

International Union of Crystallography

Report of the Executive Committee for 1995

Meetings

The IUCr sponsored the following meetings held during 1995:

1. International School on Advanced Electronic Materials, Madras, India, 6–15 February 1995.
2. BCA Fifth Intensive Course in X-ray Structure Analysis, Aston, Birmingham, UK, 1–9 April 1995.
3. International School on Quasicrystals, Balatonfüred, Hungary, 13–20 May 1995.
4. Charge Density School, La Plata, Argentina, 18–26 May 1995.
5. Erice School on Crystallography of Supramolecular Compounds, Erice, Italy, 1–12 June 1995.
6. Gordon Research Conference on Electron Distribution and Chemical Bonding, Plymouth, New Hampshire, USA, 2–7 July 1995.
7. 4th European Powder Diffraction Conference (EPDIC IV), Chester, UK, 10–14 July 1995.
8. Workshop on Structure Determination from Powder Diffraction Data, Oxford, UK, 16–20 July 1995.
9. Workshop on the Description, Understanding and Prediction of the Structure of Inorganic Solids, Montreal, Canada, 19–22 July 1995.
10. Rietveld Summer School '95-RS, Moscow, Russia, 20–22 July 1995.
11. Sixteenth European Crystallographic Meeting (ECM-16), Lund, Sweden, 6–11 August 1995.
12. International Conference on Interference Phenomena in X-ray Scattering, Moscow, Russia, 14–19 August 1995.
13. Conference on Fundamental Principles of Molecular Modelling, Skukuza, South Africa, 20–24 August 1995.
14. International Conference on X-ray Powder Diffraction Analysis of Real Structure of Matter: Size–Strain '95, Lipovsky Mikulas, Slovakia, 21–25 August 1995.
15. Summer School on Neutron Scattering, Oxford, UK, 12–21 September 1995.
16. The Sixth International Conference on Crystallization of Biological Macromolecules, Hiroshima, Japan, 12–17 November 1995.
17. International Seminar-cum-School on Macromolecular Crystallographic Data, Calcutta, India, 16–20 November 1995.
18. Asian Crystallographic School of Gems and Precious Materials, Bangkok, Thailand, 20–21 November 1995.
19. 2nd Conference of the Asian Crystallographic Association (AsCA '95), Bangkok, Thailand, 22–24 November 1995.
20. 1995 Asian Crystallographic Computing School, Bangkok, Thailand, 27–30 November 1995.

The Executive Committee met in Lund, Sweden, in August. The Finance Committee met twice, in Chester, UK, in April, and then in August in Lund immediately before the Executive Committee meeting, to prepare its advice and recommendations on finances, establishment and staff matters. The most important items of business dealt with by the Executive Committee at its meeting, and in postal ballots, were:

(1) editorial policy, pricing policy and subscription rates, approval of appointments of Co-editors, electronic publishing, special issues, 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 and expansion of this office, provision of an IUCr home page on the World-Wide Web;
- (5) cooperation with databases, including relations between the IUCr and the Cambridge Crystallographic Data Centre and between the IUCr and the Gmelin Institut/Fachinformationszentrum Karlsruhe;
- (6) the implementation of the Crystallographic Information File (CIF) for *Acta Crystallographica* 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*, approval of Volume A1 and consideration of possible further volumes;
- (8) the IUCr *Newsletter*;
- (9) the *World Directory of Crystallographers*;
- (10) approval of publications, jointly with Oxford University Press, in the IUCr/OUP Book Series;
- (11) approval of the audited accounts for the previous year;
- (12) funding and uses of the Publications and Journals Development Fund and the Research and Education Fund;
- (13) the General Fund estimates and the level of the unit contribution;
- (14) investment policy;
- (15) funding and uses of the Publications and Journals Development Fund and the Research and Education Fund;
- (16) sponsorship and financial support for meetings, including young scientists' support;
- (17) report of the Sub-committee on Statutes and By-Laws;
- (18) applications for membership of the IUCr;
- (19) discussion of the arrangements for the Seattle General Assembly and Congress and consideration of the Programme Committee proposals;
- (20) review of the activities of the Commissions;
- (21) proposals to establish new Commissions.

Publications

Volume 51 of *Acta Crystallographica*, Volume 28 of the *Journal of Applied Crystallography* and Volume 2 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

1995 was a relatively stable year for the journals, with no major changes instituted. Volume 51 of *Acta Crystallographica*

(*Acta*) included 1494 papers with an overall total of 5888 pages. The number of papers received by the Managing Editor was 1516, a 17% increase over 1994. Median publication times fell for Full Articles in Section A (5.9 months), but in Sections B (7.1 months) and D (6.8 months) publication times increased, mainly as a result of the publication of Special Issues. In Section C, the median publication time for Regular Structural Papers decreased to 6.2 months.

Volume 28 of the *Journal of Applied Crystallography (JAC)* contained 144 papers with an overall total of 860 pages. The median publication time for Full Articles decreased to 6.8 months from 7.3 months in 1994.

Volume 2 of the *Journal of Synchrotron Radiation (JSR)* included 50 papers in its first year of full publication following the inaugural issue in late 1994. Containing 319 pages, the median publication time was 2.6 months.

Comments from the individual editors follow, but everyone would agree that the dedication of the editing staff in Chester, the diligence of hard-working Co-editors and reviewers, and the continuing support of the authors who have chosen to publish in these journals have all contributed to the exceptional quality of the journals during 1995.

Acta Crystallographica Section A (A. Authier, Editor)

Section A of *Acta* contained 111 Full Articles during 1995, reflecting a steady flow of manuscripts. Two major challenges face the journal in the coming year. One is encouraging authors to write Lead Articles and Topical Reviews. There are a few coming in but much less than there should be, despite all the efforts of the Editor to solicit more such articles. The help of all crystallographers is sought to improve this situation. The second challenge is a continuing effort to reduce the time of publication by the systematic use of fax and e-mail in communications with authors and referees, and in encouraging authors to submit their manuscripts in machine-readable form.

Acta Crystallographica Section B (F. H. Allen, Editor)

Section B published 128 Full Articles in 1104 pages during 1995. This included a special conference issue in August 1995 containing 22 papers from the 1994 American Crystallographic Association Symposium on New Trends in Small Molecule Crystallography, organized by Frank Herbstein, who acted as Guest Editor for the special issue. Additionally, *Section B* published one major Lead Article and two shorter Topical Reviews in addition to five Short Communications. The number of papers received by the Editorial Office compares almost exactly with 1993 and 1994. Thus, despite losing a few papers on biological crystallography to the new *Section D*, this loss has been offset by a concomitant increase in *Section B* papers from other areas of structural science.

Section B is also building carefully on the CIF-submission procedures pioneered for *Section C*. This is now an area for development in *Section B*. A controlled policy has been adopted of publishing reports of individual crystal structures, *provided that the paper contains other experimental and computational results and/or has a detailed discussion that is scientifically appropriate*. The balance between review material and original research papers is a delicate one in a primary journal and current policy is to be reasonably selective in commissioning new review material. Having said that, it is often difficult to obtain authoritative reviews from busy potential authors. Despite its diversity of scientific content, *Section B* remains an important vehicle for the publication of results in structural crystallography and related areas.

Acta Crystallographica Section C (S. R. Hall, Editor)

There was marked improvement in the publication rate of *Section C* papers in 1995. The number of manuscripts received increased by 10% over 1994, and the number of papers published rose by over 25%. The reasons for the higher publication rate appear to be several-fold. The *Acta* staff should be congratulated on their efforts to reduce the checking and editing backlogs for *Section C* to their lowest ever level, an effort which was greatly assisted by the software innovation within that office. The much higher rate of CIF electronic submissions assisted the checking and editing processes and also meant that Co-editorial tasks were simplified. Another contributing factor was the imposition of stricter initial filtering by the Chester staff, meaning that manuscripts with serious problems were immediately returned to the authors and less time was lost in the review process of trivial omissions or errors.

In addition to the faster publication rate, the overall quality of presentation of *Section C* papers has improved noticeably. Authors are becoming more experienced with submitting material as CIFs, and the insistence on high-standard diagrams is becoming evident in the printed issues (the rejection of diagrams at the first-proof stage has decreased almost to zero). I believe that there has also been a gradual improvement in the level of expertise exhibited in *Section C*, with many of the more experienced workers in the field returning as authors. This reverses a trend that was evident in the late 1980's and early 1990's, and which was discussed in the Commission on Journals meetings. The new contents format, cover presentation and CIF entry facilities have all contributed to making *Section C* a structural science 'publication standard'.

Acta Crystallographica Section D (J. P. Glusker, Editor)

During 1995, one issue of *Section D* was devoted to manuscripts from the meeting on Structure-Based Drug Design held in Panama City Beach, Florida, USA, in April 1994. The articles in this issue cover basic concepts of structure-aided design, applications to antiviral agents, drugs involved with the immune system, protease inhibitors and antiparasitic drugs. In addition, a Lead Article by Kurt Wuthrich on NMR – This Other Method for Protein and Nucleic Acid Structure Determination, and a Topical Review by Rui Sousa on the use of stabilizing agents in protein crystallization were also published.

In all, 137 Full Articles and 8 Short Communications were published during the year. Short Communications were generally reports of crystallization and preliminary X-ray diffraction studies of biological macromolecules. Research papers covered many other aspects of macromolecular crystallography from theoretical to practical details to descriptions of results.

The influx of manuscripts to *Section D* has been excellent and the editorial staff has made extensive efforts to cut down the time between submission and acceptance.

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

The *Journal of Applied Crystallography* has continued to attract a large variety of publications, spanning powder diffraction, computing, small-angle scattering, topography and so on. The section dealing with Computer Programs seems to have become increasingly popular. In addition, there is noticeably a more widespread use of colour in research articles.

With regard to specialist areas, the section on Teaching and Education in Crystallography has not so far attracted many submissions and perhaps this section needs more publicity to

Table 1. Survey of the contents of IUCr Journals

Acta Crystallographica

Vol.	Year	Number of pages*	Number of papers	Full Articles†		Short Communications‡	
				Number	Average length	Number	Average length
A47	1991	860	123	104	7.3	19	1.4
B47		1030	137	130		7	1.7
C47		2740	1076	1069		7	0.6
A48	1992	954	117	106	7.7	11	2.2
B48		856	125	113		12	1.9
C48		2280	914	906		8	0.6
A49§	1993	901	121	108	7.7	13	2.1
B49		1075	155	149		6	2.0
C49		2186	880	869		11	0.9
D49		604	72	62		10	3.0
A50	1994	798	103	91	7.7	12	1.4
B50		782	99	94		5	2.4
C50		2102	852	847		5	0.6
D50		920	135	121		14	3.0
A51	1995	952	125	111	8.1	14	1.6
B51		1104	133	128		5	2.4
C51		2726	1091	1087		4	0.5
D51		1106	145	137		8	2.6

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
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	0	0	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
28	1995	860	144	95	7.2	10	2.8	5	3.9	16	4.7	18	1.8

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	0	0	0	0	0	0
2	1995	319	50	47	5.9	3	1.7	0	0	0	0

* 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 A49 includes, in addition, 515 pages of abstracts communicated to the Beijing Congress. ¶ Laboratory Notes, Cryocrystallography Notes, Letters to the Editor, Meeting Reports and Computer Program Abstracts.

make it viable. A new area that was begun in 1995 was Cryo-crystallography Notes. This is an important field, particularly for biological crystallographers, where many practical ideas for carrying out low-temperature experiments are being discussed. In a departure from normal procedure in *JAC*, this section has been placed under the responsibility of a single member of the Editorial Board. It is possible that this approach could be considered for other specialist areas.

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

1995 was the first full year of publication of the *Journal of Synchrotron Radiation* following the Inaugural Issue published in late 1994. The papers published covered all regions of the synchrotron-radiation spectrum as well as sources, instrumentation and methods. Nevertheless, we have sought to improve the scientific and geographical coverage via new appointments to the Editorial Board. An anxiety, however, relates to the fewer number of pages realized compared with the number estimated per issue (*i.e.* 319 pages for 1995 versus an estimated 1200 pages when the journal is fully established). The geographical impact of the journal so far can be seen from the distribution of papers published by country: UK 23, France 9, USA 8, Japan 6, Germany 4, Italy 3, Australia 2 and one each from China, Denmark and Russia. It remains the case that in the field of synchrotron radiation we see strong 'competition' from conference proceedings volumes, especially in *Review of Scientific Instruments*, which draw papers away from *JSR*. In contrast, the existence of *Synchrotron Radiation News* and its features have largely been complementary to *JSR*. The publication by *JSR* of the SRI-97 proceedings will be important for the future vigour of the journal. In the shorter term, we await the outcome of the first tranche of subscriptions as the free distribution through 1995 has finished.

Commission on International Tables

On 1 July 1995, Arthur Wilson died peacefully at his home in Cambridge in his 81st year. With him the Commission has lost its Chairman from 1982 to 1993 and Editor of Volume C. We all greatly miss his counsel, his keen interest and his friendly manner. At the time of his death, Arthur was busily engaged in preparing the Second, Revised Edition of Volume C. As the new Editor of Volume C, the Executive Committee in August 1995 appointed E. Prince of Gaithersburg, Maryland, USA. The Executive Committee has also approved the publication of Volume A1 on *Maximal Subgroups of Space and Plane Groups*, with H. Wondratschek, Karlsruhe, Germany, as Editor.

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

The Fourth, Revised Edition of Volume A was published in March 1995. It contains new diagrams for all plane groups and space groups, as well as new explanatory diagrams in Section 2.6. Furthermore, this edition contains for 17 space groups the new graphical and printed symbols for the 'double glide plane e' ', introduced in an IUCr Commission on Crystallographic Nomenclature Report in 1992. This has led to major changes in Section 1 and to modifications of the Hermann-Mauguin symbols for five space groups (Nos. 39, 41, 64, 67, 68).

Early in 1996, the material for a Corrected Reprint of Volume A, as well as for the Fourth Edition of the *Brief Teaching Edition of Volume A* was prepared.

A list of Corrigenda and Addenda to the Third, Revised Edition (1992) of Volume A appeared in *Acta Cryst.* (1995), A51, 592-595.

Volume B. Reciprocal Space; Editor U. Shmueli

1995 was marked by rather intensive editorial activities related to the preparation of the Second Edition of Volume B. Minor changes and corrections were prepared for the publication of a Corrected Reprint of Volume B. The reprint was launched mainly to make the volume available until the Second Edition is ready for printing. A list of Corrigenda and Addenda to the First Edition (1993) of Volume B appeared in *Acta Cryst.* (1996), A52, 500-501.

Most major revisions, including those in which the Editor participated as an author, were assembled during 1995 and transferred to the Technical Editor for further processing. One or two revisions of existing chapters are still outstanding at the time of writing this report.

Several final contacts with authors of new contributions were made during 1995. There was also extensive correspondence within the Commission regarding the nature and timing of these new contributions. At the time of writing (early 1996), all the preliminary editorial correspondence was concluded and all the formal invitations were issued.

Exchange of drafts is carried out predominantly by electronic mail, since files produced by \TeX -based software are ASCII and binary files produced by most word files can usually be encoded into ASCII. Most drafts are forwarded to the Technical Editor by Internet software, either by depositing them in Chester or by the Technical Editor retrieving them from Tel Aviv.

Volume C. Mathematical, Physical and Chemical Tables; Editor E. Prince

The current Editor has been appointed to try to perform the impossible task of filling the hole left by the death, on 1 July 1995, of Arthur Wilson. At the time of his death, the work of collecting material for an extensively revised and updated Second Edition was approximately 80% complete, and that work is continuing. A Corrected Reprint of the present edition of Volume C was published in February 1995, and at the current rate of sales, the stock will be exhausted in the Spring of 1997. A major effort is being made to have the Second, Revised Edition ready by that time.

A list of Corrigenda and Addenda to the First Edition (1992) of Volume C appeared in *Acta Cryst.* (1995), A51, 441-444.

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

The preparation of Volume D is progressing smoothly. The outline of Part 3 (*Symmetry Aspects of Structural Phase Transitions and Domain Structures*) was reviewed during a meeting in Aachen, Germany, with the General Editor of *International Tables* and co-authors of several chapters. The overall plan of the whole volume is now finalized and authors have been found for all chapters. About half of the manuscripts have already been submitted. Software will accompany the volume, which will include various tables (tensor invariant and group representations, phase transitions *etc.*).

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

The content of the First Edition of Volume E has been finalized. An outline is:

Part 1: *Subperiodic Group Tables: Frieze Group, Rod Group, and Layer Group Types*

Section 1: Symbols and Terms used in Part 1

Section 2: Guide to the Use of the Subperiodic Group Tables

Section 3: The 7 Frieze Groups

Section 4: The 75 Rod Groups

Section 5: The 80 Layer Groups

Part 2: *Scanning of Space Groups*

Section 6: Symbols and Terms used in Part 2

Section 7: Guide to the Use of the Scanning Tables

Section 8: The Scanning Tables

Section 9: Theory of the Scanning of Space Groups

First drafts of the sections have been written. At the present time, final drafts are being prepared or rewritten to bring about consistency of notation, terminology and style across the individual sections. Material originally to be included concerning subperiodic groups as factor groups of reducible space groups has been postponed for inclusion in a subsequent edition of this volume.

Volume 'A1'. *Maximal Subgroups of Space and Plane Groups*; Editor H. Wondratschek

In August 1995, the Executive Committee approved the publication of Volume A1, which contains amended data on maximal subgroups of space and plane groups. H. Wondratschek has been appointed Editor; Co-authors are M. I. Aroyo and Y. Billiet.

Contents: Introduction to the Tables, User's Guide, Coordinate Transformations, Subgroup Tables for Plane and Space Groups, Minimal Supergroups.

The data for each space-group type are presented in two categories:

I Maximum *translationengleich* subgroups

II Maximal *klassengleiche* subgroups with subdivisions: Loss of centring translations; Enlarged unit cell: indices 2, 3 and 4; Infinite series of isomorphic subgroups.

In contrast to the subgroup data in Volume A, the (finitely many) maximal subgroups of index up to 4 are listed individually whereas the infinite number of isomorphic subgroups are presented in (a few) infinite series. For each subgroup, either its representatives (general position) or at least a set of generators are given. The transformation to the conventional coordinate system of the subgroup is indicated by the matrix for the basis transformation and the column for the origin shift. The supergroup data are appended as a reference list only.

In addition, the group-subgroup relations are displayed by two series of diagrams: for each crystal class, one diagram for the *klassengleiche* subgroups; for the *translationengleiche* subgroups, another set of diagrams, which are similar to the subgroup diagrams of crystallographic point groups.

The volume is supplemented by a theoretical section on group-theoretical aspects and by a practical section on applications of the subgroup data.

The present status is that the data have been calculated completely and are available in principle. They are presently being transferred to \LaTeX format in order to enable printing directly from these files. The print format and the details are being discussed with the Technical Editor. One of the supplementary sections is available in draft form. The author still has to be found for the other section.

New Volumes

Three new volumes are presently under discussion or in the planning stage.

Volume 'A2'. *N-Dimensional Space Groups*; Editor T. Janssen. A proposal for this volume, which will consist of a printed volume and a CD-ROM, was extensively discussed at the Executive Committee meeting in Lund, Sweden, in August 1995 and a demonstration of the program was given. A final decision on the volume and its financial implications is awaited.

A new volume on *Macromolecular Crystallography* with M. G. Rossmann as Editor has been proposed. A memorandum on the scope and the details of this volume are being prepared by M. G. Rossmann for discussion at the Seattle Congress in August 1996.

A volume of the *Official CIF Dictionaries and Definitions* with S. R. Hall and B. McMahon as Editors has been proposed. Again, a memorandum for discussion at the Seattle Congress is being prepared.

Commission on Aperiodic Crystals

The activities of the Commission have been essentially oriented towards completing the checklist intended for the publication of incommensurate crystal structures in the journals of the Union. A great deal of effort was dedicated to coordinating international meetings specializing in the field of aperiodic crystals and serving on programme committees. The Commission maintains a WWW server relating to the activities in the field of aperiodic crystals (<http://aperiodic.smith.edu/aperiodic>). Future meetings and conferences on this topic (of which Commission members are aware) are listed on the server.

The members of the Commission participated actively in the preparation of the Aperiodic'94 conference proceedings by carefully selecting the contributions. The volume was published by World Scientific (Singapore) in 1995 and delivered to the participants 9 months after the meeting (which took place in Les Diablerets, Switzerland).

Members of the Commission had the opportunity to meet during the International School on Quasicrystals held in Balatonfüred, Hungary, 13–20 May 1995. An open discussion meeting was organized at that conference in order to exchange new ideas on the definition of aperiodic crystals. The presence of specialists from many different fields related to quasicrystals, including mathematicians, was highly productive.

The work on the checklist for the publication of incommensurate crystal structures continued actively in 1995, following comments and suggestions from members of the Commission on Journals. The final version of the checklist has been accepted by the Commission on Aperiodic Crystals and will be submitted for publication in *Acta Crystallographica*.

The Commission was active in the coordination and the preparation of sessions related to aperiodic crystals in many international conferences. In particular, members of the Commission participated actively in the Programme Committees of ECM-16 held in Lund, Sweden, in August 1995, of the NATO Advanced Study Institute on the Mathematics of Long Range Aperiodic Order held in Waterloo, Canada, in August 1995, of the Seattle Congress, and of ECM-17 to be held in Lisbon, Portugal, in 1997. The Chairman of the Commission is working closely with the Programme Committee of Aperiodic'97, which will take place in Alpe d'Huez, France, in August 1997; many members of this Commission are members of that Committee.

Commission on Biological Macromolecules

The major effort of the Commission during 1995 was concerned with the organization of an International Seminar-School on Macromolecular Crystallographic Data held in Calcutta, India, 16–20 November 1995. The meeting was held in response to the long-felt need for transferring the considerable expertise that exists in North America and European Community countries on the deposition, validation, retrieval and use of macromolecular crystallographic data to the

rest of the world. The Seminar-cum-School was organized at the Saha Institute of Nuclear Physics with Professor J. K. Dattagupta as the Convener. The Commission functioned as the International Programme Committee. The meeting was attended by 150 participants from 14 different countries and the lecturers included well known leaders in the area. The scientific programme consisted of lectures, demonstrations, discussions and hands-on sessions. The topics covered included protein and nucleic acid databases and their management; validation; database description tools; macromolecular CIF; CIF in crystallographic publications; data analysis; crystallization database; molecular modelling and biocomputing; molecular replacement; drug design; protein and nucleic acid structures; structural comparisons.

Two sessions at the Calcutta meeting were devoted to deposition policies. In fact, the discussions in these sessions followed those among the members of the Commission on this issue. Earlier, the issue was specifically raised with the Commission by the US National Committee for Crystallography. The discussion among the members of the Commission led to the conclusion that the most urgent requirement is the enforcement of the existing IUCr guidelines on data deposition. The Commission therefore recommended to the Executive Committee that it should take up the matter with major journals. There were comparatively minor divergences of views on modifications to the existing policy. It was decided that a consensus on the modifications could be arrived at through further discussions. The discussions at the Calcutta meeting also emphasized the urgency of enforcing the IUCr guidelines. The importance of depositing structure factors was also highlighted. Arising out of the discussions at Calcutta, a letter was addressed by a few of the leading participants to major journals on the need for enforcing the IUCr policy on deposition [*e.g. Nature (London)* (1996), 379, 202]. This has had the desired effect on some journals like *Nature* and *Nature Structural Biology* as evidenced by their insistence on data deposition before publication with effect from January 1996.

During 1995, the Commission extended its support to the 6th International Conference on Crystallization of Biological Macromolecules held 12–17 November 1995 in Hiroshima, Japan, and to the meeting on Experimental and Computational Approaches to Structure Based Drug Design, 8–19 May 1996, in Erice, Italy.

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 in conferences, workshops and schools, and by initiating and carrying out projects.

With great sorrow, we learned of the passing away of our member J. Alnlof in February 1996.

Meetings of the Commission

The Commission met during the Gordon Research Conference on Electron Distribution and Chemical Bonding in Plymouth, New Hampshire, USA, 2–7 July 1995. The topics discussed included the next Sagamore meeting in Saskatchewan, Canada, organized by B. Robertson. It was decided to use the same schedule as the Gordon Conference. It was also planned to have a tutorial workshop in the days before the conference. The conference proceedings would not be published. It was noted with great pleasure that the organizers of the Gordon

Conference maintained contact with the Commission and involved its members in the discussion on the organization of the next Gordon Conference. K. Schwarz and C. Lecomte were selected as Chairman and Vice-Chairman.

Conferences

La Plata. An International School and Workshop on Charge Density Analysis was held 18–26 May 1995 in La Plata, Argentina. The School was organized by G. Punte on behalf of the IUCr, our Commission and the National University of La Plata. The main topics of the School were as follows: physical principles of accurate structure analysis; X-ray and synchrotron data collection techniques (including advanced methods); crystallization techniques; electron-density modeling with diffraction data; error analysis of experimental results; theoretical methods in charge-density studies; chemical interpretation of electron density in terms of orbital concepts and topological analysis; calculation of properties from the multipole model; comparison of experimental and *ab initio* electron densities; application to structural activity problems. The lecturers were P. Coppens (USA), R. Goddard (Germany), P. Mallinson (UK), C. Lehmann (UK), V. Tsirelson (Russia), R. Boese (Germany), J. F. Piniella (Spain). The School was attended by (mainly young) participants from Argentina, USA, UK, France, Germany, Mexico, Chile, Cuba and Uruguay. A few tutorial sessions devoted to the use of the multipole model, theoretical models and error analysis took place. Much attention was paid to the new program package *XD* (Koritsansky's project of our Commission), where much progress was noted since the Brest meeting.

Gordon Conference. The Gordon Research Conference on Electron Distribution and Chemical Bonding took place at Plymouth, New Hampshire, USA, 2–7 July 1995. About 75 crystallographers and theoretical chemists discussed experimental determinations, quantum-chemical calculations, and interpretation and use of electron-density distributions. The use of the maximum-entropy method and the contribution of electron diffraction raised much interest and heated discussions.

Second International Workshop on Compton Scattering and Fermiology. The meeting was organized by N. Shiotani in Tokyo, Japan, 28–31 August 1995. 64 scientists from 12 countries attended the meeting with 44 invited talks. Synchrotron radiation has made it possible to use ultra-high momentum resolution (0.02 a.u.) and photon energies up to the electron rest energy can be employed. One of the objects of the fermiology project is to standardize procedures with Si as test case. The results of the various groups show significant differences, probably due to background contribution and multiple scattering. On the theoretical side, quite different methodologies – FLAPW and KKR – yield very similar results. Compton studies on different systems were extensively discussed. Other techniques such as positron annihilation, angle-resolved photoemission and electron Compton scattering contributed to obtain a robust picture of the underlying electronic structure. The next meeting will be hosted by Martin Blume in Brookhaven, USA, in Spring 1998.

Sagamore meeting. The next Sagamore meeting will be organized by B. Robertson in Saskatchewan, Canada, 27 July–1 August 1997.

Projects

1. *Fermiology of High- T_c Superconductors via High-Resolution Synchrotron-Based Compton Scattering.* Owing to the recent arrival of new synchrotron sources and the alertness

and initiative of our scientists, the project on fermiology and Compton scattering is thriving, as witnessed by the workshop in Tokyo. Active management by A. Bansil contributes to its success.

2. *Density Matrix Project.* Since progress seems to run in phase with the Sagamore meetings, new results are expected at the coming conference.

3. *Multipole Refinement and Related Topics.* A Chairman, C. Lecomte, has been appointed and a concept programme has been devised to make a concerted effort of assessing the various multipole programs in existence and in particular the new program *XD* that has been developed by T. Koritsanzky *et al.* under the auspices of the IUCr. The activities of the project will be carried out in close cooperation with those undertaken in the field of the Maximum Entropy Project.

4. *Maximum Entropy Project.* This topic has led to vigorous scientific discussions during the various conferences organized by the Commission. Recent results obtained by different groups show significant differences. The Chairman of the project, M. Sakata, has formulated the objects of the project and its operating procedures.

Commission on Crystal Growth and Characterization of Materials

The main activity of the Commission in 1995 was the preparation and performance 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. It continued the successful series of similar schools organized in the past by the Commission for the benefit of students and young scientists, mainly from economically disadvantaged countries. Six present and two previous Commission members were active in the International Programme Committee of the School and helped to establish a programme of 46 lectures, which were presented by 7 Indian and 16 non-Indian teachers, among them three members of the Commission. 14 lectures treated the fundamentals of crystal growth, 20 dealt with growth methods, 10 with real structure and characterization and 2 with device fabrication. The local organization was in the hands of Professor C. Subramanian, Crystal Growth Centre of the Anna University, and his staff. The total number of participants was 102 (without teachers), among them 91 scientists from India and 9 from neighbouring and East European countries. The School was financially supported by the IUCr, the International Centre for Theoretical Physics, Trieste, Italy (ICTP), the Council of Scientific and Industrial Research, Delhi, India (CSIR), the Indian Association of Crystal Growth, the Tamil Nadu Government and the Anna University, Madras. 16 attendees received IUCr Young Scientist Awards. As a result of the strong engagement of teachers and participants in the lectures and discussions and, owing to the cordial kindness and hospitality of the Indian hosts, the School was a great success.

The Commission recommended IUCr sponsorship of the following international conferences: Sixth International Conference on Crystallization of Biological Macromolecules (ICCBM-6), 12–17 November 1995, in Hiroshima, Japan. A member of the Commission, F. Rosenberger, University of Alabama, USA, was President of the International Advisory Board; Fourth International Symposium on Ferroic Domains and Mesoscopic Structures (ISFD-4), 25–30 March 1996, Vienna, Austria.

The Commission was active in making proposals, mainly in the fields of crystal growth and defect characterization, for the programme of the forthcoming Seattle Congress. Four Microsymposia on crystal growth have been established, three of them (Fundamentals of Crystal Growth, Methods and Materials, Controlling and Predicting Crystal Morphology) being subject to the responsibility and care of the Commission Chairman.

The Eleventh International Congress on Crystal Growth was held 8–13 June 1995 in The Hague, The Netherlands, with meetings of the Executive Committee, the Council and the General Assembly of the International Organization for Crystal Growth (IOCG). Following an initiative of this Commission, a stronger interaction and cooperation of the IUCr and the IOCG in fields of common interest, *e.g.* in the study of crystal perfection, was discussed. It was agreed to consider a joint Symposium on Crystal Characterization. The new President of the IOCG, Professor T. Nishinaga, Tokyo University, Japan, is a member of this Commission.

Commission on Crystallographic Apparatus

During 1995, the Commission continued promoting its two major projects: Absolute Structure Determination of Light-Atom Compounds and Precision Lattice-Parameter Determination. Activities also continued in the field of position-sensitive X-ray detectors and high-pressure crystallography.

(1) Absolute Structure Determination of Light-Atom Compounds (E. F. Weckert and L. Malakhova)

The project aims to compare different X-ray methods for the determination of the absolute structures of light-atom compounds. The group decided to concentrate on (i) exploitation of anomalous-dispersion effects and (ii) three-beam diffraction, and tried to establish the limits of the applicability of these methods as a function of radiation, content of anomalous-scattering atoms and crystal quality. It also aims to find not only the limits of what is possible but also the limits of what can be easily achieved in a routine structure determination, including a comparison of different software packages. The following sample compounds were selected, which include different contents of anomalous-scattering atoms: sucrose, $C_{12}H_{22}O_{11}$ (space group $P2_1$); L-asparagine monohydrate, $C_4H_8N_2O_3 \cdot H_2O$ (space group $P2_12_12_1$); benzil, $C_{14}H_{10}O_2$ (space group $P3_121$); BN (space group $F\bar{4}3m$); urotropin, $C_6H_{12}N_4$ (space group $F\bar{4}3m$); benzophenone, $C_{13}H_{10}O$ (space group $P2_12_12_1$); $C_{14}N_2O$ (space group $P2_12_12_1$); $C_{28}N_2$ (space group $P2_12_12_1$). One problem here was to find samples with very small anomalous-dispersion effects in large quantities.

We decided to start with compounds of high oxygen content and try the more difficult compounds later. The first batch of crystals was distributed among interested participants and experiments are on the way or have finished. The second batch of compounds will be distributed soon. Three-beam interference experiments have successfully been performed with nearly all of the compounds (except sucrose and urotropin). As this method works without anomalous-dispersion effects, the main problem is crystal quality. The participants are listed below with their roles: Professor P. Beurskens, Nijmegen, The Netherlands, numerical analysis of experimental data; Professor S. L. Chang, Taiwan, numerical evaluations of measured three-beam interference profiles; Dr Z. Dauter, York, UK, anomalous-dispersion-based measurements using image-plate detectors and numerical evaluation of experimental data; Dr J. Grochowski, Cracow, Poland,

anomalous-dispersion-based measurements and numerical evaluation of data sets; Professor A. Kirfel, Würzburg, Germany, numerical analysis of experimental data; Professor C. Kratky, Graz, Austria, anomalous-dispersion-based measurements and numerical evaluation of data sets; Dr L. Malakhova, Moscow, Russia; Dr D. Watkin, Oxford, UK, anomalous-dispersion-based measurements and numerical evaluation of data sets; Dr E. Weckert, Karlsruhe, Germany, three-beam interference measurements and anomalous-dispersion-based measurements, data analysis.

(2) *Precision and Accuracy of Lattice Parameter Determination (G. DeTina and L. Finger)*

After much delay, ten 'kits', each containing five ruby spheres and five zeolite crystals, were fabricated by M. J. Kirisits. The crystals were mounted on the tips of X-ray glass capillaries using a minimum of fast-setting epoxy, the capillaries were set in machined brass pins and each of the crystals was subjected to preliminary diffraction analysis to assess quality and to determine approximate cell parameters and orientation matrices. Over 120 crystals were screened for a suitable group of 100 representatives for the kits. A good deal of thought and work went into the design and construction of the packaging for the kit. Given that each kit would be shared among five to seven participants, there would be ample opportunities for postal mishap. The containers were inexpensive fishing-tackle boxes. Into each was placed a handmade wooden frame, fitted out to hold the ten pins securely with nylon lock screws, ten inverted glass vials to protect the crystals and two locking braces to keep the vials from moving. The wooden frame was dimensioned to fit securely and snugly in the fishing-tackle box. Test flights of the boxes indicated that crystals would survive a fall of 2 m. The tackle boxes were then placed in sturdy cardboard shipping containers filled with packing foam.

Manuals were written to instruct the participants in the use of the kits. In addition to the preliminary information concerning the orientation matrices of the crystals, there were instructions on the treatment of the ruby spheres. The idea was to ensure that information necessary to evaluate the instrumental variances in the zeolite lattice parameters would come out of the ruby-sphere measurements. References to the literature were included, as well as definitions of the various orientation matrices in use on various diffractometers.

The original list of participants was contacted again to check their continued interest in participation in the project. The kits were mailed at the end of the summer (August, September 1995) to the first ten participants. These participants in turn mailed their kits to various other participants. To date, we have received results from 24 participants. A recent letter was sent to all participants to find out where the remaining kits are (two have been returned).

The plan is now for the data to be interpreted by the organizers. The results of the ruby measurements will be used to determine the alignment of the diffraction equipment and assess its contribution to the variance in the zeolite crystal parameters. A brief report may be made to the Commission at Seattle.

(3) *Review on Position-Sensitive Detectors (G. McIntyre)*

We made a proposal for a series of review articles on the state of the art of the development of position-sensitive detectors and their application to crystallography using X-rays, neutrons and electrons. While this was intended to indicate important new developments, especially at third-generation synchrotron

sources and larger neutron facilities, we also believed that an important role of the Commission was to make recommendations for conventional diffractometry at smaller laboratories and universities.

Shortly after the proposal was made, several extensive overviews of X-ray position-sensitive detectors appeared in the *Journal of Synchrotron Radiation*, which rendered the first objective of our series unnecessary for the moment. Since then we have mainly observed developments to await the appropriate time for a new review. This should be made soon in view of the much increased use in the last two years of image plates and CCD-based position-sensitive detectors for conventional X-ray crystallography in smaller laboratories and universities and the application of image plates to quasi-Laue methods and the promising results for neutron diffraction from microstrip gaseous proportional counters in neutron diffraction.

In the meantime, we wondered if a future project of our Commission could concern guidelines for graphical user interfaces for diffractometer control. The advent of fast, and relatively cheap, workstations has seen a dramatic change in the way in which we drive crystallographic instruments, and in the visual interface to the control program. The Motif guidelines of the Open Software Foundation are followed by many, but not all, developers of graphical diffractometer control programs. Is there a need, or desire, for additional guidelines for (powder and single-crystal) diffractometer control programs so that all interfaces have a similar look and feel? We believe that there are now a sufficient number of interfaces in the different main areas of crystallography that such guidelines could be established.

(4) *High-Pressure Crystallography (R. J. Nelmes)*

The major event was a three-day international Workshop held in Tsukuba, Japan, in March 1995. This was the fourth in a series of HPG Workshops, following previous ones in Munich, Germany (1989), Daresbury, UK (1991) and Washington, USA (1992). The organizing Chairman was O. Shimomura, a member of the HPG. About 80 participants from UK, Germany, France, Russia, China, USA and Japan attended. The programme began with a technical session on new optics, detectors and high-pressure techniques for diffraction experiments. Then followed sessions on data collection using diamond-anvil cells and large-volume cells, and data analysis by the Rietveld and maximum-entropy methods. The Proceedings will appear shortly in *High Pressure Research*.

During the past year, members of the HPG have also been heavily involved in preparations for the 1996 Congress in Seattle, where there is to be a substantial high-pressure programme comprising two Keynote Lectures and six Microsymposia over the first three days of the Congress. All current members of the HPG are chairing or co-chairing sessions and several are giving talks. There are to be 39 invited speakers from the USA, Japan, France, Germany, the UK, Russia, Switzerland, Canada, The Netherlands and Spain, 8 other contributed talks, and 35 poster presentations. It is expected to be a major meeting, celebrating the vitality and exciting future prospects of the field.

It has been a long-term objective of the HPG to raise the profile of high-pressure crystallography within the IUCr – particularly following the demise of the previous Commission on High Temperature and Pressure – and we are grateful to the Congress organizers for their willingness to accommodate our plans for Seattle so generously. All the Chairs and Co-Chairs of the high-pressure sessions have worked hard to create a programme that justifies this support.

Commission on Crystallographic Computing

The main activities of the Commission during 1995 were:

1. Refereeing of the section *Computer Program Abstracts* in *J. Appl. Cryst.*, carried out by D. Watkin and M. Ramanadham.

2. The seed spread by H. D. Flack (past Chairman and consultant to the Commission) of a crystallography WWW page has grown into a very useful tree with many branches, accessed by thousands of people. Recently, P. Bourne has also set up a Commission on Crystallographic Computing (IUCrCC) home page with the address <http://rosebud.sdsc.edu/projects/pb/IUCr/IUCrCC.html>. He has also set up a software repository at the address <http://www.sdsc.edu/projects/pb/IUCr/softrep/help.html> accessible from the IUCrCC.

3. Plans for the organization of a small regional school, more oriented towards computational aspects, after the poor response to D. Watkin's explorations, were deferred and it was decided to leave the matter until the next triennium.

4. The major activity of the Commission was the organization of the Asian Crystallographic Computing School in Bangkok, Thailand, 27–30 November 1995. The School was organized jointly by the IUCr Computing and Teaching Commissions as a satellite of AsCA'95 (2nd Conference of the Asian Crystallographic Association). The Local Organizing Committee was chaired by Professor P. Phavanantha. The School program included 3.5 hour lectures in the mornings, and a 45 minute lecture and 2 hour practical session in the afternoons. The morning lectures covered all basic aspects of crystallographic computing (data treatment, Patterson and Fourier, direct methods, refinement and interpretation of results) with some introductions to more advanced topics, such as extensions to macromolecular crystallography, treatment of powder data, analysis of thermal motion and charge-density studies. The afternoon lectures were mostly dedicated to computational aspects and the practical sessions were mainly hands-on usage of a rather wide variety of crystallographic software running on PC's. Handouts with lecture notes were distributed to the participants and discussions and questions were encouraged. The lecturers who contributed to the School were: P. Coppens, G. R. Desiraju, Fan Hai-fu, C. M. Gramaccioli, S. R. Hall, C. Kennard, P. Phavanantha, M. Ramanadham, W. T. Robinson, J. Simpson, B. Skelton, H. Toraya, D. Viterbo and T. Yamane. The organizational aspects were coordinated by A. Ungkitchanukit and C. Poorakkiat. The number of participants was 42 from 7 different Asian countries. Their qualifications ranged from post-graduate students to Assistant Professor, but most participants were at the postdoctorate level. An anonymous questionnaire was distributed. Most people found the School useful and the practical sessions were greatly appreciated. The main problem was the very different crystallographic backgrounds of the participants. Despite the many difficulties encountered in its organization, in the end the School turned out to be quite successful.

5. The setting up of the Summer School on Crystallographic Computing, as a Satellite Meeting of the Seattle Congress, is now at its final stage, with P. Bourne and K. Watenpaugh acting as local organizing persons. It will take place 17–23 August 1996 at the Western Washington University in Bellingham, approximately 150 kilometres north of Seattle. The School will concentrate on the most recent aspects of macromolecular crystallography computing, both theoretical and practical. Besides lectures, there will be extensive hands-on sessions in

using the latest methods dealing with data collection (from both laboratory instrumentation and the new synchrotron beamlines), phasing, including integrated approaches, model building, refinement, and visualization. In addition, attention will be given to: analyzing and using the fast growing body of macromolecular structure data; new data formats; and new computing methods that can be applied universally. Proceedings of the meeting will be available in traditional printed form and *via* the World-Wide Web (<http://www.sdsc.edu/Events/IUCr/IUCr.html>).

6. The Commission is also contributing to the organization of the Seattle Congress. P. Bourne and G. Krüger have been nominated members of the International Programme Committee and are involved in the setting up of the Microsymposia on Computing. In particular, the Microsymposium Computing II on General Advances & Applications will take place on Saturday 10 August 1996 as an Open Commission Meeting (Chair: D. Viterbo; Co-Chair: S. R. Hall). The Commissions' consultant H. D. Flack is organizing both the Microsymposium Computing I – The Internet and two half-day workshops Surfing the Crystallographic Net.

*Commission on Crystallographic Data**(A) Cambridge Structural Database*

The CSD continues to be available to all academic institutions *via* the 32 affiliated National Data Centres. It is also supplied to industrial companies, predominantly in the pharmaceutical sector, where it is used in drug design. The availability of the CSD on CD has resulted in a steep increase in the number of academic sites registered. CCDC Web pages are being increasingly used, and the information is continually being upgraded (see <http://www.ccdc.ac.uk>).

(A1) *Database contents*. The database aims to include all published organic and metal-organic complex structures and now contains 152 464 data entries (April 1996 release). The CSD main-file growth in the last year has been 11 194 new entries.

The database of 'CSD Usage' continues to grow. This is a collection of Abstracts for scientific papers making significant use of the CSD. This is searchable by *Quest* on keywords and the text of the Abstract. There are 538 Abstract entries in the April 1996 release. A separate database is distributed for 3897 Protein Data Bank entries. Detailed statistics are available from CCDC on request.

(A2) *Protein Data Bank (PDB)*. Since April 1995, the CSD release has included the coordinate data for the Brookhaven PDB entries in compressed format on CD-ROM. It should be emphasized that these coordinates are not searchable by *Quest* as part of the 3D-search facility, rather they are provided as a convenient package for those users who search the PDB sequence information with *Quest* and wish quickly to extract and view the relevant hits. A utility program, *pdbget*, is supplied to retrieve the entries in PDB format. The PDB coordinates are provided on a separate CD for Unix and on a single CD for VMS systems.

The *Quest* program allows sequence searching *via* menu options and an automatic link to the coordinate file is provided in the form of a *RASMOL* button. This allows the user to view a current hit immediately in a *RASMOL* window.

(A3) *Platforms*. The CSD is supported on VAX/VMS, DEC Alpha VMS, DEC Alpha OS/F, SGI (Unix) and SUN (Unix) platforms. The distributed CDs also contain executables for IBM RS/6000, HP 700 Unix, DEC Alpha OS/F, which are

created on machines remote to CCDC and not supported to the same degree. Instructions are provided that enable the software to be compiled on almost any Unix system.

Distribution is now predominantly on the CD medium, though a few sites still require tape versions. This has greatly facilitated the procedure of release at CCDC (which is scheduled for April and October of each year).

(A4) *CSD-MDL Database*. This is a version of CSD in the form of an MDL registered database, which is searchable by the MDL MACCS and ISIS software. It is provided to certain users who have licences for MACCS and CSD. Update procedures have been written so that CCDC supplies a file of updated records in the SD-file format to the user, who then updates the local copy of the CSD-MDL. Some users have been supplied with the SD file direct for the complete database for loading into their own database systems. CCDC has invested in extra hardware to support the production of CSD-MDL and releases are now up to date with the main CSD database.

(A5) *CSD-UNITY Database*. This is a version of the CSD converted into a Tripos UNITY database. Software has been written that produces data entries in the Tripos SLN format, suitable for loading to UNITY. This version is available to registered users of CSD who also have a Tripos UNITY license.

(A6) *Software*. The CSD is provided with: *Quest3D*, the search program, including 3D searching, and intermolecular contacts; *VISTA*, a program for visual display of statistics on geometry parameters extracted by *Quest3D*; *PLUTO*, a program for visualization of structures, especially intermolecular contacts in the crystal.

Quest has been updated with a new output file format (MOL2) as used by the modelling program *Sybyl* (from Tripos) and widely used in other contexts. *Quest* now also allows output of simple coordinate lists for atoms, both orthogonal and fractional, and optionally by fragment selection, as in the old *GSTAT* program (COOR option).

The *VISTA* program has been significantly improved in the last year, with spread-sheet facilities, polar histograms/scatter plots and PostScript output.

PLUTO now also allows output of coordinate lists in the *GSTAT* style. This is especially useful for dumping of packing programs.

(A7) *PreQuest*. This new program has the aim of providing a facility to the crystallographic community that accepts a variety of input formats for data and creates a local CSD database. It is also the program used for in-house validation of all new data entries at CCDC. This is due for release in October 1996 and has been through extensive β testing at certain non-CCDC sites.

The main objective is to provide users with local databases in CSD format, which are searchable by the *Quest* program, concatenated with the main CSD if desired. This is particularly important to industry where many companies have as many as 1000 structures that are currently not releasable to the public domain. It is important often to academics also to be able to perform the same geometry calculations on new compounds, pre-publication, as are relevant to their current research using the main CSD. This also provides the user with a definitive check of their data before deposition at CCDC or publication. Particular emphasis has been placed on the reading of the standard CIF format.

The *PreQuest* program also allows input of non-crystallographic Cartesian data from whatever source, e.g. MO calculations, molecular modelling.

(A8) *Data deposition*. Since August 1995, the CCDC has been inviting the electronic deposition of structures as private communications. There has been no restriction on the permitted format and a 'deposition form' has been made available on the CCDC WWW page (see <http://www.ccdc.ac.uk>). In practice, there has been a steady growth in the percentage of CIF depositions (33%), which is preferred by CCDC. These files may be read directly by the *PreQuest* program and after checking can be archived to the main database. It is hoped that the number of depositions will continue to grow; the current estimate is about 500 per annum.

(A9) *The IsoStar Project*. A new development project is under way. This is an organized library of intermolecular contacts for a selected range of chemical groups of biological interest. Automatic scans are made of the CSD for each group and the contacts stored so that they may be viewed interactively. The resulting 3D distribution of contacts is very valuable in providing a picture of the most likely interactions to occur between groups, which is relevant to drug design and protein-ligand interaction. It is intended to add contact distributions taken from ligands in the protein data from the PDB. After consultation with collaborators, it is likely that the results should be available in an easy-to-use format such as a WWW browser. The scatter plots and vector plots will probably be accessed by menu under Netscape and the 3D visualization performed by *RASMOL*. It should be noted that this project is still at the prototype stage but should be substantially complete by the end of 1996.

(A10) *Version 6*. A development of the CSD system is under way, under the title Version 6. This will provide a more flexible interface for the user, especially in the areas of query formation and browsing of hits. New software is being written for the interface, which will drive the non-graphic search engine *Quest* with the same functionality as Version 5. There will be emphasis on ease of transfer of results to other software.

A second aspect of Version 6 will be a redesign of the internal storage of the database fields. This is so that the CSD will be able to accommodate new data fields if necessary and remove most of the internal hard-coded limitations of the present system (e.g. the maximum number of atom sites is 1000).

This is at an early stage of development, which will run over a two-year time scale.

(B) *International Centre for Diffraction Data*

(B1) *Databases*. The set 45 Powder Diffraction File products were released in August 1995. The set 46 products are on schedule for August 1996 release. The 1994 release of NIST Crystal Data is available, and the 1995 release is currently undergoing α testing. CD-ROMs containing both the PDF and CD are no longer available because the size of the combined databases exceeds the capacity of a single CD-ROM.

The (MS Windows) search/retrieval program *PCPDFWIN* has become very popular and a new PC Search Index, to assist in phase identification using the Hanawalt and Fink techniques, has been developed (available in August 1996). Plans are to discontinue development and support of DOS-based software and make the source code for discontinued programs available.

The ICDD continues to archive powder patterns in CIF/STAR format. A pilot full-pattern data set of clay patterns is undergoing testing.

The ICDD awarded 37 Grants-in-Aid worldwide, with the expectation of generating new entries for the Powder Diffraction File and welcomes additional grant applications.

(B2) *Science*. Poster sessions highlighting new developments in powder diffraction were held in the October 1995 and March 1996 ICDD meetings. Clinics in X-ray diffraction and X-ray fluorescence were held at ICDD headquarters in June 1995 and 1996. Four \$2000 crystallographic scholarships were awarded. Plans have been made to expand the coverage of the PDF by the inclusion of calculated powder patterns. Recommendations for the calculation of powder patterns have been derived.

An ICDD WWW site (<http://www.icdd.com:7999/>) has been established. It is planned to develop it into the electronic centre for powder diffraction – including product information, bulletin boards, discussion groups, public domain software and other features. Its development is being guided by an Electronic PDF Committee.

(B3) *Organizational items*. A new Board of Directors, chaired by R. L. Snyder, was elected. One of the major objectives of the ICDD is to increase collaboration with other database organizations. R. Jenkins has been named General Manager of the ICDD. The ICDD hopes to expand greatly its worldwide membership.

(C) NIST Crystal and Electron Diffraction Data Center

(C1) *Database*. The NIST Crystal and Electron Diffraction Data Center is concerned with the collection, evaluation and dissemination of data on solid-state materials. The Data Center maintains a comprehensive database with chemical, physical and crystallographic information on all types of well characterized substances. These materials fall into the following categories: inorganics, organics, organometallics, metals, intermetallics and minerals. During this year, the master database has been significantly augmented with respect to all categories of materials and now contains approximately 227 000 entries. From this central database, two distribution databases are produced: (1) NIST Crystal Data and (2) the Electron Diffraction Database. These databases are made available through computer-oriented modes of dissemination including PC, scientific instruments and on-line searching.

The major project in 1995 was the organization of the NIST-sponsored Workshop on Crystallographic Databases, an international meeting of representatives of all crystallographic data centers, journal editors, instrument manufacturers and database users. Manuscripts from all speakers have been collected and edited and will be published in the *NIST Journal of Research*. A number of the manuscripts describe the use of NIST data products including, for example, a manuscript entitled Using NIST Crystal Data within Siemens Software for Four-Circle and Smart CCD Diffractometers. In this paper, it is emphasized that the diffractometer/NIST-database combination creates a new analytical tool for materials research and analysis.

(C2) *NIST Workshop on Crystallographic Databases*. The NIST Workshop on Crystallographic Databases was one in a series of NIST-sponsored workshops, each focusing on a particular type of data including crystallographic, thermodynamic, phase diagram and mass spectral data. Scientific databases are becoming critical to research in the industrial and academic communities. By bringing together top scientists involved in producing crystallographic data with users of the resulting databases, this Workshop served as a forum to examine how well the scientific community is being served and what data activities the community feels are important in the future. This Meeting was sponsored by the National Institute of Standards and Technology and laid the ground work for future directions with respect to crystallographic databases.

A main goal of the Workshop was to foster interactions between users and providers of crystallographic databases and between the communities that use the different databases. During the Workshop, three sessions of scientific presentations were held: Formal Data Activities; Scientific Uses of the Databases; Data Transfer: Ensuring State of the Art Technology.

In the first session (Chair: D. Watson), a representative from each of the data centres covered present activities and projected future activities of the data centre. In the second session (Chair: C. Brock), the focus was on using crystallographic databases in analysis, in the production of materials properties and in the design of new chemicals, pharmaceuticals and materials. In the third session (Chair: B. McMahon), speakers addressed issues related to data transfer such as: (1) data exchange standards (CIF *etc.*); (2) the role of journals in the evaluation of published data; (3) data exchange between journals and crystallographic data centres; (4) computerized modes of data dissemination. Following the presentations, a discussion session (Chair: J. Flippen-Anderson) focused on Barriers to the Use of Crystallographic Data and on Partnerships for the Future. Workshop proceedings will be published in a special issue of the *NIST Journal of Research*.

As anticipated, the Workshop was of special interest to those who use crystallographic data in their research or are involved with this data in some other capacity, such as managers of scientific projects, journal editors, on-line system designers, instrument manufacturers and librarians, among others. In spite of the fact that the crystallographic databases have been in existence for many years, the workshop represents the first time that all parties have met to discuss common issues. Many attendees commented that the Workshop was very instructive, extremely useful and that it should be repeated in a few years. In addition to the invitees, many scientists have expressed a strong interest in the subject and have requested a copy of the Workshop Proceedings.

During the Workshop, representatives from the data centres as well as speakers in the third session noted that the modes of data collection and evaluation are in transition. Data transfer is facilitated by the rapid acceptance of standardized Crystallographic Information Files (CIF). Both IUCr and American Chemical Society journals use CIFs as an integral part of their publication process. With respect to data and software exchange, the data centres are establishing close cooperative ties with each other as well as with instrument manufacturers, scientific journals and users. These interactions are deemed critical to ensure the production and availability of high-quality data at an ever increasing rate. To further coordinate such efforts and to meet future challenges, the possibility of establishing a more formal federation between the data centres was discussed. It was clear to all participants that the crystallographic databases have become critical to research and analysis in many diverse areas of science. The recognized importance of such data is the result of a number of factors including the intrinsic value of evaluated crystallographic data, the vast amount of data and the evolution of modern computerized delivery systems. From the users point of view, several points were clear. First, the cost of searching the databases should be as low as possible. Second, search commands for all the databases should be simple to use. In addition, since one often wishes to search multiple databases, the command structure should be standardized. Third, with respect to scientific software, many users stated the need for new scientific algorithms to seek and recognize structural patterns, motifs, structure types *etc.*

(D) *CRYSTMET: NRC Metals Data File*

(D1) *Database.* CRYSTMET – NRC's Metals Data File presently has 55 000 entries. NRC has decided to discontinue the production of the database. J. Rodgers offered to take over production of CRYSTMET, NRC has agreed and has given him the exclusive rights to CRYSTMET. Funding for the continued production of this database is being sought. The on-line availability of this database will continue until the end of March 1996. J. Rodgers has submitted a proposal to NRC to acquire the rights to the on-line service to the crystallographic databases; this future on-line system will be developed by J. Rodgers and others.

(E) *ICSD: Inorganic Crystal Structure Database*

(E1) *Database.* The ICSD now contains 41 476 entries (1656 have been added or corrected, 1220 are completely new). The database is distributed as before by Fachinformationszentrum (FIZ) Karlsruhe, Germany, together with the retrieval system *RETRIEVE* and the 3D graphics programs *CRYSTAL VISUALIZER*, *STRUCTURE TIDY* and *LAZY PULVERIX*. For use in academic institutions, special conditions can be arranged as part of the IUCr/FIZ/Gmelin Institut Agreement.

Commission on Crystallographic Nomenclature

The work of the Commission in 1995 was accomplished, as in prior years, both internally and through the major contributions made by its sub-committees and working groups; most communications used electronic means. Membership of the Commission is entirely *ex officio*, by virtue of a primary IUCr responsibility closely related to crystallographic nomenclature.

The Commission reports with deep sadness the loss of its longest-serving and highly effective member Professor A. J. C. Wilson who died 1 July 1995, see obituary in *Acta Cryst.* (1996), A52, 7–10. Dr E. Prince was welcomed as the new Editor of *International Tables for Crystallography*, Volume C. The report of the Working Group on the Expression of Uncertainty in Measurement, entitled *Statistical Descriptors in Crystallography. II*, was published in *Acta Cryst.* (1995), A51, 565–569. The report presents the concepts of standard uncertainty and of Type A and Type B evaluations of standard uncertainties as developed by the International Organization for Standardization (ISO) and recommends replacement of the term estimated standard deviation by standard uncertainty or combined standard uncertainty in statements of the statistical uncertainties of data and results. The conclusion, long held by the IUCr, that the result of a measurement is complete only when accompanied by a quantitative statement of the uncertainty in that measurement is now fully recognized by the ISO, with legal consequences.

The Sub-committee on the Nomenclature of *N*-Dimensional Crystallography, see *Acta Cryst.* (1996), A52, 91–124 for membership, has elected N. D. Mermin of Cornell University, USA, and G. Chapuis of the Université de Lausanne, France, as advisors. Consideration of the concepts, definitions and terminology of crystallography in *N* dimensions has continued. A wide range of nomenclature views has emerged and the Sub-committee has decided to confine its attention to areas in which agreement is feasible rather than pursue a more general approach. The former includes symbols for point-group transformations, systems ordering and geometric crystal class notation in four dimensions and preferred settings and cell choices to the sixth dimension.

The Sub-committee on Atomic Displacement Parameter Nomenclature, see *Acta Cryst.* (1996), A52, 91–124 for membership, completed its report entitled *Atomic Displacement Parameter Nomenclature* in record time under the able chairmanship of K. N. Trueblood. The report was accepted by the Commission on 20 December 1995 and immediately submitted to the IUCr Executive Committee for approval [reports of the Commission's sub-committees and working groups accepted by the Commission and Executive Committee become IUCr nomenclature policy and are followed by all publications of the Union]. The report considers the confusing and inconsistent terms and symbols in current use for parameters denoting dynamic or static displacements of atoms in crystals. It focuses on individual atomic anisotropic displacement parameters representing atomic motion and possible static displacive disorder, provides clear definitions for these quantities, discusses graphical representations of the Gaussian mean-square displacement matrix and the expressions used if the Gaussian approximation is inadequate, and makes recommendations for symbols and nomenclature [see *Acta Cryst.* (1996), A52, 770–781].

The resignation of P. Toledano, Chair of the Working Group on Phase Transition Nomenclature, see *Acta Cryst.* (1996), A52, 91–124 for membership, was received with regret during the year. Professor J.-C. Tolédano was elected Chair to succeed him. 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.

Commission on Crystallographic Teaching

Visiting Professorships

Dr P. Mallinson from the University of Glasgow was Visiting Professor in the Laboratory of Crystallography at La Plata University, Argentina, in May 1995, in connection with the Charge Density School.

Professor Th. Hahn and Professor H. Wondratschek were Visiting Professors in St Petersburg, Russia, 22–29 August 1995, in connection with the School on Space Group Symmetry. Among the major organizers of this School, was Professor L. A. Aslanov from this Commission.

Contributions to Schools of Crystallography

A Fifth Intensive Course in X-ray Structural Analysis for young scientists took place at Aston, England, 2–8 April 1995 and Dr D. Watkin was one of the organizers.

Another school of crystallography (Rietveld Summer School, '95RS) took place in Moscow, Russia, 20–22 July 1995. Among the organizers of this school was Professor L. A. Aslanov.

A three-day course on Symmetry as a Basis for Structure Analysis was held during the first week of October at the University of Natal, South Africa, coordinated by Professor M. Laing.

In November 1995, two IUCr-supported schools of crystallography took place at Chulalongkorn University, Bangkok, Thailand, in connection with the Asian Crystallographic Association (AsCA) meeting. In organizing these schools, this Commission and the Commission on Crystallographic Computing were actively involved. The first, the Asian Crystallographic School of Gems and Precious Materials, took place 20–21 November, just before the AsCA meeting; the second, the Asian

Crystallographic Computing School, took place immediately after the meeting (27–30 November).

Just before the opening of these schools (16–20 November), another school of crystallography (on Macromolecular Crystallographic Data) took place in Calcutta, India, and this Commission was active in supporting this project within the IUCr and in ensuring connection and coordination with the other schools taking place in Asia.

Pamphlet Project

Professor G. D. Nigam and Professor H. Wondratschek are writing a new pamphlet on crystal symmetry. The pamphlet activity is being coordinated mainly by Dr J. P. Glusker.

Other activities

At the European Crystallographic Meeting ECM-16 in Lund, Sweden (6–11 August 1995), a Workshop on Crystallographic Teaching was held. Besides the host, Dr A. Oskarsson, who provided excellent help and contributions, several members of the Commission were present (L. A. Aslanov, K. El Sayed, J. P. Glusker, C. Gramaccioni). Here possibilities for the future were discussed, especially involving initiatives for developing countries. A seminar concerning crystallographic teaching for the Seattle Congress is currently being organized by this Commission, mainly by Dr A. Oskarsson.

Commission on Electron Diffraction

The Commission organized a very successful Winter Workshop on Electron Diffraction and Imaging at Surfaces in Arizona, USA, 3–6 January 1996. The Organizing Committee was chaired by Professor M. A. Van Hove with Professor A. Ichimiya as the Vice-Chair. About 75 people attended what was judged to be a most successful and well organized workshop. There were 16 invited speakers from five countries (Germany, Japan, Russian, UK, USA). It was supported by a grant from the IUCr.

Professors J. W. Steeds, D. L. Dorset and M. A. Van Hove have been involved with the organization of Microsymposia for the Seattle Congress. Professor J. W. Steeds is chairing a session on Strain Measurement and is the Organizing Committee member responsible for the session on Characterization of Defects, Microstructure and Texture. Professor D. L. Dorset is chair of the session entitled Methods of Structure Determination and Organizing Committee member responsible for the session on Direct Methods of Phase Determination from Surfaces.

The Commission has decided to seek a redefinition of its area of responsibility and believes that the best interests of the gas electron diffraction community, at present associated with this Commission, would be served by transfer to the Commission on Small Molecules. We are at present investigating the possibility of this transfer.

One of our members, Professor D. L. Dorset, has recently published a book entitled *Structural Electron Crystallography* with Plenum Press. This is particularly timely because there is considerable growth of interest at present on the levels of quantitative accuracy that can now be achieved by electron diffraction in modern electron microscopes.

Commission on Neutron Scattering

The Commission has continued its work over the broad field of neutron scattering during the last year. Preparations for the Seattle Congress and General Assembly and, in particular, the two Microsymposia and the Satellite Meeting on Neutron

Scattering to be held at the National Institute of Science and Technology (NIST), Gaithersburg, Maryland, USA, 5–7 August 1996, have been major activities. The latter has been organized by the Chairman, Professor J. W. White (Australian National University), and Dr E. Prince (NIST), the Commission being kept abreast of developments of the programme.

The year also saw the suggested formation of a Commission on Small-Angle Scattering and the Commission on Neutron Scattering is supportive of this. We see that from time to time specialist groups may wish to organize this way (as the Commission on Powder Diffraction has shown) but we will continue to sustain a broad interest in the whole field of neutron scattering. The current programme for the Satellite Meeting on Neutron Scattering in Gaithersburg illustrates this, since the emphasis has been placed on the science while showing the way in which new methods can be brought to bear on particular problems. In the case of the Gaithersburg meeting, giant magnetoresistance phenomena as looked at by diffraction, small-angle scattering and inelastic scattering will be one of the themes.

The Commission continues its work on two projects: International Standards for Neutron Inelastic Scattering Cross Sections (NISC) and Internationally Agreed Exchange Format for Neutron Synchrotron Data. In the NISC project, Dr Osborn and his colleagues have now not only proved the value of PrAl₃ as a standard material but also demonstrated the quality of the actual sample that was used in the original experiments. As reported in 1994, agreement of a number of major neutron scattering centres has been obtained to measure this at their instruments. We are looking forward to an interesting programme in the next few years on this subject.

Although it began independently, the internationally agreed format on neutron and synchrotron data work is expected to benefit from the support that this Commission and the IUCr (ultimately) can give to the project. Spallation neutron sources produce large data sets that should have an internationally agreed format structure. An attempt is being made to achieve uniformity with data formats from synchrotron sources. In many cases, the data are only partially used (*e.g.* looking along particular symmetry directions in single-crystal experiments) and may be reanalysed for further physical information as new aspects of problems present themselves.

The publication of *Neutron News* continues to be an important contribution to the development of neutron scattering science worldwide. I would like to thank the Editor, Dr G. Lander, for his cooperation with the Commission. I should also like to thank all members of the Commission itself for their help during the last three years and wish those members who are retiring well for the future.

Commission on Powder Diffraction

1995 was another very active year for the Commission on Powder Diffraction (CPD). The CPD was involved in the organization of three major international meetings in Chester, UK, Oxford, UK, and Liptovsky Mikula, Slovakia, was involved in ongoing projects for maintaining and updating the *World Directory of Powder Diffraction Programs* and continuing the Round Robin on Crystallite Size and Microstrain Determination, and initiated two new projects on Recommended Guidelines for Rietveld Analysis and a Round Robin on Quantitative Phase Analysis. Direct communication with powder diffractionists worldwide was maintained and enhanced with the production

of two more issues of the *CPD Newsletter* and its wide dissemination *via* an increased mailing list and its installation on the World-Wide Web.

Meetings/Workshops/Schools

After undertaking largely independent activities over the past six years, the CPD and the European powder diffraction community (in the form of the EPDIC series of meetings) started what is hoped to be an increasing level of cooperation. This interaction began with the invitation to the CPD Chairman, R. J. Hill, along with other members of the CPD, J. Fiala and D. Louër, to serve on the Programme Committee of the EPDIC IV meeting in Chester, UK, in July 1995. The collaboration will continue with similar CPD involvement in the organization of EPDIC V in Italy in 1997 and with assurances by the CPD and the ECM to coordinate their meetings in Europe so as to prevent overlap.

The CPD lent its support to the very successful International Meeting on Structure Determination from Powder Diffraction Data, held in Oxford, UK, in July 1995 and organized by W. I. F. David and colleagues from the Rutherford Laboratory, UK. CPD members L. B. McCusker, D. Louër and R. J. Hill presented invited lectures and workshops and the IUCr provided a generous grant to the Organizing Committee. This Conference was a very timely meeting with a very productive mixture of lectures and workshops that captured much of the excitement of this rapidly evolving area of powder diffraction. A book is expected to evolve which will be a member of the IUCr/OUP Monograph Series.

The CPD was also involved in the International Conference on X-ray Powder Diffraction Analysis of Real Structure of Matter: Size-Strain '95, held in Slovakia in August 1995 under the local guidance of Dr P. Sutta. CPD members J. Fiala, J. I. Langford and D. Louër and Chairman R. J. Hill served on the Programme Committee, J. Fiala as Chairman, and the IUCr again provided support in the form of a grant. Extended proceedings of this Conference will be published shortly, with advice provided by the CPD.

CPD consultant and immediate Past Chairman, R. A. Young, continued the series of CPD-organized three-day Rietveld Summer Schools with co-lecturers R. B. Von Dreele and A. K. Cheetham. The latest in this series was held in July 1995 at the Moscow State University, Russia, with Professor L. A. Aslanov as head of the local organizing group. The meeting was very well attended by 86 students and local scientists and, as usual, led to a significant enhancement of the participants' awareness of the capabilities of Rietveld analysis, particularly by young scientists. The CPD is once again grateful to the IUCr for providing financial support to assist with the travel expenses of the main lecturers and for registration and living-cost grants for students.

The CPD maintained a high profile in preparations for the IUCr Congress in Seattle through the involvement of its Chairman, R. J. Hill, and member D. E. Cox on the Programme Committee and with associated responsibility for the coordination of lecturers and other contributions to most of the powder-diffraction-related Microsymposia. The CPD's nominee, D. Louër, was invited by the IUCr to present a Plenary Lecture entitled Powder Diffraction – an Update at the Congress, and the CPD-initiated Microsymposium entitled Materials VIII – Powder Diffraction was also accepted, with R. J. Hill and J. B. Cohen as Co-Chairs.

In a novel initiative, the CPD has combined forces with the 45th Annual Denver X-ray Conference (DXC) to organize jointly the Satellite Meeting on Powder Diffraction in Denver, Colorado, USA, 3–8 August 1996, associated with the Seattle Congress. Two members of the CPD, D. E. Cox and D. K. Smith, served on the Organizing Committee and several CPD members and consultants were involved as invited speakers or workshop and special session organizers, including D. Louër (France), D. E. Cox (USA), R. J. Cernik (UK), H. Toraya (Japan), R. A. Young (USA) and R. J. Hill (Australia). In response to a joint request from the DXC and the CPD, the IUCr provided support for this ground-breaking meeting.

Projects

In conjunction with the Slovakia meeting, CPD member J. Fiala and R. L. Snyder (ICDD) co-chair a Task Group working on a Round Robin on Crystallite Size and Microstrain Determination. The preliminary results of studies on a widely circulated 'standard' sample of a ceramic material containing inclusions of crystallites of known size were reported during the Slovakia meeting.

Continued organizational and financial support was provided by the CPD for the maintenance and updating of the *World Directory of Powder Diffraction Programs*, co-organized by S. Gorter (The Netherlands) and D. K. Smith (USA). This compilation has now appeared in two updated versions and includes summary descriptions and contact information for several hundred programs. It has become a major resource that is accessible to the worldwide powder diffraction community. The grant from the CPD has been used to enable the database to be even further expanded in scope and size, and to provide hardware for it to be distributed by anonymous FTP.

Two new projects were initiated during the year. One involves the production of summary guidelines and protocols for the collection and analysis of powder data for Rietveld analysis and, related to this, the identification of a new Rietveld-method 'standard' material with higher complexity than the monoclinic zirconia sample used as a benchmark for the recently completed CPD Rietveld Refinement Round Robin project. This work is being coordinated by CPD members L. B. McCusker and D. E. Cox. The second new project is being coordinated by D. K. Smith and R. J. Hill and involves a new round robin survey of the accuracy, precision, capabilities and limitations of quantitative phase analysis by diffraction methods. The selection of appropriate multiphase samples and discussion of the protocols for the survey are well advanced, with the recommendations planned for open discussion during a workshop at the Satellite Meeting on Powder Diffraction in Denver in August 1996. The centre for distribution of survey materials and data analysis will be maintained by R. J. Hill and I. C. Madsen at Port Melbourne, Australia.

Newsletter

Production of the *CPD Newsletter* continued with the distribution of issues 14 and 15 in May and October 1995, edited by E. R. Tellgren (Sweden) and H. Toraya (Japan), respectively. These issues included feature articles on the Aminoff Prize (awarded to Hugo Rietveld), the contributions of Gunnar Hägg to powder diffraction, neutron powder diffraction at Kjeller, Norway, a tribute to Arthur C. Wilson, and current powder diffraction activities at the Photon Factory, Japan. Copies were sent to more than 850 powder diffractionists worldwide through

the CPD's extensive hard-copy mailing list. A novel feature of the *CPD Newsletter's* availability now and in the future is its recent installation on the World-Wide Web with access via a pointer from the IUCr Home Page. CPD member R. J. Cernik (Daresbury Laboratory, UK) has installed a copy of *Newsletter* 15 along with contact details and a brief introduction to the CPD and has agreed to continue this service for subsequent issues. It is expected that this innovation will ultimately provide even more widespread access and contributions to the activities of the CPD during the next triennium. The CPD is grateful to the Daresbury Laboratory for its agreement to support the distribution of the *Newsletter* in both hard and soft form in this manner.

Commission on Small Molecules

Most of the Commission's efforts during this year have been concentrated on preparations for the Seattle Congress and General Assembly. J. A. K. Howard and J. L. Flippen-Anderson are active members of the International Programme Committee, with particular responsibility for coordinating the small-molecule activities in Seattle. There will be three Plenary Lectures (V. K. Bel'sky, G. Desiraju and A. Gavezzotti) directly concerned with Commission topics of interest. In addition, F. H. Herbstein and Y. Ohashi are organizing Microsymposia on Solid State Reactions and Dynamic Properties in Molecular Crystals, respectively, while R. Harlow and R. Boese are organizing an Open Meeting of the Commission on Chemical Crystallography of the Future.

Commission-approved meetings or sessions took place at the Kloster Irsee meeting on Computational Methods in Chemical Design, Molecular Modelling – Theory and Experiment (organized by C. Kruger *et al.*) in May 1994, at the ACA Meeting in Montreal, Canada, in July 1995 (The Description, Understanding, and Prediction of the Structure of Inorganic Solids, organized by I. D. Brown), at ECM-16 in Lund, Sweden, in August 1995 (Intermolecular Interactions and Packing in Crystals organized by J. A. K. Howard and H.-B. Bürgi) and the Small Molecules Indaba in the Kruger National Park, South Africa, in August 1995 (Fundamental Principles of Molecular Modelling, organized by J. C. A. Boeyens; proceedings are being edited by W. Gans and published by Plenum).

The proceedings of the three-day symposium entitled New Trends in Small Molecule Crystallography held at the ACA Meeting in Atlanta, Georgia, USA, in 1994 has appeared as a Special Issue (edited by F. H. Herbstein) of *Acta Cryst.* (1995), B51, 385–640, which can be ordered separately. The proceedings of the 9th International Symposium on Organic Crystal Chemistry (held at Poznan-Rydzyna in August 1994), edited by D. W. Jones and A. Katrusiak, have appeared as Volume 374 of *J. Mol. Struct.* Proceedings of the session on Phase Relations and Transformations in Some Small Molecule Systems of the Symposium on Molecular Structure held in Fuzhou, China, in September 1993 will appear as an issue of *Crystallography Reports* (edited by F. H. Herbstein).

The Executive Committee has approved the Commission's suggestion that its name be changed to Commission on Structural Chemistry; this has to be approved by the General Assembly. Negotiations are being pursued to associate gas electron diffractionists with the activities of the Commission.

The Commission suffered a grievous loss with the death of Yu. T. Struchkov, an active member of long standing.

Commission on Synchrotron Radiation

Synchrotron radiation in the field of crystallography has during the last year been in a very expansive phase. New third-generation sources with strong crystallographic programs have been commissioned in Grenoble, Argonne, Trieste, Berkeley and Lund and the Japanese SPring-8 project is in an advanced construction phase. The Commission's work during this period has been concentrated on spreading information on the new experimental opportunities available by actively organizing Microsymposia and giving general review talks. Major efforts were made to organize synchrotron-based Symposia at several meetings during 1995.

Synchrotron radiation featured prominently at the 16th European Crystallographic Meeting in Lund, Sweden, 5–11 August 1995. Three different half-day Symposia, Synchrotron Radiation Applications I and II and Synchrotron Radiation Instrumentation, were organized by the Chairman and applications both in small-molecule and macromolecular crystallography were covered. The instrumentation part included talks on microcrystal diffraction, detectors and novel optics development.

The Commission was actively involved on the Programme Committee of the Third International School and Symposium on Synchrotron Radiation in Natural Sciences, 31 May–8 June 1996, Jaszowiec, Poland. This School covered a very wide area of synchrotron-radiation techniques and applications in the natural sciences. The Polish Synchrotron Radiation Society succeeded in attracting excellent lectures for the benefit of participants mainly from the central and eastern part of Europe. This year, the School was attended by approximately 100 participants.

The 17th European Crystallographic Meeting now in a detailed planning stage to be held in Lisbon, Portugal, 24–28 August 1997 includes four Microsymposia in the area of synchrotron radiation: Time-Resolved Crystallography, New Developments in Detectors, High-Energy Diffraction and Phase Contrast Imaging under the programme responsibility of the Commission Chairman.

The Commission is heavily involved in the IUCr Congress in Seattle and the Chairman has been active on the Programme Committee. Three Microsymposia: Synchrotron Radiation I, II and III have been scheduled. In addition to the main Congress in Seattle, a Synchrotron Radiation Satellite Meeting at the Advanced Photon Source in Argonne is being organized under the auspices of the Commission (4–7 August 1996). The main feature of the Satellite Meeting is to give a broad overview of the state-of-the-art developments in the synchrotron-radiation field and in particular to give a review of the impact of the new third-generation sources. More than 30 invited leading synchrotron-radiation scientists will present the latest developments in the field.

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 1995 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1995 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1996, but approved in 1995, are listed below:

1. Winter Workshop on Electron Diffraction and Imaging at Surfaces, Scottsdale, Arizona, USA, 3–6 January 1996.
2. International Symposium on Ferroic Domains and Mesoscopic Structures, Vienna, Austria, 25–30 March 1996.
3. School on X-ray and Neutron Dynamical Diffraction – Theory and Applications, Erice, Italy, 9–21 April 1996.
4. 3rd European Symposium on X-ray Topography and High-Resolution Diffraction, Palermo, Italy, 22–24 April 1996.
5. School on Experimental and Computational Approaches in Structure Based Drug Design, Erice, Italy, 8–19 May 1996.
6. IUCr Satellite Meeting on Powder Diffraction, Denver, Colorado, USA, 3–8 August 1996.
7. IUCr Satellite Meeting on Synchrotron Radiation, Argonne, Illinois, USA, 4–7 August 1996.
8. IUCr Satellite Meeting on Neutron Scattering, Gaithersburg, Maryland, USA, 5–7 August 1996.
9. Summer School on Crystallographic Computing, Olympia, Washington, USA, 17–23 August 1996.

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. Coddling. A new Chairperson will be appointed in Seattle.

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 the 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

Early in 1995, there was a lively exchange between members of the Committee on the Internet. A special meeting of the Committee held in conjunction with the American Crystallographic Association meeting in Montreal, Canada, then made recommendations to the IUCr Executive Committee. It is clear that the IUCr should disseminate crystallographic information on the Internet as soon as technically and financially feasible. It is less obvious what information can be disseminated economically and how rapidly the transition can proceed.

It was agreed at Montreal that electronic submission of manuscripts to all the Union journals should be encouraged, and that the Standard Generalized Markup Language (SGML) protocol

should become the standard for the IUCr's serial publications. What has yet to be determined is how the SGML protocol will be implemented. For example, it would be technically feasible to meet the objective by requiring all manuscripts to IUCr journals to be submitted in CIF format, which would be converted to SGML automatically by a translator. So far, the Committee has not decided to recommend that action. The rate at which the Chester office can implement the transition without undue disruption is also being assessed.

The residual uncertainties on manuscript submission are insignificant compared with those related to dissemination of information electronically on the Internet. Some members favoured having the journals provide only the titles of the articles published in the journals free of charge electronically. Others felt that the Union should supply an electronic copy of any manuscript in its journals at an appropriate fee. Planning the dissemination of information in the Union journals is complicated by the strong dependence of some crystallographic work on complex diagrams. Alternative protocols for processing graphical and pictorial information exist, but protocols preferred as *de facto* standards for different classes of information have yet to emerge. This issue has been referred to the Commission on Crystallographic Computing for advice.

The IUCr Executive Committee decided to appoint a consultant to advise on those aspects of the Chester office's work that would benefit from independent scrutiny. The consultant's report will become available for deliberation early in 1996.

Regional Associates and Scientific Associates

American Crystallographic Association (ACA)

The ACA had another highly successful year with increased membership and increased participation in their annual meeting. The meeting was held in Montreal, Quebec, Canada, 23–28 July 1995. Under the able leadership of Y. Le Page (Programme Chair) and M. Cygler (Local Chair), the meeting was packed with science and activities. The abstracts for the meeting were posted on the World-Wide Web, which proved to be a useful way to highlight the science presented at the meeting. The ACA presented Dr K. Trueblood and Dr J. P. Glusker with the Fankuchen Award at the Montreal meeting. Also, five students, Fei Gu, Peter Kuhn, Erik Martinez-Hackert, Monica Niederhut and Thomas Schneider, were presented with a Pauling Prize for their poster presentations.

The ACA remains an active member of the American Institute of Physics and provides representatives to several AIP committees. The ACA again sponsored a summer school in crystallography held in Pittsburgh. The ACA accepted an application from Mexico to join the Regional Association. Members of the ACA Council for 1995 were: President: H. Steinfink; Past-President: E. Adman; Vice-President: C. Huber; Treasurer: J. Griffin; Secretary: C. Lowe-Ma; Canadian representative: I. D. Brown; Mexican representative: M. Soriano; Executive officer: W. L. Duax.

Asian Crystallographic Association (AsCA)

The second Conference of the Asian Crystallographic Association was initially planned to be held in Kuala Lumpur, Malaysia, but circumstances forced the Organizing Committee to change its plans. Eventually, it was decided in mid-May 1994 that Chulalongkorn University in Bangkok, Thailand, would

host the Conference, and the preparations continued. The Conference was held on the campus of the University for three days, 22–24 November 1995. With Professor P. Coppens, President of the IUCr, attending the opening ceremony, Professor W. Robinson, President of the AsCA from New Zealand, declared the meeting open. The subtitle of the Conference was Three Days Conference on Frontier Topics in Crystallography. About 240 people attended the meeting, including 100 from Japan.

Each day's sessions began with two Plenary Lectures, followed by six Microsymposia in three separate rooms. Poster sessions accompanied them. The speakers at the Plenary Lectures consisted of two from Japan and one each from Australia, China, India and Taiwan. In addition, a special lecture was given by the President of the IUCr. All the lectures proved to be good and were highly valued. Each Microsymposium was a great success and crowded to capacity. Especially remarkable were the vigorous activities and interchanges among young crystallographers from Australia, Japan and Taiwan. They appeared very promising.

The total number of papers presented was a little over 200. This number is slightly less than 240 papers at the time of the first Conference of AsCA held in Singapore. Nevertheless, it may be safely said that the second Conference contributed much to the AsCA itself, which now appears to have planted its deep roots in terms of both the scale and the significance of holding conferences in the Southeast Asian area.

The second Conference turned out to be highly successful under the strenuous efforts of Professor W. Robinson (New Zealand), President of the AsCA, Professor Y. Ohashi (Japan), Chairman of the Programme Committee, Professor P. Phavanantha (Thailand), Chairman of the Local Organizing Committee, Professor Y. Wang (Taiwan), Vice-President of the AsCA, and Professor T. Uragami (Japan), a member of the International Organizing Committee, among others. There were some communication problems in organizing the Conference. Also, early in October 1995 before the start of the Conference, Professor A. Authier made an on-site inspection of progress. His detailed report greatly helped to smooth the communication between the local committee and outside committee members. As an Asian crystallographer, I would like to express my sincere appreciation to Professor Authier for his devotion.

In closing, I think it is worth mentioning that, prior to the holding of this Conference, the Asian Crystallographic School of Gems and Precious Materials was held 20–21 November. Also, after the Conference, the Asian Crystallographic Computing School was held 27–30 November. The IUCr sponsored both these Schools and extended its support to young scientists, including those attending the second conference. Excluding those from Australia and Japan, the scholarships were distributed among 14 young attendees (Taiwan 3, Vietnam 3, India 2, Russia 2, Armenia 1, China 1, Malaysia 1, Sri Lanka 1) out of the 18 applicants.

European Crystallographic Committee (ECC)

The IUCr representative, Yu. T. Struchkov, sadly died in 1995.

International Organization of Crystal Growth (IOCG)

During 1995, the activity of the IOCG was governed by the preparation and performance of the Eleventh International Conference on Crystal Growth (ICCG-11), The Hague, The Netherlands, 18–13 June 1995, and the Ninth International Summer

School on Crystal Growth (ISSCG-9), Papendaal/Arnhem, The Netherlands. Both events were organized by the Dutch Association for Crystal Growth, the Chairpersons C. F. Woensdregt (for ICCG-11) and J. P. van der Eerden (for ISSCG-9) were both from Utrecht University.

ICCG-11 was attended by more than 1000 scientists from all over the world. Eight plenary lectures on modern topics and novel developments in various fundamental and practical fields of crystal growth were presented, and 32 Microsymposia of 2 hours duration were held in four parallel sessions, resulting in a total of 196 oral contributions. In addition, 10 videos and about 630 posters were shown. The Conference Proceedings are published in the *Journal of Crystal Growth*.

During ICCG-11, meetings of the IOCG Executive Committee, of the Council and of the General Assembly were held under the direction of its (retiring) President, B. Cockayne. The following resolutions, among others, were approved: the Brazilian Society for Crystal Growth, the Czech and Slovak Association for Crystal Growth and the Romanian Materials Science Crystal Growth Society are formally accepted into the IOCG.

The offer of the Japanese Association for Crystal Growth to hold ISSCG-11 and ICCG-13 in 2001 in Japan should be accepted.

The possibility of the IOCG becoming an International Scientific Associate affiliated to ICSU, with a possible change of name to International Union for Crystal Growth, will be explored by the new President and Executive Committee.

An honorary post entitled Honorary Principal Founder of IOCG was created on the Executive Committee for the period 1995–1998 for the retiring Secretary and Principal Founder of the IOCG, Michael Schieber, Jerusalem, Israel, in recognition of his distinguished service to this organization.

The following officers and Executive Committee members are elected for the period 1995–1998, from the end of ICCG-11 through ICCG-12, which will be held in Jerusalem in 1998. President: T. Nishinaga (Japan); Vice-Presidents: K. W. Benz (Germany), R. F. Sekerka (USA); Secretary: G. B. Stringfellow (USA); Treasurer: C. F. Woensdregt (The Netherlands); Past-President: B. Cockayne (UK); Honorary Principal Founder of IOCG: M. Schieber (Israel). Executive Committee: P. Bennema (The Netherlands), A. A. Chernov (Russia), J. J. Favier (France), A. Horowitz (Israel), Jiang Min-Hua (People's Republic of China), H. Komatsu (Japan), H. J. Scheel (Switzerland), J. N. Sherwood (UK). *Ex officio* members: C. F. Woensdregt (The Netherlands), Chairman of ICCG-11; M. Schieber (Israel), President of ICCG-12; P. M. Dryburgh (UK), IOCG representative to the IUCr; H. Klapper (Germany), IUCr representative to the IOCG; J. N. Sherwood (UK), IOCG representative to IUPAC; D. J. Buttrey, IUPAP representative to the IOCG.

In addition, 35 councillors representing National Associations, 5 councillors representing nations who do not have a National Association and 4 *ex officio* councillors representing International Unions have been approved. The *ex officio* councillor representing the IUCr is M. H. Dacombe. The following IOCG Prizes, sponsored by the Dutch Association for Crystal Growth and the ICCG-11 Organizing Committee, were awarded: the Frank Prize to P. Bennema (The Netherlands) and the Laudise Prize to R. F. Feigelson (USA).

The first IOCG Distinguished Service Award, sponsored by the Japanese, Italian and British Associations for Crystal Growth, was presented to M. Schieber (Israel).

An important item considered during the IOCG Executive Committee and Council meeting was the stronger interaction of the IUCr and the IOCG in fields of common interest. It was agreed to consider holding a joint International Symposium on Crystal Characterization.

The Twelfth International Congress on Crystal Growth (ICCG-12) will be held in Jerusalem, Israel, in July 1998, the Tenth International Summer School on Crystal Growth (ISSG-10) at Lake Garda, Italy, in June 1998.

International Centre for Diffraction Data (ICDD)

The International Centre for Diffraction Data (ICDD) is a non-profit scientific organization that collects, edits, publishes and distributes powder diffraction data for the identification of crystalline materials.

Mission Statement

The International Centre for Diffraction Data will continue as the world centre for quality diffraction data to meet the needs of the technical community. The ICDD promotes the applications of materials characterization methods in science and technology by providing a forum for the exchange of ideas and information.

The ICDD Organization

The ICDD membership comprises scientists from various affiliations – educational, governmental, industrial. Approximately 100 scientists from around the world constitute the active membership from which the organization draws its Board of Directors, Committees and Sub-committees. The members, who are volunteers, are actively engaged in developments in the field of X-ray powder diffraction and related disciplines. A paid scientific and administrative staff is responsible for the production of the various databases offered by the ICDD.

Technical Committee (Chairman elected for two-year term)

At present, the Technical Committee consists of 15 active Sub-committees: Ceramics, Crystal Data, Data Collection and Analysis, Diffraction Problems, Education, Electron Diffraction, Metals and Alloys, Minerals, New Product Research & Development, Organic and Forensic, Pattern Calculations, PDF Database, PDF Editorial Staff, Search/Match Methods and Target Systems for Technical Committee Activity. These Committees meet twice a year to report on their progress.

ICDD Assisted Research

The ICDD sponsors a Grants-in-Aid Programme to provide high-quality data and to develop search techniques for the identification of materials by powder diffraction methods.

ICDD Educational Commitments

The ICDD sponsors a worldwide program of workshops, seminars and schools. The ICDD Clinic on X-ray Powder Diffraction (XRD) comprises two one-week courses in the fundamentals of qualitative and quantitative X-ray diffraction. The ICDD also sponsors the Clinic on X-ray Fluorescence Spectrometry (XRF) in the fundamentals of qualitative and quantitative X-ray fluorescence. Both the XRF Clinic and the XRD Clinic are conducted annually during the summer months. Schedules and fees for educational activities may be obtained from ICDD headquarters.

Activities of the ICDD for 1995

The International Centre for Diffraction Data announced the award of four Crystallography Scholarships for 1996. Mr P. M. Leu, University of California, Davis, USA, Mr A. Oakley, St Vincent's Institute of Medical Research, Australia, Ms L.

Shimoni, Fox Chase Cancer Center, USA, and Mr H. Xu, Princeton University, USA, have been designated recipients by the ICDD Scholarship Award Selection Committee. P. Leu's research centres on the theoretical development of a holographic technique to determine atomic crystal structure from electron or fluorescent X-ray diffraction data. A. Oakley is exploring crystal structure function by X-ray crystallography and computer graphics techniques. L. Shimoni is determining the crystal structure of various enzymes and H. Xu is studying high-temperature TEM and X-ray diffraction of the order-disorder phase transition in β -eucryptite.

At the Fall meeting of ICDD, CPD member D. K. Smith was elected by the Board as a Distinguished Fellow. Professor Smith has contributed greatly over the past 30 years as a scientist, Board member (Chairman), Grantee, Journal Editor and principal teacher of ICDD XRD Clinics. His international contributions to conferences in Australia, Denver (USA) and Egypt are well recognized by his colleagues and his current activity with the CPD *World Directory of Powder Diffraction Programs* has saved many scientists from 're-inventing the same software'. He recently retired from Penn State after 27 years as a Professor of Mineralogy.

On 20 December 1995, Chairman G. C. Johnson Jr announced to staff and ICDD members that D. Richardson had submitted his resignation as the General Manager of ICDD as of 1 January 1996. D. Richardson brought new perspective to the Centre and leaves the organization on a strong financial footing. The Executive Committee has begun the process of locating a new General Manager.

On 22 February 1996, the results of the recent election were announced. Chairman: R. L. Snyder; Vice-Chairman: CPD consultant and former Chairman R. A. Young; Technical Committee Chairman: T. C. Huang; members-at-large: C. R. Hubbard, J. A. Kaduk, T. N. Blanton, C. E. Crowder and C. Lowe-Ma will continue as members-at-large. G. C. Johnson Jr fills the position of Past-Chairman.

The ICDD X-ray Clinics will be held in June 1996 at the International Centre for Diffraction Data headquarters in Newtown Square, Pennsylvania, USA. The ICDD Clinic on X-ray Powder Diffraction will be held in two week-long sessions as follows: Fundamentals of X-ray Powder Diffraction (3–7 June 1996); Advanced Methods in X-ray Powder Diffraction (10–14 June 1996).

The ICDD Clinic on X-ray Fluorescence Spectrometry will be held 17–21 June 1996.

Highlights of 1995 technical activities

ICDD Products

PDF – Set 45, Alphabetical Index & Search Manual: 2000 new patterns edited by Editorial Staff, Metals and Alloys, and Minerals Sub-committees.

Electron Diffraction Database – 1993 Release (actually released in 1995): total entries 82K (new 10K), tested by Electron Diffraction Sub-committee.

Crystal Data Identification File – 1994 Release (Update G): total entries 200K (new 15K), assisted by Crystal Data Sub-committee

Round robin studies

Crystallite Size and Microstrain Determination (R. L. Snyder and J. Fiala, co-sponsored by ICDD and CPD); Evaluation of Practices in *Ab Initio* Pattern Indexing (D. Louër, Data Collection & Analysis Sub-committee); Profile Fitting (Cline, Data Collection & Analysis Sub-committee); Preferred Ori-

entation (E. Crowder, Diffraction Problems Sub-committee); X-ray Reflectivity (N. Blanton, Data Collection & Analysis Sub-committee).

Conferences/Workshops

Denver X-ray Conference (August, Colorado Springs, CO, USA): Basic Crystallography for Diffractionists (Organizers: D. K. Smith and R. L. Snyder); Crystallographic and Phase Diagram Databases (T. C. Huang, A. Mighell and W. Wong-Ng); Open Session on Attacking Problems in XRD and XRF Analysis (G. J. McCarthy and R. Jenkins); Parallel Beam Optics (Eatough and Goehner); PDF and New Techniques in Phase Analysis (R. Jenkins and C. M. Foris); Rietveld Analysis (J. A. Kaduk and L. Iyengar); Use of Spreadsheets in X-ray Analysis (R. Jenkins and Klimasers).

EPDIC IV (July, Chester, England): Powder Diffraction File (R. Jenkins, J. W. Visser and Rysel).

BCA Annual Spring Meeting (March, Cardiff, UK): Use of Powder Diffraction File (R. Jenkins).

Representatives on Other Bodies

IUPAC Interdivisional Committee on Nomenclature and Symbols (IDCNS)

The annual meeting of the IDCNS was held 8–9 August 1995 in Guildford, UK. As has often been the case, it overlapped one or other major crystallographic meeting. This year, it coincided with the 16th European Crystallographic Meeting. Neither the IUCr representative, the alternate, nor several other qualified crystallographers approached were able to participate in this IDCNS meeting. However, it proved possible for IDCNS to pay adequate attention to a primary IUCr concern regarding the ångström. Our strong objections, as expressed by many of our Editors and others associated with IUCr publications, to the 1994 proposal by the Comité Consultative d'Unités (CCU) of the Bureau International des Poids et Mesures (BIPM) to deprecate the ångström were presented in advance of the meeting. The Chair of IDCNS agreed to transmit these objections to CCU. IDCNS now supports a different approach to the classification of units, in which non-SI units would simply be listed without indication of status but with an account of their usage by various communities. The Chair reported that the 1994 recommendations would be reviewed further at the CCU meeting in April 1996 before they might be submitted to the Comité International des Poids et Mesures (CIPM) for final action. Authority to act in all matters touching on the demands for higher accuracy, wider range and greater diversity in measurement standards between nations has been given jointly to the Conférence Générale des Poids et Mesures, the CIPM and the BIPM by the Convention du Mètre. This Convention, which dates to 1875, is a diplomatic treaty that has now been signed by 48 nations.

Among other matters discussed of interest to the IUCr, IUPAC's Green Book *Quantities, Units and Symbols in Physical Chemistry* is presently in revision with the aim of publishing the third edition in 1998. It will contain, *inter alia*, a new section on uncertainties in measurement for consistency with the recent International Organization for Standardization's Guide to the Expression of Uncertainty in Measurement. The IUCr is already in conformity with this document, see *Acta Cryst.* (1995), A51, 565–569. The proposal has been made to CCU that the terms kilobyte (kb) and megabyte (Mb) be used only for

10^3 (not 10^{24}) and 10^6 (not 10^{24^2}) bytes, respectively. New related prefixes have been proposed for these common units as follows: 2^{10} = kibi (kilobinary), symbol kb; 2^{20} = mebi (megabinary), symbol Mb; 2^{30} = gibi (gigabinary), symbol Gb; and 2^{40} = tebi (terabinary), symbol Tb. In consequence, the unit for 2^{10} bytes would become kibibyte (kibyte), that for 2^{20} bytes mebibyte (mibyte) *etc.* Symbols for the bit and the byte are under discussion. These proposals have not been accepted by CCU and alternatives are under consideration. Interested crystallographers are invited to suggest less confusing terminology for large binary quantities either to the representative or alternative representative for consideration by the CCU.

43 nomenclature reports originating in the divisions and commissions of IUPAC were received by the representative in the course of the year. Reports containing matters likely to be of interest or concern to the IUCr were reviewed with care and corrections made where necessary. Following revision, as required by the IDCNS, all accepted nomenclature reports are published in *Pure Appl. Chem.* and constitute the current nomenclature policy of IUPAC.

International Council for Scientific and Technical Information (ICSTI)

All major ICSTI activities were scrutinized at its General Assembly, which in 1995 was conducted under the auspices of the European Patent Office (EPO). The programme included an extended technical presentation on the use of information by the EPO itself. The proceedings had implications for the IUCr's scientific publishing.

A Survey on the Use of Networks, conducted by ICSTI, assessed the use of networks for disseminating information in the wide range of environments spanned by ICSTI membership. While the project produced few surprises, it was reassuring to see many common prejudices confirmed.

A significant new trend was strong support on ICSTI for the SGML protocol, which has gained such widespread acceptance that its future role as a *de facto* publishing standard is assured. There is also widespread expectation that the WWW will become the future medium for disseminating scientific information on the Internet eventually, but there are significant financial and technical obstacles to its realization.

On the basis of earlier experience with the TULIP project, which tested electronic delivery of scientific information in libraries, commercial publisher members of ICSTI could not foresee their commercial publishing on the Internet becoming financially viable within five years. They believed that electronic delivery would remain expensive compared with alternatives for the foreseeable future. In a decision that is mainly cost driven, several members intend focusing on magnetic media and CD-ROM delivery.

The approach of typical not-for-profit members of ICSTI differed strongly from that of the commercial publishers. Not-for-profit publishers favoured presenting material on the Internet, provided that did not compromise the viability of their hard-copy core publishing.

Notwithstanding its important role in electronic publishing, raster graphics' cipher-like properties limit it to applications where human observers synthesize the graphic or pictorial information. ICSTI is considering a study of alternative protocols for representing and disseminating graphic and pictorial information as a topic for a future project.

International Council of Scientific Unions (ICSU)

(A) *Report on the 34th Meeting of the ICSU General Committee held in Chang Mai, Thailand, 7-9 October 1995*

I. Administrative

(a) *Assessment of ICSU*: an independent Assessment Panel has been established to assess the work and mode of action of ICSU. Its Chairman, R. Schmitt, attended the 34th Meeting of the General Committee. The Panel was to meet in Paris in early 1996 and the conclusions will be reported to the 25th General Assembly of ICSU in 1996.

(b) *Frequency of the General Committee Meetings*: a vote of the General Committee confirmed the straw vote taken in Rabat, Israel, in 1994 in favour of 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) *Admissions*: it was recommended to admit as National Scientific Associates the National Academy of Sciences of Kazakhstan and the Uganda National Council for Science and Technology and as International Scientific Associates the International Society for Photogrammetry and Remote Sensing and the Engineering Committee on Oceanic Resources.

(d) *Informatics*: the meeting of experts from various Unions which was convened by the International Mathematics Union in May 1995 will probably lead to the creation of an International Union of Computing Science and Informatics. The Chairman of the IUCr Commission on Crystallographic Computing was consulted.

(e) *Ethics*: the General Committee discussed the possibility of establishing a Standing Committee for Scientific Responsibility and Ethics in Science and agreed that the mandate of such a Committee still needed to be sharpened by a working group before the next General Assembly. The Norwegian Academy of Science and Letters has offered to provide a secretariat for this Standing Committee.

II. Review of Interdisciplinary ICSU Bodies and Scientific Associates

The following bodies were discussed: CODATA; WDC; FAGS; IASA; IFSEM; IRPA.

III. Scientific Priority Setting

(a) *Agriculture*: a Workshop on Food Security for the 21st Century was held in Senegal in November 1995 with the aim to formulate specific recommendations for action by ICSU in agriculture, forestry and aquaculture. Food security is an issue of relevance for many members of the ICSU family. Stress on such issues as nutrition security, impact of pesticides, effect of poverty on food security *etc.* will be included.

(b) *Water Research*: a report from SCOWAR was discussed and the microbiological aspects of water quality and water safety were stressed by several members.

(c) *ICSU involvement in the Human Dimensions of Global Environmental Change Programme*: it was recommended that ICSU should interact more closely with the social sciences and that ICSU should co-sponsor this Programme.

(d) *Arctic Science*: it was recommended that ICSU should be more involved in the Arctic; as a possible means of cooperation, the International Arctic Science Committee might apply for Associate status in ICSU.

(e) *Science in the Year 2000*: IUPAP plans to celebrate Science in the Year 2000 and it was suggested that other Unions might do the same and that their efforts should be coordinated. It was recommended that ICSU should also organize a special

event at its 1999 General Assembly and that it should act as a focal point for other such initiatives sponsored by ICSU bodies.

IV. Report on Follow-up to Recommendations of 33rd Meeting of the General Committee

(a) *Towards Managing the Earth System*: W. Fyfe reported on plans for mounting a programme on managing the Earth system, which should include both scientists and politicians.

(b) *Energy*: it is recommended that a meeting be convened in 1996 to define a strategy for ICSU for all problems concerning energy.

(c) *Biodiversity*: the original sponsors of DIVERSITAS (IUBS, SCOPE and UNESCO) have been joined by ICSU, IUMS and GCTE/IGBP. A Scientific Committee, a Chair and an Executive Director will be named for the programme, which would be financed by CNRS, France, and housed at UNESCO.

(d) *Committee on Capacity Building in Science*: ICSU is planning to launch an important and ambitious programme on Capacity Building in Science, which will be presented at the 1996 ICSU General Assembly. All ICSU bodies are invited to mobilize their resources to support this programme. It is felt that capacity building, including education and public understanding of science issues, is the area in which ICSU can make the most significant contribution to the future of humanity.

(e) *Universality and UN Decisions about Sanctions*: the General Committee has revised its statement on Freedom in the Conduct of Science (see Appendix 1) and has produced, after advice from legal experts, a document on the impacts of UN Sanctions on Freedom in the Conduct of Science (see Appendix 2). Members of the ICSU family are encouraged to use these documents whenever necessary.

V. Scientific Programme

The following lectures were presented during the scientific sessions, which were open to scientists from Thailand:

(a) *Science in Asia: Science and Technology in Thailand* (S. Sabhasri), *Why Basic Sciences in Asia* (M. Ito).

(b) *Informatics and Basic Sciences: Informatics a Cultural Revolution* (A. Authier), *Informatics and the Wealth of Nations* (J. E. Fenstad), *Information and the Changing Global Environment* (G. I. Pearman).

(c) *21st Century Issues in Biosciences: New Frontiers in Biotechnology, Marine Biotechnology as a Paradigm* (R. Colwell), *Biodiversity and Ecosystem Services* (H. A. Mooney).

VI. Next Meeting

The next meeting of the ICSU General Committee will be held on 23 September 1996, just prior to the 25th General Assembly which will be held in Washington, DC, USA, at the invitation of the US National Academy of Sciences.

*Appendix 1**ICSU statement on freedom in the conduct of science**

The International Council of Scientific Unions (ICSU) is the oldest existing non-governmental body committed to international scientific cooperation for the benefit of humanity. Created in 1931 when its predecessor, the International Research Council, was dissolved because of discrimination against scientists from certain countries, ICSU has consistently and vigorously pursued a policy of non-discrimination. ICSU maintains that

* Approved by the Executive Board and General Committee of ICSU, Lisbon, Portugal, October 1989, revised by the Executive Board, Rabat, Israel, October 1994, and further revised by the General Committee at its meeting in Chiang Mai, Thailand, October 1995.

discrimination hinders the free communication and exchange of ideas and information among scientists and thereby impedes scientific progress, which is dependent on their collective efforts.

ICSU's members are 23 International Scientific Unions and 94 National Academies of Science or Research Councils. Together these organizations set up international mechanisms to carry out scientific programmes of an interdisciplinary nature which are concerned with issues such as protection of the environment, research in Antarctic regions or space research. An important factor in the success of these activities is that they are carried out under the aegis of such a respected independent and international scientific body as ICSU. Each of the International Scientific Unions, the National Scientific Members, ICSU interdisciplinary bodies, and Scientific Associates – the organizations comprising the ICSU family – strictly adheres to the basic principles of the Council's Statutes when involved in activities carried out within the scope of ICSU's concern.

One of the basic principles in these Statutes is that of the universality of science (see Statute 5), which affirms the right and freedom of scientists to associate in international scientific activity without regard to such factors as citizenship, religion, creed, political stance, ethnic origin, race, colour, language, age or sex. Such rights are embodied in a variety of articles in the International Bill of Human Rights.†

ICSU seeks to protect and promote awareness of the rights and fundamental freedoms of scientists in their scientific pursuits. ICSU has a well established non-political tradition which is central to its character and operations, and it does not permit any of its activities to be disturbed by statements or actions of a political nature.

As the intrinsic nature of science is universal, its success depends on cooperation, interaction and exchange, often beyond national boundaries. Therefore, ICSU strongly supports the principle that scientists must have free access to each other and to scientific data and information. It is only through such access that international scientific cooperation flourishes and science thus progresses.

On these grounds, ICSU works to resolve such cases as do, nevertheless, arise from time to time when such open access is denied or restricted and in cases primarily involving members of the ICSU family. In most cases, private consultations involving members of the ICSU family have been successful. Where private consultations have failed, ICSU has publicized acts of discrimination against scientists and taken steps to prevent their repetition, including, if necessary, such measures as encouraging members of the ICSU family to decline invitations to hold or attend meetings in the country concerned.

On the basis of its firm and unwavering commitment to the principle of the universality of science, ICSU reaffirms its opposition to any actions which weaken or undermine this principle.

Appendix 2

Implications of the impacts of UN sanctions on freedom in the conduct of science

The role of science and scientific enquiry in the promotion of human welfare is undeniable. But in order to ensure the

proper functioning of this progress, it is essential to maintain the possibility of communication and cooperation beyond national boundaries. This is all the more so in a world in which the interconnection of different branches of science is becoming increasingly important as the opportunities for scientific contribution to the solution of developmental and environmental problems become increasingly obvious.

The promotion of international scientific work and its use for the benefit of humanity has been the central purpose of the International Council of Scientific Unions (ICSU) since its creation in 1931. ICSU has strongly upheld the principle of the universality of science without which science, a vital and necessary component of human development, cannot flourish. That belief is embodied in the attached Statement on Freedom in the Conduct of Science. ICSU has consultative status with ECOSOC, with UNESCO, and with other relevant UN organizations. Thus, ICSU is recognized as 'providing a natural and appropriate forum for the international organization of science'.‡

In the course of performing its statutory functions in this regard, ICSU has increasingly encountered difficulties related to the implementation of UN Security Council decisions on sanctions under Article 41 of the UN Charter. These difficulties fall mainly into the following categories:

(i) *Bona fide* scientists engaged in wholly peaceful research have been refused entry visas necessary for their participation in international scientific activities, such as conferences or visits to research institutes.

(ii) The free flow of scientific communication has been interrupted in the belief that such communication violates UN sanctions; examples include refusals to publish scientific works and embargoes on the sale of scientific books and journals.

(iii) The collection and interpretation of scientific data and information have been hindered, particularly with regard to the environment and despite the fact that such data are essential to progress in implementation of the Rio Declaration on Environment and Development.

(iv) The purchase of scientific equipment and materials having only peaceful applications has been impeded.

The difficulties described above appear to contravene several fundamental principles embodied in the UN Charter (notably Articles 1 and 55), the Universal Declaration of Human Rights (Articles 2, 19 and 27), and the UNESCO Constitution (Article 1).

Aware of the fact that the UN Security Council is willing to minimize the unintended adverse side effects of UN sanctions in this area, and given the importance of freedom in the conduct of international science to the well being of humanity, ICSU recommends that appropriate measures be taken by the UN Security Council to permit and facilitate the free flow of all legitimate international scientific communication and exchange among *bona fide* scientists engaged in wholly peaceful research.

Such measures should include:

the issuance of a statement supporting the free flow of all legitimate international scientific communication and exchange among such scientists;

the unequivocal lifting of any and all sanctions related to legitimate international scientific exchange among such scientists, irrespective of nationality;

the notification of all UN member countries that such action be taken, accompanied by a recommendation that any national

† The International Bill of Human Rights includes three documents: the Universal Declaration of Human Rights (1948), the International Covenant on Civil and Political Rights and the International Covenant on Economic, Social and Cultural Rights (1966).

‡ UNESCO-ICSU Agreement signed in 1947.

legislation enacted to conform to the UN sanctions be modified to exempt scientific exchange;

a resolution that international scientific communication and exchange among such scientists will be exempted from sanctions imposed in the future.

Document drawn up by meeting of invited legal and other experts, ICSU, Paris, France, July 1995, and subsequently modified by members of the Standing Committee on Freedom in the Conduct of Science and the Executive Board of ICSU, October 1995.

(B) ICSU Press Conference on Electronic Publishing

A Conference on Electronic Publishing in Science, organized jointly by ICSU Press and UNESCO, was held during the week 19–26 February 1996 in the UNESCO Headquarters in Paris, France. The IUCr representative, A. Authier, was Co-Chairman of the Local Organizing Committee. It was attended by 150 experts in electronic publishing, scientists, publishers, librarians and lawyers. Invited speakers (including the Editor of *Acta Crystallographica Section C*, S. R. Hall) surveyed the field before participants split into five workshops to discuss specific issues. Main topics included: 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.

The Conference overwhelmingly recommended that strict peer review should be applied to all scientific material submitted for publication in electronic journals. ICSU and UNESCO are invited to organize a forum involving scientific societies in order to formulate codes of ethics and of conduct for electronic publication on such matters as peer review, citation, integrity, priority of publication and authentication of material and archiving. It was recommended that scientific societies, publishers and librarians come together to establish principles and guidelines for electronic archiving and that consultation with the International Organization for Standardization (ISO) should be ensured concerning the use and development of appropriate standards. Funding agencies should regard the costs both of the publication of research results and access to required information as an essential component of research funding. An international committee should be established by ICSU in coordination with ICSU members and associates and involving representatives of the library and scientific publishing communities to conduct a technical study of the costs and benefits of electronic publication. ICSU and UNESCO should promote good access to computer communications for scientists in all countries with all available means. All scientists should receive training in the use of information resources and libraries and in good authoring skills as undergraduates. The scientific community in developing countries should become more involved in the development of methodologies, tools and standards relating to electronic publishing and archiving and regional cooperation should be encouraged. UNESCO should support pilot projects to this end. Further details may be found in the ICSU home page on the World-Wide Web at <http://www.lmcp.jussieu.fr/icsu/>.

ICSU Committee on Capacity Building in Science (CCBS)

This Committee met in Paris, France, on 21 June 1995 at the ICSU Headquarters. On this occasion, the outstanding problem discussed was the needs of scientists in developing countries;

the Visiting Professorship Programme and schools supported by the IUCr were deeply appreciated. An excellent feature of that meeting concerned the active interactions with Chairmen of Teaching Commissions of other scientific societies.

ICSU Committee on Data for Science and Technology (CODATA)

Introduction

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, 15 Scientific Unions, 5 co-opted Members and 29 Supporting Organizations.

Vital statistics

For the period of the report, number of members: 39, number of scientific meetings organized: 14, number of publications produced: 7 (3 Reports, 4 Newsletters) plus at least 4 World-Wide Web sites established including the main CODATA home page along with Task Group sites with contents ranging from symposium proceedings to directories to databases.

Organizational matters

The annual meetings of the Executive Committee and the Officers were held in conjunction with each other. This year, CODATA was reviewed in the ICSU cyclical evaluation process; documentation was assembled for presentation to the ICSU Review Committee. Upon receipt of their report, a detailed response was prepared for consideration by the ICSU Executive Board, which, at its fall meeting, approved the report and the continuation of CODATA.

In connection with CODATA's impact on the scientific, technical and medical community, an agreement was made with Springer-Verlag to become the publisher for CODATA's two monograph series, one relating generally to scientific aspects of data, the other relating more specifically to reference books of data.

In response to suggestions made in the ICSU evaluation report and to recommendations made in the Long Range Planning meeting held in 1994, CODATA embarked on a plan to organize current and select future Task Groups and Commissions more strategically. Other changes to integrate CODATA more fully into the activities of the Unions and to be more relevant to the outside world are under way. Finances continued to be troublesome as worldwide fiscal and political conditions made it difficult for some National Members to pay their dues on time. The Secretariat in Paris is maintained with a full-time Executive Director and part-time clerical assistance.

Activities undertaken during 1995

Scientific Meetings. 14 meetings were convened by Commissions and Task Groups, which focus on biology. The Commission on Standard Terminology for Access to Biological Data Banks (STABD) was particularly active with meetings taking place on three fronts: Species 2000, World ICTV Virus Database and Biological Terminology. The Steering Committee for Species 2000, a joint effort with IUBS and IUMS, developed plans for this worldwide program involving a federation of taxonomic databases covering, for instance, viruses, bacteria, marine invertebrate groups, vertebrates, insects, fungi, plants

and fossils. Spectacularly successful, this program has been adopted by UNEP as part of its Global Biodiversity Work Program and is the subject of major applications for funding. For the World Virus Database, meetings were required to support the standardization of virus names and characteristics. This activity has already attracted one grant of US\$50 000 and given rise to an application for another of US\$450 000. The terminology subgroup convened a workshop on Interdisciplinary Harmonization of Terminology for Microbial Spores, which brought together 20 international experts on spore morphology and physiology to develop a manual of definitions and instructions on accurate and standardized descriptors of spores. Here, grants of US\$45 000 from external sources were used to supplement those funds that CODATA could supply.

Task Groups. The Task Group on Biological Macromolecules convened a symposium and a technical workshop related, respectively, to the policies and technical problems of interlinking the major macromolecular databases. Keeping up with the times, the Group published the symposium proceedings on the WWW. Five other sponsors joined CODATA in providing funding for this symposium.

The second of the two meetings of the Task Group on Global Plant Checklist Network was particularly useful as it facilitated liaison between members of the Task Group and the Species 2000 Steering Committee as well as the International Working Group on Taxonomic Databases. This Group, too, is publicized on the WWW as described below under *Electronic Publication*.

The Task Group on Thermodynamic Data for Key Chemical Substances met in Paris in October 1995, bringing together experimental scientists from the primary calorimetric measurement laboratories in the world. The group prepared its initial reports on barium and strontium and their compounds in preparation for producing recommended values in 1996.

Likewise, the Task Group on Fundamental Constants met in Boulder in June 1995 to review available data pertaining to the fundamental constants together with the current experiments under way that were likely to yield useful results relevant to the constants in the next one to two years. The next least-squares adjustment of the constants is planned for 1998.

Publications

Data Access, CODATA Special Reports Series, No. 15 (1995), by the Working Group on Data Access.

In 1996, six books will be published, to be based in part on papers presented at the 14th International CODATA Conference in 1994.

The Task Group on Materials Database Management produced two reports, one of which will be adapted to become part of a book to be published in 1996. This report, entitled *The Costs of Building and Operating Numeric Databases: Results of a CODATA Survey*, is especially noteworthy in that it represents one of the first attempts to quantify the costs of developing and maintaining this type of database.

CODATA Newsletter, Nos. 70–73 (four issues; distribution of 6000 copies each).

Electronic publications - World-Wide Web Proceedings of the Symposium in Commemoration of B. Keil: Towards a Federation of Macromolecular Databases, May 1995 (URL <http://cis.gmu.edu/michaels/codata>).

The data model for the Checklist database, the Data Definitions document describing the fields for the database and

the Database of Plant Databases on the IOPI site at URL <http://iop.csu.edu.au/iopi>. The last item is an especially useful resource for those seeking information about what plant-based databases exist.

Fundamental Constants, the major product of the Task Group by that name, appears at many WWW sites throughout the world. World ICTV Virus Database is at URL <http://life.anu.edu.au:80/viruses/ictv.html>.

Special Projects. CODATA will investigate the issues of data exchange more systematically with a view to issuing a formal statement; CODATA formed a Working Group on Data Access, which met in March 1995 and produced their first report as cited above. The mandate is to examine problems, policies and possible solutions to the issue of international access and exchange of data for scientific research.

New areas of interest. A rapidly expanding area of interest is that associated with the Species 2000 program mentioned previously. From its early stages, the program has attracted interest from the United Nations Secretariat for the Convention on Biological Diversity. The Convention defines the rights of individual nations over their biological diversity but only a project such as Species 2000 can offer even the first steps towards a global catalogue of the diversity that exists.

Building on work initiated by the Working Group on Electronic Information Transfer, plans are being proposed to enhance CODATA's use of the WWW, especially as it relates to the dissemination of scientific and technical data. The IUCr delegate to CODATA is the current Chairperson of this Working Group.

Report of use of 1995 ICSU Grant and UNESCO Subvention

Under the Task Group on the Survey of Data Sources in Asian–Oceanic Countries, a Subgroup, on Asian–Oceanic Microbial Research Network, met in Beijing with members of the Asian Network on Microbial Research to discuss the needs and feasibility of a proposed information network for the study of microbial diversity in Asia, to be known as the Asian Microbial Information Network (AMIN). It is planned that AMIN should be functional by early 1997. 15 participants attended from Korea, Thailand, China and Japan.

The other Subgroups, Databases on Animal Viruses in Asian–Oceanic Countries and the Survey of Databases on Fishes in Asian–Oceanic Countries, carried on their activities without formal meetings in order to use travel funds most efficiently. As a by-product of the Task Group activities, it is expected that other countries from the region will be joining CODATA as National Members.

Task Group on Materials Database Management. The Task Group held a meeting in Paris where they evaluated work to date and made plans for the next biennium. Two reports of considerable interest, described above, were prepared during the year. One will be adapted to become part of a forthcoming book on materials.

Meetings

The 15th International CODATA Conference and General Assembly will be held in Tsukuba, Japan, 29 September–3 October 1996.

Conclusions 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 be reviewed and refined as an effective means of charting future directions.

In general, CODATA enjoyed an effective year. Its Task Groups and Commissions continued to be productive and some of the new work being proposed for approval at the next General Assembly is both scientifically important and exciting. 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.

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). New officers have been appointed by the ICSU Executive Board as of 1 January 1996: Chairman: R. Nichols (USA); Vice-Chairman: A.-M. Cetto (Mexico); Scientific Secretary: G. T. Thyagarajan (India).

A regional Secretariat for COSTED-IBN has been established in South Africa with the following aims: capacity building in research in basic and applied science; a concerted drive to encourage all countries of Southern and East Africa to join ICSU and COSTED-IBN; development of a framework for science and technology indicators for African countries; launching of the new Academy of Sciences of South Africa.

The question of including the countries of Central and Eastern Europe in the activities of COSTED-IBN was raised and it was agreed that this should be pursued as a matter of urgency.

ICSU Committee on Space Research (COSPAR)

The main activities of COSPAR were the preparations for the 31st COSPAR Scientific Assembly and Associated Events, held 14–21 July 1996 at the University of Birmingham, UK.

Finances

The audited accounts of the year 1995 are given at the end of this Report. For comparison, the figures for 1994 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 1995 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 744 005. This loss has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1995. 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 1995. The total of SwFr 365 159 with the banks at the end of the year was represented by US\$ 20 418 with Merrill Lynch, £156 454 with National Westminster Bank and SwFr 59 473 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 744 005 resulting from fluctuations in rates of exchange, have decreased during the year, from SwFr 5 352 197 to SwFr 5 224 690.

Transfers of SwFr 100 000, SwFr 50 000, SwFr 25 000, SwFr 50 000 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, the *International Tables* Fund and the General Fund, respectively. Transfers of SwFr 60 000 and SwFr 50 000 were made to the Research and Education Fund from the *Acta Crystallographica* Fund and the *Journal of Applied Crystallography* Fund, respectively. A transfer of SwFr 25 000 was made to the President's Fund from the General Fund. A transfer of SwFr 50 000 was made to the Ewald Fund from the General Fund. A transfer of SwFr 75 000 was made to the *Newsletter* Fund from the General Fund. A transfer of SwFr 200 000 was made to the *Journal of Synchrotron Radiation* Fund from the *Acta Crystallographica* 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 there is an additional entry for 'Movement in investment market value in the year'.

The General Fund account shows a profit of SwFr 139 839 before the transfers totalling SwFr 200 000 to the *Newsletter* Fund, the President's Fund, the Ewald Fund and the Publication and Journals Development Fund, as compared with a profit of SwFr 12 296 in 1994, before a transfer of SwFr 150 000 to the *Newsletter* Fund. The administrative expenses were SwFr 218 220 in 1995 as compared with SwFr 217 980 in 1994. Of this amount, SwFr 76 249 was charged to the publications of the Union.

SwFr 21 691 was given for general support of scientific meetings, in addition to SwFr 90 709 for financial support to young scientists attending meetings, which appears in the expenses of the Research and Education Fund, and SwFr 5964 in special grants from the President's Fund. SwFr 8107 was spent in assisting the work of the non-publishing Commissions. The expenses of the Union representatives on other bodies were SwFr 4601. The cost of the Finance Committee meetings held in 1995 was SwFr 12 870, while the Executive Committee meeting cost SwFr 24 822. The Union received SwFr 13 572 from the UNESCO subvention to ICSU. The subscriptions from Adhering Bodies were SwFr 147 991. Interest on bank accounts and investments credited to the General Fund was SwFr 219 918.

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 1704. Grants totalling SwFr 5964 were paid from the Fund.

The *Acta Crystallographica* account for 1995 shows a surplus of SwFr 181 465 before the transfer of SwFr 360 000

to other fund accounts, as compared with a surplus of SwFr 364 303 in 1994 before transfers of SwFr 200 000.

The subscription rates were increased for 1995. The number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 67 personal subscriptions, was 719. The number of paid subscriptions to *Sections A+B+C* of *Acta*, including 11 personal subscriptions, was 133. For 1994, the number of paid subscriptions to all sections of *Acta*, including 74 personal subscriptions, was 778. For the number of paid subscriptions to the separate sections of the journal, those to *Section A* decreased from 293 in 1994 to 285, those to *Section B* decreased from 222 to 217, those to *Section C* increased from 139 to 144 and those to *Section D* increased from 134 to 162. The cost of the technical editing office has been divided between the *Acta Crystallographica*, the *Journal of Applied Crystallography* and the *Journal of Synchrotron Radiation* accounts in percentages based on the number of text pages published during the year. The technical editing costs for *Acta Crystallographica* were SwFr 637 345 as compared with SwFr 620 283 in 1994. 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 77 743 before transfers of SwFr 100 000 to other fund accounts, as compared with a surplus of SwFr 10 642 in 1994 before transfers of SwFr 50 000. The number of subscriptions, including 107 personal subscriptions in 1994 and 105 in 1994, decreased from 931 in 1994 to 907 in 1995.

The *Journal of Synchrotron Radiation* Fund was started in 1995 and received a transfer of SwFr 200 000 from the *Acta Crystallographica* Fund. In 1995, the *Journal of Synchrotron Radiation* was distributed free of charge to existing subscribers to *Journal of Applied Crystallography* and *Section D* of *Acta Crystallographica*.

The *Structure Reports* series ended in 1993. The *Structure Reports* account shows a surplus of SwFr 14 391 in 1995 before

a transfer of SwFr 25 000 to the Publications and Journals Development Fund as compared with a surplus of SwFr 17 603 in 1994 before transfers of SwFr 95 000 to other fund accounts. The net income from sales was SwFr 14 391 in 1995 as compared with SwFr 18 120 in 1994.

The *International Tables* account shows a surplus of SwFr 156 576 before a transfer of SwFr 50 000 to the Publication and Journals Development Fund as compared with a surplus of SwFr 50 786 in 1994 before transfers of SwFr 75 000 to other fund accounts. The net sales income was SwFr 245 749 in 1995 as compared with SwFr 79 974 in 1994. 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. The main income and expense involved the Ninth Edition of the *World Directory of Crystallographers*, which was published in 1995.

The *Newsletter* Fund Account was started in 1994 and received transfers of SwFr 75 000 and SwFr 150 000 from the General Fund in 1995 and 1994, respectively. In 1995, the handling of the advertizing was transferred to the editorial office at Buffalo; in 1994 it had been handled by the American Institute of Physics and used to offset the printing costs.

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 170 246 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 a one-year project to develop an SGML implementation for the Union's journals are charged to this account. SwFr 90 709 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.

Auditors' Report to the International Union of Crystallography

We have audited the financial statements on pages 984 to 995 which have been prepared under the accounting policies set out on page 996.

Respective responsibilities of Executive Committee and Auditors

In accordance with the Statutes and By-laws of the International Union of Crystallography the Executive Committee is responsible for all the financial affairs of the Union and for appointing an external auditor, on the recommendation of the Treasurer, to audit 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 Unions affairs as at 31 December 1995 and of the excess of income over expenditure for the year then ended.

Deloitte & Touche Chartered Accountants
Liverpool, England
10 June 1996

General Fund Account for the year ended 31 December 1995

	1995	Swiss Francs	1994		1995	Swiss Francs	1994
Subscriptions to ICSU and ICSU bodies				Grant received from UNESCO			
Administration expenses:			7,340	subvention to ICSU	13,572	1,5750	
General Secretary and Treasurer:				Subscriptions from Adhering Bodies	147,991	148,000	
Honorary and secretarial	8,214	9,333		Income from investments (Note 7)	177,652	188,124	
Audit and accountability charges	29,959	26,796		Profit on disposal/redemption of	42,266	44,854	
Legal and professional fees	4,867	1,721		investments (Note 8)	23,076	-	
Postage and sundries	(121)	1,030		Amounts charged to the following			
Travelling expenses	6,520	7,105		journals and publications:			
Bank charges	1,506	1,878		<i>Acta Crystallographica</i>	63,287	55,889	
Executive Secretary's office:				<i>Journal of Applied</i>	9,150	13,110	
Salaries and expenses	166,879	167,866		<i>Journal of Synchrotron</i>			
Depreciation of office equipment	396	2,251	217,980	<i>Radiation</i>	3,812	68,999	
		218,220					
Seventeenth General Assembly and							
Congress							
Expenses	136	2,797					
Programme Committee	18,445	-					
Meeting of the Executive Committee	24,822	21,520					
Finance Committee expenses	12,870	7,924					
Travel Expenses of IUCr Representatives							
on other bodies	4,601	9,368					
STAR/CIF	4,265	9,940					
Commission expenses	8,107	16,028					
Sponsorship of meetings	21,691	27,866					
President's secretary	19,161	20,778					
Transfers to other Funds:							
<i>Newsletter</i> Fund	75,000	150,000					
President's Fund	25,000	-					
Ewald Fund	50,000	-					
Publications and Journals							
Development Fund	50,000	-					
IUCr/FTZ agreement	1,860	-	266,221				
		315,958					
Loss on disposal/redemption of							
investments (Note 8)		-	111,890	Excess of expenditure over income	60,161	137,704	
		540,967	603,431	carried to summary below left			
					540,967	603,431	
Balance at 1 January		980,148	929,049				
Difference between income and	(60,161)	(137,704)					
expenditure							
Movement in investment market value in	440,128	268,328	130,624				
the year (Note 5)			(79,525)				
Fluctuations in rates of exchange			980,148				
Balance at 31 December		1,190,554					

President's Fund Account for the year ended 31 December 1995

	Swiss Francs		Swiss Francs	
	1995	1995	1995	1994
Grants	5,964	18,284	1,704	2,162
			25,000	-
			174	-
			-	16,122
			<u>26,878</u>	<u>18,284</u>
<i>Excess of income over expenditure carried to balance sheet</i>	20,914	-		
	<u>26,878</u>	<u>18,284</u>		
Balance at 1 January	34,363	54,324		
Difference between income and expenditure	20,914	(16,122)		
Fluctuations in rates of exchange	(6,891)	(3,839)		
Balance at 31 December	<u>48,386</u>	<u>34,363</u>		

Acta Crystallographica Account for the year ended 31 December 1995

	Swiss Francs		Swiss Francs	
	1995	1994	1995	1994
Publication expenses:				
Printing and binding Volume 51 (1994 Volume 50)	721,857	613,783	1,892,514	1,921,146
Distribution and postage	92,158	90,978	15,545	32,325
Airfreight costs	40,460	41,739	53,271	55,316
	<u>854,475</u>	<u>746,500</u>	<u>5,338</u>	<u>1,806</u>
Net loss on reprints Index to Volume 50 (1994 Volume 49)	15,127	-	1,966,668	2,021,638
Supplement to Volume A49 Microfiche costs	2,380	2,356		
	<u>88</u>	<u>6,427</u>		
		85		
		<u>755,368</u>		
Editorial expenses:			133,952	136,751
Editorial honoraria	55,911	47,674		
Secretarial assistance	6,462	17,708		
Postage, travel and sundries	16,697	25,208		
Technical Editing:				
Salaries and expenses	607,218	594,730		
Computer expenses	27,483	21,660		
Depreciation of office equipment	2,644	3,893		
		<u>716,415</u>		
Administration expenses recharged from				
General Fund		63,287		
Transfers to other Funds:				
Publications and Journals				55,889
Development Fund	100,000			
Research and Education Fund	60,000			
Journal of Synchrotron Radiation Fund	200,000			200,000
			178,535	-
			<u>2,011,772</u>	<u>1,886,433</u>
Excess of income over expenditure - see below				
			178,535	-
			<u>2,011,772</u>	<u>1,886,433</u>
Balance at 1 January	1,943,228	1,996,023		
Difference between income and expenditure	(178,535)	164,303		
Fluctuations in rates of exchange	(219,997)	(217,098)		
Balance at 31 December	<u>1,544,696</u>	<u>1,943,228</u>		

Journal of Synchrotron Radiation Account for the year ended 31 December 1995

	Swiss Francs 1995	Swiss Francs 1995
Publication expenses:		
Printing and binding Volume 2	62,622	
Distribution and postage	12,306	
Airfreight costs	8,977	
	<u>83,905</u>	
Net loss on reprints	108	
Editorial expenses:		
Editorial honoraria	6,317	
Secretarial assistance	2,760	
Postage, travel and sundries	2,441	
Technical Editing:		
Salaries and expenses	40,306	
Computer expenses	1,656	
Depreciation of office equipment	159	
Administration expenses recharged from General Fund	53,639	
	3,812	
	<u>81,722</u>	
<i>Excess of income over expenditure</i>	<u>223,186</u>	
– see below		<u>223,186</u>
Balance at 1 January	81,722	
Difference between income and expenditure	(10,186)	
Fluctuations in rates of exchange		
Balance at 31 December	<u>71,534</u>	<u>8,874</u>
		<u>14,312</u>
		<u>200,000</u>
		<u>10,031</u>
		<u>613</u>
		<u>10,644</u>
		<u>1,770</u>
		<u>8,874</u>
		<u>14,312</u>
		<u>200,000</u>

Structure Reports Account for the year ended 31 December 1995

	1995	Swiss Francs 1994	1995	Swiss Francs 1994
Publication expenses:				
Printing and binding (1994 Volumes 47B and 50B)	-	517		
Transfers to other funds:				
Research and Education Fund	-	25,000		
Publications and Journals Development Fund	25,000	45,000		
Ewald Fund	-	25,000	5,056	6,184
	<u>25,000</u>	<u>95,000</u>	<u>14,391</u>	<u>18,120</u>
<i>Excess of income over expenditure - see below</i>	-	-	10,609	77,397
	<u>25,000</u>	<u>95,517</u>	<u>25,000</u>	<u>95,517</u>
Balance at 1 January	108,833	198,389		
Difference between income and expenditure	(10,609)	(77,397)		
Fluctuations in rates of exchange	(12,245)	(12,159)		
Balance at 31 December	<u>85,979</u>	<u>108,833</u>		

International Tables Account for the year ended 31 December 1995

	1995		1994		1995		1994	
	Swiss Francs		Swiss Francs		Swiss Francs		Swiss Francs	
Publication expenses:								
Printing and Typesetting Volume A	36,619	-	-	-	175,068	12,918		
Printing and Typesetting Volume C	38,225	74,844	-	-	32,248	63,512		
Editorial expenses:								
Editorial honoraria	3,085	6,500			4,711	6,103		
Secretarial assistance, postage and office equipment	7,619	19,466			4,362	5,399		
Technical Editing	3,625	3,222		29,188	118,185	20,141		
Transfers to other funds:					334,574	108,073		
Research and Education Fund	-	25,000						
Publications and Journals Development Fund	50,000	50,000		75,000	88,825	28,099		79,974
<i>Excess of income over expenditure - see below</i>	106,576	245,749	-	104,188	-	-		24,214
								104,188
Balance at 1 January	195,075		241,083					
Difference between income and expenditure	106,576		(24,214)					
Fluctuations in rates of exchange	(37,606)		(21,794)					
Balance at 31 December	264,045		195,075		245,749			104,188

Book Fund Account for the year ended 31 December 1995

	Swiss Francs			Swiss Francs	
	1995	1994		1995	1994
Publication expenses:			Sales of copies, net of		
Book series expenses	-	204	Publisher's commission on sales	857	1,153
Atlas of Crystallography	-	300	Atlas of Crystallography (1995 net)	25,548	-
World Directory of Crystallographers			9th Edition	1,178	1,550
9th Edition	24,134	9,713	Sundry publications		
			Royalties	2,017	4,035
			IUCr/OUP Book series		
Excess of income over expenditure	5,466	-	Excess of expenditure over income	-	3,479
- see below			- see below left		
	<u>29,600</u>	<u>10,217</u>		<u>29,600</u>	<u>10,217</u>
Balance at 1 January	8,839	13,305			
Difference between income and expenditure	5,466	(3,479)			
Fluctuations in rates of exchange	(1,783)	(987)			
	<u>12,522</u>	<u>8,839</u>			
Balance at 31 December					

Publications and Journals Development Fund Account for the year ended 31 December 1995

	Swiss Francs		Swiss Francs	
	1995	1994	1995	1994
Expenses:				
Computer expenses:				
Purchase of computer equipment and software	57,462	96,774	50,000	25,000
Programming and development	112,784	120,910	25,000	45,000
	170,246	217,684	50,000	50,000
			100,000	100,000
Electronic Publishing Committee/ Section Editors Meeting	17,047	16,029	275,000	220,000
JSR expenses (1995 - page 989)	-	132,817	22,112	23,477
Electronic Publishing Project	4,597	-	-	-
	105,222	-	-	123,053
<i>Excess of income over expenditure - see below</i>	297,112	366,530	297,112	366,530
Balance at 1 January	556,554	741,785		
Difference between income and expenditure	105,222	(123,053)		
Fluctuations in rates of exchange	(82,501)	(62,178)		
Balance at 31 December	579,275	556,554		

Research and Education Fund Account for the year ended 31 December 1995

	Swiss Francs		Swiss Francs	
	1995	1994	1995	1994
Expenses:				
Young Scientists' Support	90,709	83,728	60,000	100,000
1989 ECM Fund creditor	-	1,024	50,000	25,000
Visiting Professorship Programme	3,861	6,668	-	25,000
	94,570	91,420	-	175,000
			110,000	39,652
<i>Excess of income over expenditure - see below</i>	56,965	123,232	41,535	214,652
	151,535	214,652	151,535	214,652
Balance at 1 January	787,530	752,281		
Difference between income and expenditure	56,965	123,232		
Fluctuation in rates of exchange	(105,191)	(87,983)		
Balance at 31 December	739,304	787,530		

Ewald Fund Account for the year ended 31 December 1995

	Swiss Francs		Swiss Francs	
	1995	1994	1995	1994
Selection Committee and expenses	632	103		
			Transfers from other funds: <i>Structure Reports</i> General Fund	25,000
				25,000
<i>Excess of income over expenditure</i> - see below	65,556	40,499	Investment income (Note 7)	16,188
	66,188	40,602	<i>Excess of expenditure over income</i> - see below left	
				40,602
Balance at 1 January	270,428	260,141		
Difference between income and expenditure	65,556	40,499		
Fluctuations in rates of exchange	(41,886)	(30,212)		
Balance at 31 December	294,098	270,428		

Newsletter Fund Account for the year ended 31 December 1995

	Swiss Francs		Swiss Francs	
	1995	1994	1995	1994
Editorial honoraria	4,060	4,375	Income from advertisements	
Editorial expenses	20,974	29,998	Reimbursement for CGA-17	
Newsletter printing and distribution	96,053	56,039	second circular	
Advertising costs	11,517	-	Transfers from other funds: General Fund	150,000
				75,000
<i>Excess of income over expenditure</i> - see below	5,511	59,588		
	138,115	150,000		
Balance at 1 January	53,599	-		
Difference between income and expenditure	5,511	59,588		
Fluctuation in rates of exchange	(7,369)	(5,989)		
Balance at 31 December	51,741	53,599		

Cash Flow Statement for the year ended 31 December 1995

		Swiss Francs	
	Note	1995	1994
Net cash outflow from operating activities (see below)		(243,902)	(221,604)
Returns on investments			
Interest received		42,266	44,854
Investment income		259,191	269,017
Net cash inflow from returns on investments		301,457	313,871
Investing activities			
Purchase of fixed assets		(65,404)	(1,663)
Purchase of investments	5	(666,238)	(681,186)
Disposal of investments	8	511,189	372,146
Net cash outflow from investing activities		(220,453)	(310,703)
Decrease in cash and cash equivalents	10	(162,898)	(218,436)
Reconciliation of excess of income over expenditure to net cash outflow from operating activities			
Excess of income over expenditure		616,498	234,623
Deduct:			
Increase in market value of investments	5	(440,128)	(268,328)
Operating profit/(loss) before fluctuations in rate of exchange		176,370	(33,705)
Exchange rate fluctuations attributable to operating activities	9	(119,833)	(36,721)
Interest received	6	(42,266)	(44,854)
Investment income	7	(259,191)	(269,017)
(Profit)/loss on disposal of investments	8	(23,076)	111,890
Depreciation charges		3,581	7,058
(Increase)/decrease in debtors		(71,695)	70,645
Increase/(decrease) in creditors		92,208	(26,900)
Net cash outflow from operating activities (see above)		(243,902)	(221,604)

Notes to the Accounts

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 of existing leasehold premises 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.

(iii) Leasehold property improvements related to new leases are depreciated over the term of the lease.

(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.

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:

	1995	1994
Netherland Guilders	1.3534	1.3258
Danish Crowns	4.7847	4.6364
Pounds Sterling	0.5618	0.4848
US Dollars	0.8621	0.7476

The net assets of the Union at 1 January 1995 (Sw Fr 5,352,197) would have had the value of US \$4,001,302 or £2,594,745 if expressed in those currencies.

At 31 December 1995, these net assets (Sw Fr 5,224,690) would have had the value of US \$4,504,205 or £2,935,231 respectively, being an increase of US \$502,903 or an increase of £340,486 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. Tangible fixed assets

	Leasehold property improvements Sw Fr	Office equipment Sw Fr	Total Sw Fr
Cost			
As at 1 January 1995	-	14,320	14,320
Additions	57,790	7,614	65,404
As at 31 December 1995	57,790	21,934	79,724
Accumulated depreciation			
As at 1 January 1995	-	7,055	7,055
Charge for year	-	3,581	3,581
As at 31 December 1995	-	10,636	10,636
Net book value 31 December 1995	57,790	11,298	69,088
1 January 1995	-	7,265	7,265

5. Investments

Swiss Francs

	Holding at market value 1 January 1995	Additions during the year	Disposals/ redemptions during the year	Fluctuations in rates of exchange	Increase/ (decrease) in market value	Holding at market value 31 December 1995	Holding at revalued cost 31 December 1995	Holding at revalued cost 31 December 1994
Held by Merrill Lynch								
Corporate Government Securities								
GNM P146535-2016 (US\$)	5,739	-	(93)	(695)	290	5,241	4,741	5,498
4,232 Units								
GNM P169332-2016 (US\$)	36,600	-	(6,340)	(4,437)	1,729	27,552	24,924	35,043
22,247 Units								
ML Capital Fund/CLB (US\$)	124,762	-	(107,748)	(17,014)	-	-	-	118,874
3,730 Units								
Hausmann Holdings (US\$)								
443 Units	362,923	-	-	(43,990)	79,554	398,487	202,412	200,991
Global Allocation Portfolio Class A (US\$)								
5,700 Units	75,691	-	-	(9,174)	14,612	81,129	69,757	79,378
Meridian Funds Global Government Fund (US\$)								
9,503 Units	127,453	10,157	-	(15,449)	7,482	129,643	139,898	147,735
Permal Investment Holdings NV (US\$)								
77 Units	131,547	-	-	(15,945)	25,839	141,441	117,943	134,211
Meridian Charter Income Fund (US\$)								
12,234 Units	143,612	9,098	-	(17,407)	11,989	147,292	149,208	159,487
British Gas Finance (US\$)								
75,000 Units	100,430	-	-	(12,174)	4,133	92,389	89,453	101,792
GEC (US\$)								
75,000 Units	98,984	-	-	(11,998)	624	87,610	87,797	99,907
US Treasury Note 6.875% (US\$)								
100,000 Units	130,226	-	-	(15,785)	3,045	117,486	116,168	132,592
US Treasury Bill 0% (US\$)								
179,000 Units	231,531	-	(199,958)	(31,573)	-	-	-	230,384
Lehman Brothers Holdings (US\$)								
80,000 Units	-	90,168	-	1,582	1,375	93,125	91,750	-
ECS Capital Portfolio CLB (US\$)								
20,764 Units	-	236,709	-	4,153	20,715	261,577	240,862	-
Held by Foreign & Colonial								
Reserve Asset Fund Class D (US\$)								
16,887 Units	488,252	32,073	-	(59,182)	34,411	495,554	472,636	501,331
Reserve Asset Fund Class L (£)								
21,581 Units	490,370	123,119	-	(67,268)	74,123	620,344	508,439	446,582
Reserve Asset Fund Class X (£)								
9,581 Units	476,258	15,119	(173,974)	(65,333)	(67)	252,003	262,317	496,937
Reserve Asset Fund Class C (US\$)								
25,471 Units	550,989	27,540	-	(66,786)	41,419	553,162	545,078	588,922
Reserve Asset Fund Class M (US\$)								
11,080 Units	271,982	14,914	-	(32,967)	51,754	305,683	249,308	266,724
Reserve Asset Fund Class E (£)								
7,937 Units	170,701	106,408	-	(23,417)	10,086	263,778	272,356	192,332
Reserve Asset Fund Class N (Yen)								
17,828.27 Units	152,063	933	-	(20,749)	(2,941)	129,306	133,067	153,013
UK Treasury 7.75% 22.9.2006 (£)								
375,000 Units	718,504	-	-	(98,564)	59,956	679,896	707,082	819,500
	4,888,617	666,238	(488,113)	(624,172)	440,128	4,882,698	4,485,196	4,911,233

6. Bank interest

	Swiss Francs			
	1995		1994	
National Westminster Bank PLC				
Manchester Business Reserve Account	7,487		4,710	
Manchester Capital Reserve Account	10,661	18,148	13,820	18,530
Merrill Lynch				
CMA Account	7,055		8,123	
Foreign & Colonial				
Cash balance	657		182	
Petty cash accounts	8		3	
Interest from Munksgaard	16,398	17,063	18,016	18,201
Allocated to General Fund	42,266		44,854	

7. Investment income

	Swiss Francs			
	1995		1994	
GNM P146535-2016	456		885	
GNM P169332-2016	2,679		3,771	
ML Capital Fund/CLB	-		10,248	
Hausmann Holdings	1,028		4,425	
Meridian Funds Global - Government Fund	10,157		15,211	
Meridian Charter - Income Fund	9,098		12,324	
British Gas Finance	8,072		9,056	
GEC	6,704		7,914	
US Treasury Note 6.875% 31.10.1996	7,872		-	
Foreign and Colonial - Reserve Asset Fund Class D	32,073	35,376		
Foreign and Colonial - Reserve Asset Fund Class L	34,119	29,367		
Foreign and Colonial - Reserve Asset Fund Class X	15,119	29,088		
Foreign and Colonial - Reserve Asset Fund Class C	27,540	39,955		
Foreign and Colonial - Reserve Asset Fund Class M	14,914	11,550		
Foreign and Colonial - Reserve Asset Fund Class E	17,408	13,513		
Foreign and Colonial - Reserve Asset Fund Class N	933	855		
Lehman Brothers	3,200	-		
UK Treasury 7.75% 22.9.2006	54,889	45,479		
UK Treasury 7.75% 22.9.2006 - Tax on 1994 income	12,930	-		
	259,191	269,017		
Allocated to:				
President's Fund	1,704	2,162		
Ewald Fund	16,188	15,602		
Publication and Journals Development Fund	22,112	23,477		
Research and Education Fund	41,535	39,652		
Balance left in General Fund	177,652	188,124		
	259,191	269,017		

8. Profit/(loss) on disposal/redemption of investments

	Swiss Francs	
	1995	1994
Proceeds	511,189	372,146
Book value	488,113	484,036
Profit/(loss) allocated to General Fund	23,076	(111,890)

Book value represents market value at 1 January 1995.

9. Exchange rate fluctuations attributable to operating activities

	Swiss Francs	
	1995	1994
Total fluctuations in exchange rates dealt with in fund accounts	(744,005)	(567,972)
Adjustments for exchange differences attributable to:		
Investments	624,172	482,831
Fixed assets	-	1,117
Cash and bank balances	-	47,303
Attributable to operating activities	(119,833)	(36,721)

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

	Swiss Francs	
	1995	1994
Balance at 1 January 1995	562,935	828,674
Net cash (outflow)/inflow	(162,898)	(218,436)
Fluctuations in rates of exchange on cash and bank balances	-	(47,303)
Balance at 31 December 1995	400,037	562,935

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

	Swiss Francs			
	1995	1994	Change 1995	Change 1994
Cash at bank and in hand	400,037	562,935	(162,898)	(265,739)

12. Capital commitment

	Swiss Francs	
	1995	1994
Contracted for but not provided	34,491	-
Authorized but not yet contracted for	35,600	-

13. Operating lease commitments

At 31 December 1995, the Union was committed to making the following payments during the next year in respect of operating leases.

	Land and buildings	Other
	Swiss Francs	Swiss Francs
Leases which expire:		
within two to five years	64,080	5,511
after five years	-	-
	64,080	5,511

Income and Expenditure Account for the year ended 31 December 1995

Income	Note	Swiss Francs			Note	Swiss Francs		
		1995	1994			1995	1994	
Income								
Membership subscriptions		147,991	148,000					
Sales								
Journals	2,290,217		2,318,524		170,246		217,684	
Books	364,174		114,811					
Back numbers and single issues	39,298	2,693,689	60,413	2,493,748	17,047		16,029	
Investment income								
Income from investments	7	259,191	269,017		4,597	191,890	-	233,713
Bank interest	6	42,266	44,854					
Profit on sale of investments	8	23,076	-	313,871				
Other income								
Grants		13,746	15,750					
Royalties and copyright fees		6,434	3,468					
Advertising income		61,725	2,040					
Reimbursement for CGA-17 second circular		17,048	98,953	21,258				
TOTAL INCOME		3,265,166	2,976,877					
Expenditure								
Journals								
Publication costs	1,236,290		1,059,457					
Editorial expenses	98,133		111,865					
Technical editing	777,373	2,111,796	740,069	1,911,391				
Books								
Publication costs	192,859		45,017					
Editorial expenses	14,329		25,966					
Technical editing	-	207,188	3,222	74,205				
Newsletter								
Publication costs	107,570		56,039					
Editorial expenses	25,034	132,604	34,373	90,412				
<i>Journal of Synchrotron Radiation</i> costs		-		132,817				
President's Fund								
Grants and Young Scientists' support		96,673		102,012				
General Assembly costs		18,581		2,797				
Committee meetings and expenses		38,324		29,547				
Carried forward		2,605,166		2,343,181				
Expenditure (cont.)								
Brought forward						2,605,166		2,343,181
Publications and journals development General					170,246		217,684	
Electronic Publishing Committee/Section Editors meeting expenses					17,047		16,029	
Electronic publishing project					4,597	191,890	-	233,713
Subscriptions paid						6,789		7,340
Visiting Professorship Programme						3,861		6,668
ECM creditor						-		1,024
Administration expenses:								
General Secretary and Treasurer:								
Honorarium and secretarial assistance					8,214		9,333	
Audit and accountancy charges					29,959		26,796	
Legal and professional fees					4,867		1,721	
Postage and sundries					(121)		1,030	
Travelling expenses					6,520		7,105	
Bank charges					1,506		1,878	
Executive Secretary's office: Salaries and expenses					166,879		167,866	
Travel expenses of IUCr representatives on other bodies					4,601		9,368	
STAR/CIF Commission expenses					4,265		9,940	
Sponsorship of meetings					8,107		16,028	
President's secretary IUCr/FLZ agreement					21,691		27,866	
Loss on sale of investments					19,161	277,509	-	299,709
Depreciation					1,860			
Loss on sale of investments	8					-		111,890
Depreciation						3,581		7,057
TOTAL EXPENDITURE		3,088,796		3,010,582				
<i>Excess/(deficit) of income over expenditure</i>						176,370		(33,705)
Increase in market value of investments	5					440,128		268,328
Excess before fluctuation in rates of exchange (page 984)						616,498		234,623