations for a session Chairman and possible topics. Similarly, arrangements were put in place for a Satellite Meeting on Powder Diffraction to be held in Denver in August 1996, in conjunction with the 45th Meeting of the Denver X-ray Conference.

Two CPD *Newsletters* were issued in April and October, edited by CPD members Professor Deane Smith of the Pennsylvania State University, USA, and Dr Bob Cernik of Daresbury Laboratory, England, respectively. Feature articles included the explanation, establishment and use of crystallographic news groups on the world-wide Internet (by Lachlan Cranswick of CSIRO in Melbourne, Australia), use of synchrotron diffraction information from single powder grains for structure solution prior to Rietveld refinement using bulk powder diffraction data (by Bob Cernik of Daresbury Laboratory, England), description and use of CIF for powder diffraction (by Brian Toby, Terrytown, USA), introduction to the SPring-8 project (by Hideo Toraya, Nagoya, Japan) and the new high-resolution neutron powder diffractometer at the high-flux isotope reactor, Oak Ridge, USA (by Brian Chakoumakos, Oak Ridge National Laboratory, USA).

The CPD remained active in the execution of its existing projects and in the initiation of new ones. Part II of the Rietveld Refinement Round Robin Project was published in *J. Appl. Cryst.* (1994), **27**, 802–844. This part of the project provided outcomes of the analysis of Rietveld refinements of the monoclinic zirconia crystal structure based on X-ray and neutron powder diffraction data collected on a 'standard' sample with a wide spectrum of instruments located in 12 countries around the world. Work on Part III commenced during the year – this part will focus on a multivariate analysis of the results obtained from the zirconia refinements.

The CPD confirmed its on-going support for the *World Directory of Powder Diffraction Programs*, co-produced by CPD member Professor Deane Smith from the USA and Dr Syb Gorter from The Netherlands, through the provision of a grant for the purchase of computer hardware. Organization of a new round robin project on Phase Quantification by Diffraction Methods, coordinated by Deane Smith, continued during the year with a call for expressions of interest and suggestions for the type of tests and samples that might be used. Also, arrangements continued for a survey of methods and models in use for the determination of crystallite size and microstrain from powder diffraction data under the auspices of a Task Group co-chaired by Dr Jaroslav Fiala and Professor Bob Snyder of the USA.

#### *Commission on Small Molecules*

The major achievement of the Commission during 1994 was undoubtedly the three-day Symposium (26–28 June) entitled *New Trends in Small Molecule Crystallography* held, in conjunction with the American Crystallographic Association, at the 1994 ACA Meeting in Atlanta, Georgia. The Symposium Organizing Committee [F. H. Herbstein (Haifa), Chairman; W. L. Duax (Buffalo); G. Ferguson (Guelph); Yu. T. Struchkov (Moscow)] set up a programme emphasizing the tremendous qualitative and quantitative changes to be expected in the

nature of the next century's structural information because of the anticipated advances in experimental and computational diffraction techniques. Perhaps the appeal and the strength of the Symposium lay in the fact that about half of the topics were not 'pure' diffraction and that about half of the invited speakers would not class themselves as professional diffractionists. Eight of the speakers were from North America, four from the United Kingdom, eleven from Europe and two from Asia; four were under 35, describing their own research. The topics covered included direct methods, synchrotron and neutron sources and techniques, low temperatures and their advantages, perfect crystals, chemical theory, arrangements of atoms and molecules in crystals, comprehensive multidimensional crystallography, electron microscopy, surface crystallography, diffuse scattering, thermal motion, reactions in crystals, thermodynamic studies, the chemical crystallography of high- $T_c$  superconductors and single-crystal nuclear magnetic resonance and nuclear quadrupole studies. The proceedings will appear in a Special Issue of *Acta Crystallographica Section B* (August, 1995). The published papers (all refereed) will cover the same ground as the lectures but will be considerably extended.

Members of the Commission met in Atlanta during the ACA Meeting and in Dresden during the 15th European Crystallographic Meeting to discuss further activities, with special emphasis on the Commission's role at the Seattle Congress. An Open Meeting of the Commission and, possibly, a Satellite Meeting, are being considered, as well as nominations for Plenary Lecturers. Judith Howard is organizing, together with Hans-Beat Bürgi, a session on Intermolecular Interactions and Packing in Crystals at the 16th European Crystallography Meeting in Lund in August 1995. The Commission has approved (in so far as content is concerned) the Workshop on Inorganic Solids to be held at McGill, USA, 19–22 July 1995 (I. D. Brown) and the Small Molecules Indaba in the Kruger National Park, South Africa, 20–24 August 1995 (J. C. A. Boeyens). Other future Meetings are currently under consideration. The Commission will also be suggesting to the Executive Committee a change of name to Commission on Structural Chemistry.

#### *Commission on Synchrotron Radiation*

In this period, the main activities involved several Meetings and Workshops with active participation from the Commission. These Meetings included a Symposium on Frontiers of Materials Science in Synchrotron Radiation in Kobe, Japan, a Summer School on Synchrotron Radiation in Natural Sciences in Jaszowice, Poland, the organization of a Microsymposium on Synchrotron and Neutron Diffraction: Results and Perspectives at the International Mineralogical Association General Meeting in Pisa, Italy, and the organization of a Microsymposium on Methods and Instrumentation in Synchrotron Radiation at the 15th European Crystallographic Meeting in Dresden, Germany.

The Polish Summer School on the topic of the use of synchrotron radiation in natural science is an on-going Summer School organized every two years by the Polish synchrotron users community, notably Professor Auleyner and his colleagues in Warsaw. The School brings users from predominantly the Eastern countries together and all aspects of synchrotron-radiation research in natural sciences are covered by invited leading synchrotron scientists in the various fields. The Commission has actively participated in the Organizing

Committee for several years. Detailed reports are published in *Acta Physica Polonica*.

The Microsymposia directly organized by the Commission presented the latest developments in synchrotron radiation of interest to the mineralogical community. In particular, the rapid progress in high-pressure instrumentation and methods were highlighted.

A well attended Microsymposium on Instrumentation and Methods in Synchrotron Radiation at ECM-15 in Dresden focused its interest mainly on the new development trends in detectors and microcrystal diffraction.

The Commission has also been active in planning Meetings for the coming years. The most prominent one being the Synchrotron Satellite Meeting in connection with the Seattle Congress in 1996. The Satellite Meeting will be held at Argonne National Laboratory, 4–7 August 1996. The Commission has organized four different Microsymposium sessions on synchrotron-radiation-related topics at the European Crystallographic Meeting (ECM-16) in Lund, Sweden, to be held in August 1995.

#### 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 1994 the Executive Committee approved sponsorship of several Schools and Meetings, mostly with financial support. Those held in 1994 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1995, but approved in 1994, are listed below:

1. BCA Fifth Intensive Course in X-ray Structure Analysis, Aston, England, 1–9 April 1995.
2. International School on Quasicrystals, Balatonfüred, Hungary, 13–20 May 1995.
3. Charge Density School, La Plata, Argentina, 18–26 May 1995.
4. Erice School on Crystallography of Supramolecular Compounds, Erice, Italy, 2–12 June 1995.
5. Gordon Research Conference on Electron Distribution and Chemical Bonding, Plymouth, USA, 2–7 July 1995.
6. Fourth European Powder Diffraction Conference (EPDIC IV), Chester, England, 10–15 July 1995.
7. Workshop on Structure Determination from Powder Diffraction Data, Oxford, England, 16–20 July 1995.
8. Rietveld Summer School '95-RS, Moscow, Russia, 19–21 July 1995.
9. Workshop on the Description, Understanding and Prediction of the Structure of Inorganic Solids, Montreal, Canada, 19–22 July 1995.
10. Conference on Fundamental Principles of Molecular Modelling, Skukuza, South Africa, 20–24 August 1995.
11. International Conference on X-ray Powder Diffraction Analysis of Real Structure of Matter: Size-Strain '95, Lipovsky Mikuls, Slovakia, 21–25 August 1995.
12. Summer School on Neutron Scattering, Oxford, England, 12–21 September 1995.

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 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

At a Meeting of the Committee in March 1994, the Committee proposed plans for continued development of electronic publishing by the IUCr. The document submission aspects of electronic publishing are improving steadily, with procedures introduced by the IUCr now being adopted by other publishers. In addition to continuing improvement in manuscript submission, the extraction of CIFs from the IUCr archives and the transmission of checked CIFs to database producers are progressing. High priority has been given to providing CIF checking as an automatic service, because that will reduce the incidence of errors in the published literature, and hence reduce costs for the crystallographic databases.

For the time being, the document delivery aspects of electronic publishing are characterized by very high uncertainties about future trends. During the year, what were previously difficult problems regarding the use of networks for semi-commercial purposes were unexpectedly resolved. Similar changes associated with the use of the new medium for publishing are expected in the future. Any plan to use electronic publishing for document delivery must allow for unexpected changes. The *World Directory of Crystallographers*, in addition to serving its main purpose, is being used as a medium for testing some aspects of document delivery that will be helpful as the IUCr moves towards publishing its journals in electronic form. A staged programme, moving towards greater use of electronic media for document delivery, will be submitted to the IUCr Executive Committee for consideration.

#### Regional Associates and Scientific Associates

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

The American Crystallographic Association continues to enjoy a growing number of members, increasing participation

in the Annual Meeting and a sound financial base. The Annual Meeting of the American Crystallographic Association was held in Atlanta, Georgia, 25 June–1 July 1994. Highlights of the Meeting included awarding the Bertram E. Warren Award to Dr Michael J. Bedzyk and the Martin J. Buerger Award to Professor Philip Coppens and a three-day Symposium on New Trends in Small Molecule Crystallography co-sponsored by the ACA and the Commission on Small Molecules, which provided an interesting and well attended opening session for the Meeting. The ACA continues to foster junior scientists: part of the programme was organized by the young scientists' interest group and five students received Pauling Prizes for their outstanding poster presentations. The 1995 Meeting will be held in Montreal in July 1995 and the programme will be available on the Internet.

The ACA continues to expand its representation as Regional Associate of the IUCr. At the June ACA Council Meeting, Dr Manuel Soriano was appointed as interim Representative of Mexico pending organization of the Mexican Division. The ACA also maintains close ties with the American Institute of Physics and has Representatives on key committees of the larger organization. The officers of the ACA for 1994 are Elinor E. Adman, President; Hugo Steinfink, Vice-president; S. N. Rao, Treasurer; Charlotte Lowe-Ma, Secretary; Richard E. Marsh, Past-president; I. David Brown, Canadian Representative; William I. Duax, Executive Officer.

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

The Asian Crystallographic Association is a Regional Associate of the International Union of Crystallography and one of its prime functions is the promotion of better communication and contacts between Asian crystallographers. The second Conference of the Asian Crystallographic Association is scheduled to be held in Chulalongkorn University, Bangkok, Thailand, 22–24 November 1995. The Chairman of the International Organizing Committee is Professor W. T. Robinson (New Zealand), the Chairman of the International Programme Committee is Professor Y. Ohashi (Japan) and the Chairman of the Local Organizing Committee is Professor Phathana Phavanantha. Students or young scientists early in their careers attending the Conference are eligible to apply for support towards registration and accommodation costs. Funds for this support have been provided by the IUCr.

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

The main event of the ECC activities in 1994 was the 15th European Crystallographic Meeting (ECM-15) in Dresden, Germany (28 August–2 September) with 775 registered participants and 65 accompanying persons (at the preceding ECM-14 in Enschede, The Netherlands, 2–7 August 1992, there were 450 participants). 820 abstracts were received but some were rejected, in particular because of non-registration of the presenting authors in time. The normal registration fee was DM 250. For students, a reduced registration fee of DM 50 was available. About 60% of participants registered before the deadline and paid a reduced registration fee. Financial support was obtained from the IUCr (for young scientists), the Free State of Saxony, the International Science Foundation, Deutsche Forschungsgesellschaft and The Netherlands Association of Crystallography. There were 146 applications for support, of which 84 received some financial help to the sum of DM 40 000. 38 young scientists were supported by the

IUCr. Most of the support went to the scientists from Eastern and Central Europe. The total income and expenditure of the Conference totalled DM 350 000.

The Conference agenda included 10 Plenary Lectures, 21 Microsymposia and 4 poster sessions. The book of abstracts contains 618 abstracts on all traditional and 'hot' topics of modern crystallography. Several commercial and non-commercial exhibitions (modern equipment, computing facilities, software, books) and demonstrations as well as *ad hoc* Meetings and panel discussions were well organized.

The Conference was accompanied by a rather large, interesting and diverse social programme, special events and tours, including an evening lecture (one of the Plenary Lectures) by Professor A. Authier (Paris) on Real and Ideal Crystals, attended by an audience broader than participants of the ECM-15, the Conference excursion in 'Saxon Switzerland', a performance of the Dresden Opera, a sightseeing tour of Dresden, a trip to Meissen with its world-famous porcelain factory and a visit to the Gallery of the Old Masters (the Zwinger Museum), and a Saxon farewell evening.

As usual, ECM-15 was supplemented by interesting Satellite and related Meetings: the Second European Symposium on X-ray Topography and High-Resolution Diffraction (Berlin, Germany, 5–7 September), the 16th General Meeting of the International Mineralogical Association (Pisa, Italy, 4–9 September), the Aperiodic '94 International Conference on Aperiodic Crystals (Lausanne, Switzerland, 18–22 September), the XVI Conference on Applied Crystallography (Cieszyn, Poland, 22–26 August), a Meeting on Practical Aspects of Crystal Structure Analysis (Dresden, Germany, 26–28 August), a Workshop on High-Pressure Crystallography (Dresden, Germany, 3 September) and the especially productive traditional pre-ECM-15 (now the ninth) Symposium on Organic Crystal Chemistry OCC94 (Poznan-Rydzyna, Poland, 23–27 August). The latter had 130 registered participants (60 local and 70 foreign) and numerous unregistered. 22 participants were sponsored by Poznan University, the Batory Foundation, the IUCr, the Polish Committee of Crystallography and the Polish Scientific Research Committee. The scientific programme covered 20 invited lectures (including a Special Plenary Lecture by the Nobel Prize winner, Professor J. Karle), 16 oral communications and over 80 posters. A special scientific session was held to commemorate the late Professor M. C. Etter.

During ECM-15, the Meeting of the European Crystallographic Committee (ECC) was held on 31 August. The Representative of the IUCr Executive Committee, Professor A. Kálmán, and 26 delegates from 29 member countries (including 5 new members) were present, as well as the Chairman (K. Huml), the Vice-chairman (H. Fuess) and the Secretary (H. Flack) of the ECC Executive and the Chairmen of the Organizing Committees of ECM-15 (P. Paufler), ECM-16 (A. Oskarsson) and the future ECM-17 in 1997 (Representatives of the three potential host countries) and several guests.

The minutes of the ECC Meeting in Enschede at ECM-14 (3 August 1992) and of its informal Meeting at the Beijing Congress (25 August 1993) were approved without modification. In his report, the ECC Chairman Professor K. Huml pointed out that the ECC *Newsletter* had been stopped because of the appearance of the IUCr *Newsletter* and the computerized information systems CONCISE and WWW. Moreover, attempts to coordinate the organization of Conferences (Workshops, Schools) of interest to crystallographers in Europe have met no success.

By open vote, five new member countries of the ECC were elected: Russia, the Czech and Slovak Republics (joint membership), Serbia, Estonia and Moldova (Georgia's request for collaboration was not voted on because of the lack of a Representative and the as yet limited contacts with the country's crystallographers).

Professor A. Oskarsson reported on ECM-16 in Lund, Sweden, 6–11 August 1995, and the delegates and guests made some useful proposals. Now all information on this Meeting is published in the second circular and on the crystallographic WWW server in Geneva.

After presentation of the various invitations (by J. Hasek for Prague, M. O. Figueiredo for Lisbon and K. El Sayed for Cairo), Portugal was chosen as the site for ECM-17 in 1997. Further invitations are very welcome for future ECM's.

Among reports on other activities, J. Drenth and K. Wilson presented their ESF network on biological macromolecules, A. Preisinger described the past and future Meetings of European Powder Diffraction Conferences (EPDIC) and H. D. Flack reported on the good progress of WDC9.

The traditional discussion on the formation of the European Crystallographic Association (ECA) and collaboration with other parties concerned with crystallography in Europe took place. Earlier, there were various suggestions about the formation of the ECA. However, some members of the ECC consider formation of the Association unnecessary as its aims and objectives will coincide with those of the ECC. H. Fuess remarked that the new ECC would definitely produce a set of varied proposals corresponding to the different models of the ECA as expressed by delegates. Hopefully, this problem will find a more constructive decision at ECM-16 in Lund.

Elections to the new Executive of the ECC were performed according to the IUCr rules and its period of office is 1994–1997. The new officers are Professor Harmut Fuess (Germany), Chairman; Professor Joel Bernstein (Israel), Vice-chairman; Dr Arnold J. Smith (UK), Secretary.

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

No formal IOCG Meeting was held in 1994. The main activity of the IOCG was directed to the preparation of the Eleventh International Conference on Crystal Growth (ICCG-XI), The Hague, The Netherlands, 18–23 June 1995, and to the Ninth International Summer School on Crystal Growth (ISSCG-IX), Papendaal/Arnhem, The Netherlands, 11–16 June 1995.

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

Dr Daniel Louër, CPD Secretary, attended the ICDD October (11–14 October 1994) and March (20–24 March 1995) Meetings as Chairman of the Data Collection & Analysis Subcommittee of ICDD and Consultant to the Board of Directors. While there, he acted as proxy for the CPD Chairman as the Representative of the IUCr to the ICDD and this report is largely based on his feedback.

The Meetings were held in the new ICDD Headquarters located in Newtown Square (PA, USA). In addition to the working sessions, poster sessions were organized during the two weeks (it has been decided that the collected abstracts will be published in *Powder Diffraction*). Two general papers were also presented by Dr H. E. Goebel (Munich) in October

on A New Multilayer Optic for Parallel-Beam Applications and by Dr R. J. Cernik (Daresbury Laboratory, England) in March on Powder Diffraction at Daresbury Laboratory and EPDIC IV Programme. Among the important news items is the announcement of the retirement of the General Manager of ICDD and Corporate Secretary, Julian Messick, after 29 years of dedicated service to the ICDD. From 1 January 1995, this position has been assumed by Daniel C. Richardson.

Numerous activities were discussed during the Meetings, which were of special scientific interest for the community of powder diffractionists. These were:

(i) The Round Robin on Silver Behenate, a possible candidate for a low-angle standard sample ( $d_{001} = 58.38 \text{ \AA}$ ), chaired by T. Blanton (Eastman Kodak). The results have been published recently in *Powder Diffraction*. [(1995), **10**, 91–95].

(ii) A Round Robin on Profile Fitting, chaired by J. Cline (NIST, USA).

(iii) A Round Robin on Reflectometry, chaired by T. Blanton (Eastman Kodak).

(iv) The preparation of recommendations on the calculation of powder diffraction patterns and the use of these data for the characterization of crystalline materials. The Task Group is chaired by C. Lowe-Ma.

(v) Discussion on using a fixed value for  $\text{Cu } K\alpha_1$  in ICDD products. The Task Group is chaired by T. C. Huang.

Each year, the ICDD provides grants for the production of new powder diffraction patterns. For the Grants-In-Aid Programme 1994–1995, 29 proposals from 13 countries (only 2 proposals were from the United States) were supported, with a value of US\$203 600. The projected return is more than 650 patterns. The selection of the proposals is based on the following criteria: materials of scientific or technical importance, specific materials needed in the PDF, sample quality, instrumental method used, data-analysis methods used and quality of sample data.

A number of International Conferences were supported by the ICDD, including the 1994 Denver Conference, AXAA in Australia and EPDIC IV in Chester. Crystallography scholarship awards were provided to three applicants from over 43 applications: L. R. MacGillivray (USA), K. F. Peters (USA) and A. Vailionis (Sweden).

In June 1995, four clinics were organized by the ICDD on the following topics: Fundamentals of X-ray Powder Diffraction, Advanced Methods in X-ray Powder Diffraction, Fundamentals of X-ray Fluorescence, and Advanced Methods in X-ray Fluorescence.

Dr J. Visser was named Distinguished Fellow of ICDD by the Board of Directors, chaired by G. G. Johnson.

The above list of significant activities clearly demonstrates the high level of activity in the ICDD and underscores the very international character of its membership and support.

The ICDD Representative to the CPD, Dr Ludo Frevel, plays an important linking role with the CPD and ensures that each body is aware of the activities of the other. The major area of direct collaboration between the CPD and the ICDD at the moment is the joint organization and planning of the Size–Strain Conference in Slovakia in August 1995 and of the associated round robin on size–strain analysis. A standard sample for this survey has now been distributed to a selection of leading workers in the field and results should be forthcoming in the next few months.

### Representatives on Other Bodies

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

The Annual Meeting of IDCNS was held 26–27 August 1994 in Reading, England. The agenda contained several matters of direct interest to the IUCr, of which the principal was the ‘proposed deprecation’ of the ångström by the Comité Consultative d’Unités of the Bureau International des Poids et Mesures (BIPM). Acceptance of this change, proposed by ISO Technical Committee ISO/TC12, would result in the ångström no longer being approved by BIPM for ‘temporary use with SI units’ but categorized instead as ‘should be avoided for use with SI units’ and replaced either by nm or pm. Motivation for the proposal came from the perceived need to improve international communication across all fields by encouraging the use of standard units and quantities; ISO/TC12 was convinced that this improvement could not be accomplished over the long run if the special names in Table 10 in the 6th edition of *Le Système International d’Unités* published by BIPM in 1991, all of which are associated with special fields including ångström, barn, curie, röntgen, rad and rem, were continued to be recognized for use. It was noted, for example, that the rapidly growing field of nanotechnology will experience error and/or confusion with mixed units of Å, nm and pm. The suggestion was made that crystallographers and structural chemists should be able to convert easily to SI units. The IUCr Representative, together with a few others but not the majority present, argued strongly for BIPM retaining the present status for the ångström at least for another decade or so while we gradually introduce the nm and pm in place of the Å in our journals. The consensus was that the deprecation proposal could not be postponed indefinitely.

Another item of interest was the ISO recommendation (in ISO Standard 31-0, published in 1992) to accept *only* the comma on the line as the SI decimal sign, with digits grouped in threes and separated only by a thin space. Most IDCNS members were unaware of this Standard, and much concern was expressed over its introduction since the majority of the world’s population used the period as the decimal marker. It was agreed that, since adequate input had not been solicited in advance of issuing the Standard and the logic favouring the comma over the period was questionable, member Unions need not follow this Standard in the meantime. There was full agreement on the use of the thin space separator. A third item of interest to the IUCr was the ISO recommendation to accept both lower case ‘l’ and upper case ‘L’ as symbols for the litre. IDCNS agreed to this recommendation, but pointed out the possibility of confusion between the symbols 1 and l. Other matters of interest to the IUCr included recommendations that c.g.s. units with special names (erg, dyne, poise, stokes, gauss, maxwell, stilb and phot as given in Table 11) be deprecated, also that the units radian (rad) and steradian (sr) be listed with other Derived Units of SI. Liaisons between the IUCr Working Group on Phase Transitions and both IUPAP and IUPAC, see Commission on Crystallographic Nomenclature report, were appointed by the Representatives of these Unions to IDCNS. Nearly 50 nomenclature proposals originating in the Divisions and Commissions of IUPAC were viewed, and commented on where appropriate, by the Representative. All accepted proposals are published in *Pure Appl. Chem.*

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

The principal ICSTI activity during 1994 was the 1994 General Assembly, held in the Garden House Hotel, Cambridge, 7–11 July. The highlights of the Meeting were the presentations in the Technical Session on Friday 8 July on

- (i) The RightPages System and Other Developments in STN Publishing;
- (ii) The Development of an Electronic Library for a New University;
- (iii) Impact of Project TULIP;
- (iv) World Wide Web: a Global Scientific Enabler.

The programme was structured to provide the viewpoints of a publisher, two librarians from different environments and an expert user on document delivery services, all based on practical experience. The publisher was naturally concerned with the difficulties of dealing with a multiplicity of protocols, of the wide range of expertise among potential users and with the difficulty of identifying a viable market. The librarians, while cautiously optimistic about the performance of systems within the limited domains that they described, identified technological and organizational problems requiring resolution if those ideas were to be extended to a larger clientele. The expert user described exciting applications of electronic publishing but it was not obvious how these could be extended to commercial or semi-commercial operations.

Other sessions on The Coming User Environment, Responding to the Challenge and Assessment and Integration were more philosophical and somewhat less informative.

ICSTI is also engaged in projects to provide information to benefit its members, the most notable being the Network Utilization Survey Project, in which the IUCr is participating. The previous IUCr Representative on ICSTI often commented that the IUCr was better equipped to contribute to ICSTI than was ICSTI to the IUCr. With increased emphasis being given by ICSTI to document delivery, in which the Class A members, including the IUCr, are vitally concerned, that is less true than it was. I remain very much in favour of improved communication, and eventual amalgamation of ICSTI and CODATA. I regret to report that, if anything, the situation has become even more complicated by the Publishing Service of the International Council of Scientific Unions now setting out to study Electronic Publishing in the Scientific Domain. There are too many bodies undertaking the same tasks. What is less clear is how to persuade some of those that are redundant to withdraw. I favour a concerted approach to ICSTI and CODATA, asking both to pursue amalgamation actively. I recommend pointing out to ICSU that Electronic Publishing in the Scientific Domain is already being studied by other international bodies.

#### *International Council of Scientific Unions (ICSU)*

The 33rd Meeting of the ICSU General Committee was held in Rabat, Morocco, 13–15 October 1994, the first to be held on the African continent. ICSU is constituted by Scientific Union Members and by National Scientific Members and, for the first time, the General Committee met in its new composition, one Representative per Union Member and an equal number of National Scientific Members. The following points were discussed.

### I. Administrative

(a) *Assessment of ICSU*: following the report of the Standing Committee on Membership, Structure and Statutes, the General Committee has recommended that an independent assessment be made of the mission, the organizational structure and the operational modes of ICSU, considering ICSU's role in international science to meet the needs of society. The Executive Board is charged with establishing the terms of reference and selecting the membership of an independent team to conduct the assessment. The conclusions will be reported to the 25th General Assembly in 1996.

(b) *Frequency of the General Committee Meetings*: a straw vote indicated a preference of the majority of the members of the General Committee for reducing the frequency of the Meetings of the GC (from every 12 months to every 18 months). A decision will be made at the 25th General Assembly in 1996.

(c) *Informatics*: the General Committee recommended that the general area of informatics be better represented in the activities of ICSU in order to take into account new developments and the wide range of applications of informatics to many fields of interest within the ICSU family. A working group is to be constituted which will make proposals.

### II. Review of Interdisciplinary ICSU Bodies and Scientific Associates

The following bodies were discussed:

- Inter-Union Commission on the Lithosphere;
- Scientific Committee for the International Decade for Natural Disaster Reduction;
- World Climate Research Programme & International Geosphere-Biosphere Programme;
- International Union for Quarternary Research;
- International Union of Forestry Research Organizations;
- International Union of Toxicology.

### III. Discussion of Scientific Areas of Common Concern

(a) *Nuclear Waste Disposal*: the report of the International Union of Geological Sciences Nuclear Waste Disposal Group was presented. A paper for publication in a major scientific journal providing an independent scientific view is under preparation.

(b) *Biodiversity*: the results of the International Forum on Biodiversity were presented. The General Committee recommends that a Working Group be established to work with the members of *Diversitas* (co-sponsored by the International Union of Bio-sciences, the programme SCOPE and UNESCO) to consider the potential contributions of the various ICSU bodies to the science of biodiversity.

(c) *Capacity Building in Science*: a report was presented on the first Meeting of the Committee on Capacity Building in Science, which has replaced the Committee on the Teaching of Science (CTS). The new Committee is working towards the possibility of launching a global programme in capacity building at the 1996 General Assembly. The clearinghouse function that the CTS served in bringing together the Representatives of the teaching Commissions of the scientific Unions will be continued.

(d) *Science in the Former Soviet Union and Central and Eastern Europe*: a Meeting was organized in Leeds Castle (UK) in June 1994 on the role of science in rebuilding the countries of the former Soviet Union. It was attended by 28 persons from 14 different countries and led to very fruitful discussions. A Meeting of heads of independent national research funding

organizations from the FSU, EEC and selected OECD countries to share experiences on the way science is funded is planned for 1996.

(e) *Freedom in the Conduct of Science*: the General Committee has recommended that the scope of the Standing Committee on Free Circulation of Scientists be expanded to cover issues about the ethical responsibility of scientists, among other things, concerning such issues as human genome research, plagiarism and the deposition of data (the IUCr policy of data deposition in its journals was given as example of what should be done, the case of commercial publishers who do not have such policies was given as an example of what should not!).

(f) *Population*: ICSU's involvement in the various actions in the area of population was recalled, for instance the organization of the ASCEND 21 Conference.

### IV. Scientific Programme

(a) *Seminar on Confronting Complexity*: talks were given by members of the General Committee on various examples of complexity in chaotic and dynamical systems, in physical, chemical and biological systems, in psychology and neurosciences.

(b) *Science in Morocco*: a lecture was given on Environment, Natural Hazards and Development: some Aspects of Science in Morocco.

### V. ICSU Press Conference on Electronic Publishing

A Conference on Electronic Publishing is planned for 19–26 February 1996, to be held in the UNESCO Headquarters in Paris. Main topics will include:

- Electronic data storage and archiving;
- Legal issues in electronic publishing;
- Protection and control of data;
- Scientists' view of electronic publishing and issues raised;
- Economics and organization of primary electronic publishing.

### VI. Resolutions

- The other recommendations of the General Committee are:
  - that a working group be appointed to examine the appropriate role of ICSU in providing advice on the utilization, maintenance and restoration of the Earth's resource base;
  - that a small Meeting on energy problems be organized in 1995 with the participation of experts to be nominated by the various relevant Unions;
  - that a Committee on Food Security be established.

### VII. Next Meeting

The next Meeting of the ICSU General Committee will be held 7–9 October 1995 in Thailand.

### ICSU Committee on Capacity Building in Science (CCBS)

The IUCr Representative will be attending the CCBS Meeting in Paris, 21 June 1995.

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

CODATA is an interdisciplinary Scientific Committee of the International Council of Scientific Unions (ICSU) which seeks to improve the quality, reliability, management, accessibility and intelligent exploitation of data of importance to all fields of science and industry.

### Membership

The current membership of CODATA includes 19 National Members, 16 Scientific Unions, 5 Co-opted Members and 27 Supporting Organizations.

### Organizational matters

Regular Meetings of the Executive Committee and the Officers were held along with the biennial General Assembly. As one means of keeping its vision clear and current, CODATA convened a two-day long-term planning session in conjunction with its General Assembly. All aspects of its activities, including its structure and mandate, were scrutinized. The recommendations of the report being prepared will help the Executive Committee chart a path for CODATA for the next five years.

### Activities undertaken during 1994

*Scientific Meetings.* The highlight of the year was the 14th International Scientific Conference held in Chambry, France, 18–22 September. Attended by 341 scientists and engineers representing 32 countries, the Conference was a scientific success. In March, the Task Group on Survey of Data Sources in Asian–Oceanic Countries convened a two-day Symposium in Taipei, Taiwan, in conjunction with their regular Task Group Meeting. Approximately 80 scientists from the region (Australia, China, Taipei, India, Indonesia, Japan, Pakistan and the Philippines) attended this very vibrant Meeting. CODATA was a co-sponsor of the Workshop on the Problems of Technological Cooperation in the Asia–Pacific Region organized by the Asia Society for Advanced Materials (APSAM) in Tashkent, Uzbekistan, 25–30 September 1994. Five other Task Group Meetings were held and the Commission on Standardized Terminology for Access to Biological Data organized a special one-day session during the International Conference.

*Activities involving developing countries.* CODATA carried on the distribution, free of charge, of copies of the CODATA Referral Database to developing countries. Scientists from any country, depending on their interests and expertise of course, are welcome on CODATA Task Groups or Commissions; currently six Task Groups have members from developing countries. The CODATA Task Group on Data Sources in Asian–Oceanic Countries, especially, continued to provide a dynamic forum for such countries to participate in data activities.

### Publications

*Database Developments in Asian–Oceanic Countries*, edited by Yaruo Hu and Edgar F. Westrum Jr.

*New Data Challenges in Our Information Age (Proceedings of the Thirteenth International CODATA Conference, Beijing, China, 19–22 October 1992)*, edited by P. S. Glaeser and M. T. L. Millward.

*Data Sources in Asian–Oceanic Countries (Proceedings of the CODATA Task Group on Data Sources in Asian–Oceanic Countries, Taipei, China, March 1994)*, edited by J.-L. Wu, Y. Hu and E. F. Westrum.

*CODATA Newsletter*, Nos. 66–69 (4 issues; distribution of 6000 copies each).

### Electronic publication

*CODATA Referral Database* (Produced by the CODATA Task Group on a Referral Database), 1400 computer-searchable sources of scientific and technical data.

*Special projects.* At the request of ICSU that CODATA should investigate the issue of data exchange more systematically with a view, potentially, of issuing a formal statement,

CODATA has formed a Working Group on Data Access. Their mandate is to examine problems, policies and possible solutions to the issue of international access and exchange of data for scientific research. To keep the work focused, it is proposed initially to concentrate on the problems associated with global change research before extending its studies.

*New areas of interest.* One of the new Task Groups approved at the General Assembly has taken the initiative to support the development of a master inventory of the world's plants. This massive undertaking, which will involve the collaboration of relevant biological Unions, will ultimately provide a checklist against which species diversity, genetic resources and pharmaceutical materials can be assessed.

The new Working Group on Electronic Information Transfer (chaired by the IUCr delegate) seeks to develop means to distribute the products of CODATA-sponsored programmes to the scientific community via electronic means and to exploit the Internet in assisting the work of CODATA's Task Groups, Commissions, Secretariat and Executive Committee.

### Report of use of 1994 ICSU grant and UNESCO subvention

*Commission on Standardized Terminology for Access to Biological Data.* The Commission worked with groups such as the Federation of Scientific Editors and the IUBS Commission on Plant Taxonomic Databases to encourage policies that will result in more uniform use of terminology and hence easier development of comprehensive taxonomic data networks. They collaborated with the International Committee on the Taxonomy of Viruses and the International Leishmaniasis Network in developing standardized descriptors for viral characteristics and setting up pilot databases, respectively.

*Task Group on Geothermodynamic Data.* This Group continued its work on obtaining critical thermodynamic data for the study of problems of geological, planetary and industrial importance. One of their major contributions to the scientific community is the integration of data obtained by calorimetry, phase equilibrium studies, modeling, spectroscopy and other experimental methods into one internally consistent critically evaluated database.

*Task Group on Databases for Experimental Data and Electronic Publishing (EXPERIDAT) and Working Group on Electronic Information Transfer (WGEIT).* The Task Group's objective was to study practical means of exploiting current telecommunications and computer technology to effect high-quality cost-efficient production of numerical databases and electronic publishing. For practical reasons, the work of this group metamorphosed part way through 1994 to that of the WGEIT. As cited above under *New areas of interest*, they began to distribute the products of CODATA-sponsored programmes to the scientific community via electronic means and to exploit the Internet in facilitating the work of CODATA's Task Groups, Commissions, Secretariat and Executive Committee.

### Conclusion and future plans

CODATA plans to support the work plans of its Task Groups, Commissions and Working Groups during the next biennium as it pursues its role as the ICSU body addressing the interdisciplinary issues associated with scientific and technical data. The output of the Long Range Planning Meeting will help to chart our future course.

In general, CODATA enjoyed an effective year. Its Task Groups and Commissions continued to be productive and some of the new work approved at the General Assembly is scientifically both important and interesting. Similarly to related

organizations, one of CODATA's most significant challenges is that of raising adequate financial resources to respond to the many challenges and opportunities it foresees during the prevailing global economic restraint.

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

It was decided at the 24th General Assembly of ICSU in 1993 to merge the ICSU Committee on Science and Technology in Developing Countries (COSTED) and the International Biosciences Network (IBN). The President of the newly formed body is Professor G. K. Menon. The first joint Meeting was held in Ghana in April 1994 where it was decided that COSTED-IBN, which will be cosponsored by UNESCO, would, in the future, work along the lines of the IBN, by allowing the regional networks to set their own priorities and their own modalities for action. These regional offices will be located in Accra and Dakar for Africa, Amman for the Arab Region, Madras for Asia and Santiago de Chile for Latin America. The Central Secretariat is located in Madras (India), where a new building is being funded by the government of India.

Modest support may be made available by COSTED-IBN for one or two participants from developing countries at Meetings such as those organized by the IUCr, depending on the priorities of the regional offices, which should be directly contacted by the organizers of these Meetings.

*ICSU Committee on Space Research (COSPAR)*

The 51st COSPAR Bureau Meeting was held 23–24 March 1994 under the Chair of its resigning President, Professor W. I. Axford. The most important items on the agenda were concerned with the 30th COSPAR Scientific Assembly and Associated Activities, which were held a few months later on 11–21 July 1994 in the Congress Centre of Hamburg and with the elections of the new President, Vice-presidents, COSPAR Bureau Members and Finance Committee for the period 1994–1998. The elections took place during the COSPAR Council Meeting in Hamburg on 11 July 1995. The new COSPAR President for the term 1984–1998 is Professor Gerhard Haerendel, Max-Planck-Institut für Extraterrestrische Physik (MPE) in Garching (near Munich) and Technical University of Braunschweig, Germany. The new Vice-presidents are Professor Louis J. Lanzerotti, AT&T Bell Laboratories, Murray Hill, NJ, USA, and Professor A. Nishida, University of Tokyo, Japan. The 31st COSPAR Meeting will be held in 1996 in Birmingham, England, and the 32nd Meeting in 1998 in Tokyo, Japan.

### Finances

The audited accounts of the year 1994 are given at the end of this Report. For comparison, the figures for 1993 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 1994 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 loss has arisen on the assets of the Union, in terms of Swiss Francs, amounting to SwFr 567 972. This loss has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1994. It should be noted that this loss in Swiss Francs is not a real loss of money, but rather a loss 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 1994. For 1994, an adjustment to show the difference between revalued cost and market value has not been made. This change in accounting policy has been made so that the value of the investments is presented more realistically. (For 1993, the difference between revalued cost and market value was shown as an adjustment in order that the investments could be stated at cost. This prevented the fluctuations in value from influencing the General Fund. The revalued cost was 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 530 158 with the banks at the end of the year was represented by US \$176 029 with Merrill Lynch, £130 476 with National Westminster Bank and SwFr 26 848 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, excluding stocks of unsold publications but including the loss of SwFr 567 972 resulting from fluctuations in rates of exchange, have decreased during the year, from SwFr 5 685 546 to SwFr 5 352 197.

Transfers of SwFr 100 000, SwFr 25 000, SwFr 45 000 and SwFr 50 000 were made to the Publications and Journals Development Fund from the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Structure Reports* Fund and the *International Tables* Fund, respectively. Transfers of SwFr 100 000, SwFr 25 000, SwFr 25 000 and SwFr 25 000 were made to the Research and Education Fund from the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Structure Reports* Fund and the *International Tables* Fund, respectively. A transfer of SwFr 25 000 was made to the Ewald Fund from the General Fund. A transfer of SwFr 150 000 was made to the *Newsletter* Fund from the General Fund.

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. Note that for the General Fund the 'Release from valuation reserve' results from the change in accounting policy mentioned above.

The General Fund account shows a profit of SwFr 12 296, before the transfers totalling SwFr 150 000 to the *Newsletter* Fund, as compared with a deficit of SwFr 96 228 in 1993, before transfers totalling SwFr 40 000 to the President's Fund and the Ewald Fund. The administrative expenses were SwFr 217 980 in 1994 as compared with SwFr 263 472 in 1993. Of this amount, SwFr 68 999 was charged to the publications of the Union.

SwFr 27 866 was given for general support of scientific Meetings, in addition to SwFr 83 728 for financial support to young scientists attending Meetings, which appears in the expenses of the Research and Education Fund, and SwFr 18 284 in special grants from the President's Fund. SwFr 16 028 was spent in assisting the work of the non-publishing Commissions.

The expenses of the Union Representatives on other bodies were SwFr 9368. The cost of the Finance Committee Meeting held in 1994 was SwFr 7924, while the Executive Committee Meeting cost SwFr 21 520. The Union received SwFr 15 750 from the Unesco subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 148 000. Interest on bank accounts and investments credited to the General Fund was SwFr 232 978.

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 6% per annum, on the balances in the funds.

The President's Fund therefore received interest of SwFr 2162. Grants totalling SwFr 18 284 were paid from the fund.

The *Acta Crystallographica* account for 1994 shows a surplus of SwFr 364 303 before the transfer of SwFr 200 000 to other fund accounts, as compared with a surplus of SwFr 286 923 in 1993 before transfers of SwFr 100 000.

The subscription rates were increased for 1994. The number of paid subscriptions to *Sections A + B + C + D* of *Acta*, including 74 personal subscriptions, was 778. The number of paid subscriptions to *Sections A + B + C* of *Acta*, including 41 personal subscriptions, was 132. For 1993, the number of paid subscriptions to all sections of *Acta* (*Section D* was distributed free in 1993), including 89 personal subscriptions, was 962. For the number of paid subscriptions to the separate sections of the journal, those to *Section A* decreased from 294 in 1993 to 293, those to *Section B* increased from 218 to 222 and those to *Section C* decreased from 147 to 139. There were 134 paid subscriptions to *Section D*. As usual, the costs 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; part of the technical editing costs have also been assigned to the *Journal of Synchrotron Radiation* development costs. The technical editing costs for *Acta Crystallographica* were SwFr 620 283 as compared with SwFr 614 311 in 1993. 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 10 642 before transfers of SwFr 50 000 to other fund accounts, as compared with a surplus of SwFr 57 026 in 1993. The number of subscriptions, including 105 personal subscriptions in 1994 and 108 in 1993, decreased from 971 in 1993 to 931 in 1994.

The *Structure Reports* series ended in 1993. The *Structure Reports* account shows a surplus of SwFr 17 603 in 1994 before transfers of SwFr 95 000 to other fund accounts as compared with a surplus of SwFr 61 777 in 1993. The net income from sales was SwFr 18 120 in 1994 as compared with SwFr 241 560 in 1993.

The *International Tables* account shows a surplus of SwFr 50 786 before transfers of SwFr 75 000 to other fund accounts as compared with a surplus of SwFr 113 426 in 1993 before a transfer of SwFr 40 000. The net sales income of SwFr 79 974 derived mostly from Volume B. Volumes A and C were out of print for part of 1994.

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, and from royalties from the IUCr/OUP Book Series.

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 217 684 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. Expenses of SwFr 132 817 incurred in connection with the launch of the *Journal of Synchrotron Radiation* were charged to the Publication and Journals Development Fund. SwFr 83 728 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.

The *Newsletter* Fund account was started in 1994 and received a transfer of SwFr 150 000 from the General Fund.

**Auditor's Report to the International Union of Crystallography**

We have audited the financial statements on pages 111 to 124 which have been prepared under the accounting policies set out on page 122.

*Respective responsibilities of Executive Committee and Auditors*

The Executive Committee is responsible for ensuring the preparation and audit of the financial statements. It is our responsibility to form an independent opinion, based on our audit, on those statements and to report our opinion to you.

*Basis of opinion*

We conducted our audit in accordance with Auditing Standards issued by the Auditing Practices Board. An audit includes examination, on a test basis, of evidence relevant to the amounts and disclosures in the financial statements. It also includes an assessment of the significant estimates and judgements made in the preparation of the financial statements, and of whether the accounting policies are appropriate to the Union's circumstances, consistently applied and adequately disclosed.

We have not been requested by the Union to consider the requirements of Swiss Company Law as regards these financial statements.

We planned and performed our audit so as to obtain all the information and explanations which we considered necessary in order to provide us with sufficient evidence to give reasonable assurance that the financial statements are free from material misstatement, whether caused by fraud or other irregularity or error. In forming our opinion we also evaluated the overall adequacy of the presentation of information in the financial statements.

*Opinion*

In our opinion, the financial statements give a true and fair view of the state of the Union's affairs as at 31 December 1994 and of its excess of income over expenditure for the year then ended.

Touche Ross & Co Chartered Accountants  
Manchester, England  
14 June 1995

**International Union of Crystallography**  
**Balance Sheet as at 31 December 1994**

	Swiss Francs		1994	1993
	1994	1993	1994	1993
<b>FUND ACCOUNTS</b>				
General Fund	929,049	929,049		
President's Fund	54,324	54,324	40,156	27,803
<i>Acta Crystallographica</i>	1,996,023	1,996,023	490,002	762,588
<i>Journal of Applied Crystallography</i>	499,166	499,166	530,158	790,391
<i>Structure Reports</i>	198,389	198,389	32,777	38,283
<i>International Tables</i>	241,083	241,083	132,794	215,649
Book Fund	13,305	13,305		
Publications and Journals Development Fund	741,785	741,785	25,560	13,350
Research and Education Fund	752,281	752,281	721,289	1,057,673
Ewald Fund	260,141	260,141		
Newsletter Fund	-	-		
	5,685,546	5,685,546	(264,974)	(291,874)
			456,315	765,799
				790,778
			4,888,617	5,696,748
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*Journal of Applied Crystallography Account for the year ended 31 December 1994*

	1994		1993		1994		1993	
	Swiss Francs		Swiss Francs		Swiss Francs		Swiss Francs	
Publication expenses:								
Printing and binding Volume 27 (1993 Volume 26)	111,309		87,190		324,442		351,586	
Distribution and postage	17,058		20,433		3,784		7,148	
Airfreight costs	8,627		7,595		6,575		7,714	
	<u>136,994</u>		<u>115,218</u>		<u>1,662</u>		<u>1,038</u>	
Net loss on reprints	7,369	144,363	3,141	118,359	336,463		367,486	
Editorial expenses:								
Editorial honoraria	8,636		7,078		22,975		25,111	
Secretarial assistance	3,254		2,510					
Postage, travel and sundries	9,385		11,897					
Technical Editing:								
Salaries and expenses	118,598		118,101					
Computer expenses	5,081		6,670					
Depreciation of office equipment	913	145,867	974	147,230				
Administration expenses		13,110		19,760				
Transfers to other Funds:								
Publications and Journals	25,000							
Development Fund	25,000	50,000						
Research and Education Fund								
<i>Excess of income over expenditure</i>				57,026				
<i>carried to balance sheet</i>						39,358		
		<u>353,340</u>		<u>342,375</u>		<u>353,340</u>		<u>342,375</u>
Balance at 1 January	499,166		435,705					
Difference between income and expenditure	(39,358)		57,026					
Fluctuations in rates of exchange	(46,208)		6,435					
Balance at 31 December	<u>413,600</u>		<u>499,166</u>					





## Book Fund Account for the year ended 31 December 1994

	Swiss Francs		Swiss Francs	
	1994	1993	1994	1993
Publication expenses:				
Book series expenses				
<i>Atlas of Crystallography</i>	204	933		
<i>World Directory of Crystallographers</i>	300	783		
9th Edition	9,713	3,676	1,153	3,013
Sundry publications	—	136	25	—
			209	—
			178	215
			51	324
			225	639
			862	—
			4,035	3,015
			3,479	—
			10,217	7,226
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			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
			3,479	—
			10,217	7,226
			4,035	3,015
</				



## Ewald Fund Account for the year ended 31 December 1994

	Swiss Francs		Swiss Francs	
	1994	1993	1994	1993
Selection Committee and expenses	103	-	-	-
Ewald prize	-	37,250	25,000	15,000
			15,602	17,910
<i>Excess of income over expenditure carried to balance sheet</i>	40,499	-	-	4,340
	<u>40,602</u>	<u>37,250</u>	<u>40,602</u>	<u>37,250</u>
Balance at 1 January	260,141	261,126		
Difference between income and expenditure	40,499	(4,340)		
Fluctuations in rates of exchange	(30,212)	3,255		
Balance at 31 December	<u>270,428</u>	<u>260,141</u>		

## Newsletter Fund Account for the year ended 31 December 1994

	Swiss Francs		Swiss Francs	
	1994	1993	1994	1993
Editorial Honoraria	4,375	-	-	-
Editorial Expenses	29,998	-	150,000	-
AIP Expenses	56,039	-	-	-
<i>Excess of income over expenditure carried to balance sheet</i>	59,588	-	-	-
	<u>150,000</u>	<u>-</u>	<u>150,000</u>	<u>-</u>
Balance at 1 January	-	-	-	-
Difference between income and expenditure	59,588	-	-	-
Fluctuation in rates of exchange	(5,989)	-	-	-
Balance at 31 December	<u>53,599</u>	<u>-</u>	<u>53,599</u>	<u>-</u>

**Cash Flow Statement for the year ended 31 December 1994**

		Swiss Francs	
	Note	1994	1993
Excess of income over expenditure		234,623	286,346
Deduct:			
Interest received	5	(44,854)	(47,482)
Investment income	6	(269,017)	(245,242)
Loss/(profit) on disposal of investments	7	111,890	(33,243)
Change in market value of investments	8	(268,328)	-
Operating loss		<u>(235,686)</u>	<u>(39,621)</u>
Exchange rate fluctuations attributable to operating activities	9	(36,721)	(30,214)
Depreciation charges		7,058	8,963
Decrease in debtors		70,645	157,940
(Decrease)/increase in creditors		<u>(26,900)</u>	<u>120,098</u>
Net cash (outflow)/inflow from operating activities		(221,604)	217,166
Returns on investments			
Interest received		44,854	47,482
Investment income		269,017	245,242
Net cash inflow from returns on investments		313,871	292,724
Investing activities			
Purchase of office equipment		(1,663)	(6,454)
Purchase of investments		(681,186)	(1,854,509)
Disposal of investments		372,146	1,672,322
Net cash (outflow)/inflow from investing activities		<u>(310,703)</u>	<u>(188,641)</u>
(Decrease)/increase in cash and cash equivalents after financing	10	<u>(218,436)</u>	<u>321,249</u>

## Notes to the Financial Statements

## 1. Accounting policies

*(a) Accounting convention*

The financial statements are prepared under the historical cost convention with the exception of investments which are stated at market value 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.

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 recognised when received.

*(h) Investments*

Investments are stated at market value. This represents a change in accounting policy (they were previously stated at revalued cost) effective from 1 January 1994. The financial effect of this change in policy is given in Notes 7 and 8 to the accounts.

## 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:

	1994	1993
Netherland Guilders	1.3258	1.2887
Danish Crowns	4.6364	4.5662
Pounds Sterling	0.4848	0.4496
US Dollars	0.7476	0.6711

The net assets of the Union at 1 January 1994 (SwFr 5,685,546) would have had the value of US \$3,815,569 or £2,556,221 if expressed in those currencies.

At 31 December 1994, these assets (SwFr 5,352,197) would have had the value of US \$4,001,302 or £2,594,745 respectively, being an increase of US \$185,733 or an increase of £38,524 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 1994	Adjustment to restate at market value 1 January 1994	Holding at market value 1 January 1994	Swiss Francs	Fluctuations in rates of exchange	Increase/ (decrease) in market value	Holding at market value 31 December 1994	Holding at revalued cost 31 December 1994
<b>Held by Merrill Lynch</b>								
<b>Corporate Government Securities</b>								
4,311 Units GNM P146535-2016 (US\$)	16,460	1,761	18,221	(11,352)	(784)	(346)	5,739	5,498
27,487 Units GNM P169332-2016 (US\$)	52,100	5,587	57,687	(13,891)	(4,997)	(2,199)	36,600	35,043
<b>Mutual Funds/Unit Investment Trusts</b>								
3,730 Units ML Capital Fund/CLB (US\$)	134,183	19,263	153,446	(458,793)	(17,507)	(11,177)	124,762	118,874
443 Units Haussmann Holdings (US\$)	453,241	465,382	918,623	(458,793)	(52,464)	(44,443)	362,923	200,991
5,700 Units Global Allocation Portfolio Class A (US\$)	89,601	(934)	88,667	-	(10,116)	(2,860)	75,691	79,378
9,503 Units Meridian Funds Global Government Fund (US\$)	150,490	3,263	153,753	-	(18,330)	(23,181)	127,453	147,735
77 Units Permal Investment Holdings NV (US\$)	151,496	6,644	158,140	-	(18,043)	(8,550)	131,547	134,211
11,464 Units Meridian Charter Income Fund (US\$)	166,688	2,898	169,586	-	(19,856)	(18,442)	143,612	159,487
<b>Certificates of deposit</b>								
75,000 British Gas Finance (US\$)	114,902	10,097	124,999	-	(14,262)	(10,307)	100,430	101,792
75,000 Units QEC (US\$)	112,774	6,614	119,388	-	(13,622)	(6,782)	98,984	99,907
100,000 Units US Treasury Note 6.875% (US\$)	-	-	-	-	7,031	(2,366)	130,226	132,592
179,000 Units US Treasury Bill 0% (US\$)	-	-	-	-	12,218	1,147	231,531	230,384
<b>Held by Foreign &amp; Colonial</b>								
16,887 Units Reserve Asset Fund Class D (US\$)	525,964	46,204	572,168	-	(65,282)	(54,010)	488,252	501,331
18,081 Units Reserve Asset Fund Class L (£)	449,775	127,523	577,298	-	(41,792)	(74,503)	490,370	446,582
16,619 Units Reserve Asset Fund Class X (£)	504,361	(12,557)	491,804	-	(35,603)	(9,031)	476,258	496,937
25,471 Units Reserve Asset Fund Class C (US\$)	619,667	26,382	646,049	-	(73,710)	(61,305)	550,989	588,922
11,080 Units Reserve Asset Fund Class M (US\$)	288,038	21,416	309,454	-	(35,307)	(13,715)	271,982	266,724
5,028 Units Reserve Asset Fund Class E (£)	192,775	6,962	199,737	-	(14,459)	(28,090)	170,701	192,332
375,000 Units UK Treasury 7.75% 22.9.2006 (£)	883,455	54,273	937,728	-	(67,884)	(151,340)	718,504	819,500
17828.27 Units Reserve Asset Fund Class N (Yen)	-	-	-	-	1,938	(950)	152,063	153,013
	4,905,970	790,778	5,696,748	(484,036)	(482,831)	(522,450)	4,888,617	4,911,233

**5. Bank interest**

	Swiss Francs	
	1994	1993
National Westminster Bank PLC		
Manchester Business Reserve Account	4,710	4,065
Manchester Capital Reserve Account	13,820	19,778
Amsterdam-Rotterdam Bank NV		
Current Guilder Account	-	3
Union Bank of Switzerland		
Current Swiss Francs Account	-	-
Merrill Lynch		
CMA Account	8,123	4,801
Foreign & Colonial		
Cash balance	182	152
Petty cash accounts	3	5
Interest from Munksgaard	18,016	18,678
	<u>44,854</u>	<u>47,482</u>

**6. Investment income**

	Swiss Francs	
	1994	1993
Meridian Funds Global – Government Fund	15,211	-
Meridian Charter – Income Fund	12,324	2,635
GEC	7,914	8,859
British Gas Finance	9,056	9,647
ML Capital Fund/CLB	10,248	8,327
GNM P146535-2016	885	1,949
GNM P169332-2016	3,771	6,105
Temple Worldwide Fund G	-	698
Temple Worldwide Fund I	-	6,454
Foreign and Colonial – Reserve Asset Fund Class M	11,550	8,493
Hausmann Holdings	4,425	-
Foreign and Colonial – Reserve Asset Fund Class X	29,088	28,244
Foreign and Colonial – Reserve Asset Fund Class D	35,376	32,780
Foreign and Colonial – Reserve Asset Fund Class L	29,367	20,016
Foreign and Colonial – Reserve Asset Fund Class C	39,955	23,095
Foreign and Colonial – Reserve Asset Fund Class E	13,513	14,456
Foreign and Colonial – Reserve Asset Fund Class N	855	-
FHLMC	-	2,560
MLST World income portfolio	-	3,241
CITI CDT Cards	-	5,548
National Westminster Bank deposit account	-	62,135
UK Treasury 7.75% 22.9.2066	45,479	-
	<u>269,017</u>	<u>245,242</u>
Allocated to:		
President's Fund	2,162	2,120
Ewald Fund	15,602	17,910
Publication and Journals Development Fund	23,477	46,831
Research and Education Fund	39,652	52,043
Balance left in General Fund	188,124	126,338
	<u>269,017</u>	<u>245,242</u>

**7. (Loss)/profit on disposal/redemption of investments**

	Swiss Francs	
	1994	1993
Proceeds	372,146	1,672,322
Book value	484,036	1,639,079
(Loss)/profit allocated to General Fund	<u>(111,890)</u>	<u>33,243</u>

Book value represents market value at 1 January 1994 for 1994 and revalued cost for 1993 (see Note 1 for details of change in accounting policy). If there had been no change in accounting policy there would have been a gain of £159,443 to transfer to reserves.

**8. Change in market value of investments**

	Swiss Francs
Revaluation of investments at 1 January 1994 from revalued cost to market value	790,778
Decrease in market value in 1994	522,450
	<u>268,328</u>

**9. Exchange rate fluctuations attributable to operating activities**

	Swiss Francs	
	1994	1993
Total fluctuations in exchange rates dealt with in fund accounts	(567,972)	73,291
Adjustments for exchange differences attributable to:		
Investments	482,831	(106,915)
Fixed assets	1,117	(339)
Cash and bank balances	47,303	3,749
	<u>(36,721)</u>	<u>(30,214)</u>

**10. Analysis of changes in cash and cash equivalents during the year**

	Swiss Francs	
	1994	1993
Balance at 1 January 1994	828,674	511,174
Net cash (outflow)/inflow	(218,436)	321,249
Fluctuations in rates of exchange on cash and bank balances	(47,303)	(3,749)
Balance at 31 December 1994	<u>562,935</u>	<u>828,674</u>

**11. Analysis of balances of cash and cash equivalents as shown in the balance sheet**

	Swiss Francs			
	1994	1993	Change 1994	Change 1993
Cash at bank and in hand	<u>562,935</u>	<u>828,674</u>	<u>(265,739)</u>	<u>317,500</u>