

## International Union of Crystallography

### Report of the Executive Committee for 1996

#### Seventeenth International Congress and General Assembly

The Seventeenth General Assembly and International Congress of Crystallography were held at the Washington State Trade and Convention Center, Seattle, USA, 8–17 August 1996, by invitation of the US National Committee for Crystallography, in collaboration with the American Crystallographic Association and the US National Academy of Sciences – National Research Council. A report, including a detailed report of the General Assembly, has been published in *Acta Crystallographica Section A* [*Acta Cryst.* (1997), **A53**, 692–748].

The General Assembly and Congress were attended by 2311 scientists, 252 accompanying members and 150 exhibitors from 51 countries. The Fourth Ewald Medal and Prize were presented to Professor M. G. Rossmann at the Opening Ceremony. There were 24 Keynote Lectures and 104 Microsymposia and open Commission meetings. Nobel Laureate talks were presented at lunch times and the early afternoons were reserved for poster sessions. There were two evening sessions and three Workshops. The abstracts in the published book of Collected Abstracts were prepared from hard-copy and electronic submissions and these abstracts also appeared as a Supplement to *Acta Crystallographica*, Volume 52, dated 1 September 1996. A commercial exhibition comprising 33 companies, booksellers and software demonstrations was organized.

The General Assembly met on the evenings of Saturday 10 August, Sunday 11 August and Wednesday 14 August. The proposed changes to Statutes 3-2 and 3-3 to allow the admission of the Academy of Sciences Located in Taipei were approved. Applications for membership of the IUCr from the Academy of Sciences Located in Taipei (Category II) and from the Korean Federation of Science and Technology Societies (Category I) were accepted. The Minutes of the Sixteenth General Assembly in 1993 were approved. Proposed changes to Statutes 5-4 and 5-5 to allow postal ballots of the General Assembly were approved. Proposed changes to the By-Laws to incorporate the existence of the Finance Committee, to establish officially the position of Convener and to incorporate the existence of the Sub-committee on the Union Calendar were approved. It received the triennial financial report and the reports of the Executive Committee, the Commissions, the Scientific Associates and Regional Associates and the Union Representatives on Other Bodies since the Sixteenth General Assembly in 1993. New Officers of the Union, Chairmen and members of Commissions and Union Representatives were elected; the full list of these people will be given as an Annex to the report of the Seventeenth General Assembly and Congress. A Commission on XAFS and a Commission on Small-Angle Scattering were established. The Commission on Crystallographic Data was terminated and replaced by a Committee on Crystallographic Databases. The Commission on Crystallographic Apparatus was renamed Commission on High Pressure and the Commission on Small Molecules was renamed Commission on Structural Chemistry. The report of the Chairman of the Sub-committee on Electronic Publishing, Dissemination and Storage of Information was accepted. The good progress of the IUCr/Oxford University Press Book Series

was noted. The General Assembly approved the recommendation that the unit contribution should remain unchanged at CHF 1000 for the years 1997–1999 inclusive. It reaffirmed its decision to hold the Eighteenth General Assembly and Congress in Glasgow, UK. It also provisionally accepted an invitation from the Israel Crystallographic Society to hold the Nineteenth General Assembly and Congress in Jerusalem, Israel, in 2002.

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

#### Other meetings

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

IUCr Satellite Meeting on Powder Diffraction, Denver, Colorado, USA, 3–8 August.

IUCr Satellite Meeting on Synchrotron Radiation, Argonne, Illinois, USA, 4–7 August.

IUCr Satellite Meeting on Neutron Scattering, Gaithersburg, Maryland, USA, 5–7 August.

Summer School on Crystallographic Computing, Bellingham, Washington, USA, 17–22 August.

Other meetings held in 1996 and sponsored by the Union were:

Winter Workshop on Electron Diffraction and Imaging at Surfaces, Scottsdale, Arizona, USA, 3–6 January.

International Symposium on Ferroic Domains and Mesoscopic Structures, Vienna, Austria, 25–30 March.

School on X-ray and Neutron Dynamical Diffraction – Theory and Applications, Erice, Italy, 9–21 April.

3rd European Symposium on X-ray Topography and High Resolution Diffraction, Palermo, Italy, 22–24 April.

School on Experimental and Computational Approaches in Structure Based Drug Design, Erice, Italy, 8–19 May.

#### Executive Committee

The membership of the Executive Committee, including new members elected at the General Assembly in 1996, is as follows:

President: Professor E. N. Baker (New Zealand); Vice-President: Dr R. Chidambaram (India); General Secretary and Treasurer: Professor S. Larsen (Denmark); Immediate Past President: Professor P. Coppens (USA); Ordinary members: Professor L. A. Aslanov (Russia), Professor J. C. A. Boeyens (South Africa), Professor H. Fuess (Germany), Professor M. Hart (USA), Professor H. Schenk (The Netherlands), Professor M. Tanaka (Japan).

#### Publications

Volume 52 of *Acta Crystallographica*, Volume 29 of *Journal of Applied Crystallography*, Volume 3 of *Journal of Synchrotron Radiation*, the Fourth, revised edition of Volume A, the Fourth,

revised and enlarged *Brief Teaching Edition* of Volume A, and a revised edition of Volume B of *International Tables for Crystallography* 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 Seventeenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (1997), A53, 692–748].

### Work of the Commissions

#### *Commission on Journals*

In 1996, Professor C. E. Bugg retired as Editor-in-Chief and Chairman of the Commission at the Seattle General Assembly. He was succeeded by Professor J. R. Helliwell, who wishes to thank the outgoing Editor-in-Chief, on behalf of the whole Editorial Board and the Chester staff, for his excellent work in the last 12 years and for ensuring a smooth hand over. Again, 1996 was a relatively stable year for the journals, with no major changes instituted.

Volume 52 of *Acta Crystallographica (Acta)* included 1702 papers with an overall total of 6596 pages representing an increase of 8% over 1995. The number of papers received by the Managing Editor in Chester was 1336. Median publication times generally improved by 4–6 weeks, and were, for full articles in *Section A* (4.7 months), *Section B* (6.5 months), *Section C* (5.1 months) and *Section D* (5.2 months). Volume 29 of the *Journal of Applied Crystallography (JAC)* contained 131 papers with an overall total of 759 pages and a median publication time for Full Articles of 6.1 months. Volume 3 of the *Journal of Synchrotron Radiation (JSR)* included 45 papers in its second year of full publication and comprised 326 pages with a median publication time of 2.9 months. All of the IUCr journals are taking advantage of electronic communication (e-mail and ftp) to speed up editorial review. Also, the cooperation of authors in submitting final versions of their manuscripts on diskette has assisted production efficiency of issues as well as their quality.

The individual Editors' comments are summarized below. The dedicated efforts of Co-editors and of the editing staff in Chester have again been outstanding and high quality of the articles and subsequent technical production has been realized. This has been accompanied by new initiatives involving electronic publishing (including the WWW) as well as more detailed (and yet more automatic) checking of structures. Moreover, major conference proceedings, such as SRI-97, as well as special issues on focused topics, are in preparation. Finally, links with database centres are being extended, in association with the IUCr Committee on Crystallographic Databases.

The summary over *Acta*, *JAC* and *JSR* is as follows. The total number of pages published in 1996 was 7681, which compares with 7067 in 1995 and 5786 in 1994. The number of manuscripts submitted to the journals was 2031 (up from 1800 in 1995 and 1768 in 1994). Electronic submission of CIFs for *Section C* of *Acta* increased during the year to 97% and is now mandatory. Significant gains in publication times were made, typically of 4–6 weeks.

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

*Section A* contained 96 articles in 1010 pages during 1996. This included 2 Lead Articles, 2 Topical Reviews and 85 Research Papers. *Section A* remains in a steady state and a popular vehicle for papers on the foundations of crystallography. Authors are required to send their manuscript in machine-readable form as part of a continuous effort to reduce publication time. It is hoped that more Lead Articles and Topical Reviews will be received and the Editor will welcome any suggestion.

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

*Section B* published 1078 pages in 1996, comprising 125 Full Articles, 4 Short Communications and 1 Topical Review. These figures are almost identical to 1995 data and indicate that *Section B* has fully recovered from a decrease in submissions that accompanied the launch of *Section D*. Since the 1995 data included 22 papers arising from a special symposium issue, it appears that *Section B* is on a gradual rising trend from 1993/1994. An increase in papers discussing inorganic materials, results using novel experimental techniques and database studies is noted. Thus, there is continued strong support for *Section B* as a valuable outlet for high-quality papers in structural crystallography.

Although a delicate balance between review material and original research must be preserved in a primary journal, it proved difficult to attract suitable Topical Reviews in 1994/1995. This situation has been rectified, and a number of high-quality articles have now been commissioned.

Publication times from the date of original submission are a matter for some concern, even though *Section B* is a bi-monthly journal. While delays are sometimes caused by the slow response of authors to the comments of referees or Co-editors, the journal is now requiring, whenever possible, (a) all crystallographic data in CIF format, and (b) word processor versions of the final accepted manuscript. Such information is readily available in the vast majority of cases and will significantly speed the processing of accepted manuscripts.

I should like to thank all Co-editors, referees and the editorial staff at Chester for their work on behalf of *Section B* and, of course, the authorship for choosing to publish their work in the journal.

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

The *Section C* Editorial Board has been successful with all of its key objectives for the last triennium. It has increased its authorship from a low of 852 papers in 1994 to 1289 papers (1511 structures and 3262 pages) in 1996. It completed the transition to fully electronic submissions in May of 1996. During this period, the CIF approach has become the industry standard for exchanging, archiving and handling data in the structural sciences, and is widely used by other journals and databases.

An important part of the CIF submission process to *Acta* is the archiving of these files at the Chester Office and their availability to the crystallographic community over the Internet. Currently there are over 5000 *Section C* CIFs in this archive and it is increasing at a rate of over 100 CIFs per month. This is an extremely valuable scientific resource for the community and the IUCr in the future.

The size of the *Section C* issues grew quickly in 1996 for three main reasons. First, its initiative to provide for electronic submissions (and the associated services for checking and printing the manuscripts) has been very popular and is, in fact,

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
A48	1992	954	117	106	7.9 } 7.7	11	2.2 } 1.7
B48		856	125	113		12	
C48		2280	914	906		8	
A49§	1993	901	121	108	7.9 } 7.7	13	2.1 } 2.0
B49		1075	155	149		6	
C49		2186	880	869		11	
D49		604	72	62		10	
A50	1994	798	103	91	8.1 } 7.7	12	1.4 } 2.1
B50		782	99	94		5	
C50		2102	852	847		5	
D50		920	135	121		14	
A51	1995	952	125	111	8.3 } 8.1	14	1.6 } 1.8
B51		1104	133	128		5	
C51		2726	1091	1087		4	
D51		1106	145	137		8	
A52§	1996	1010	96	85	10.4 } 9.1	11	1.8 } 2.5
B52		1078	130	126		4	
C52		3262	1289	1284		5	
D52		1246	187	109		78	

*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
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
29	1996	759	131	84	7.5	5	3.0	5	4.4	17	2.6	20	2.3

*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
3	1996	326	45	43	6.9	2	3.5	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, and Volume A52 includes, in addition, 688 pages of abstracts communicated to the Seattle Congress. ¶Laboratory Notes, Cryocrystallography Notes, Letters to the Editor, Meeting Reports and Computer Program Abstracts.

being adopted by other journals. Second, there is an accelerating number of structures determined due to better instrumentation and faster computers. Third, the reputation of *Section C* in the structural science community as a provider of concise and well checked structural information is important for many authors.

It was clear, however, that, in the absence of a commensurate growth in journal income (either from increased or higher subscriptions), this growth could not be sustained. This is especially true at a time of some uncertainty for the scientific journal industry when subscriptions are decreasing and publishing costs are soaring. These factors are important in determining the viability of a journal independently of its scientific reputation. Submission and delivery modes are also changing with a shift from the traditional print-on-paper approaches to electronic services and presentation modes. *Section C* is well placed to compete both scientifically and financially in the changing scientific publication market as it is already a leader in using and determining the new publication technologies.

These considerations were foremost in the discussions of the *Section C* Editorial Board at the Seattle Congress in August. Some major policy changes were decided on at these meetings and these have, in the main, been encompassed in the 1997 *Notes for Authors*. In summary these include:

The provision for two separate modes of 'full' and 'CIF-access' papers. Authors must nominate the mode on submission.

The automation of the preliminary data checking of CIFs and stricter requirements for 'initial entry' into the review process.

The submitted CIFs satisfying the validation requirements will be assigned a Data Validation Number (DVN) which is embedded in the file. The DVN will be used as the publication reference code or as an archival access code.

The format of printed papers will be reduced by printing only coordinate tables which contain high symmetry sites, by condensing slightly the *Experimental data* section, by enforcing the requirement that printed geometry details contain only unique and novel values, and by allowing only one printed diagram per structure.

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

During 1996, *Section D* has published 187 articles and communications on various aspects of biological crystallography. Of these, 39 described crystal structures of macromolecules, many of which were refined, and details of their three-dimensional structures and their biological relevance were included. Another 39 articles involved methods that can be used to work with intensity data, determine phases, or refine structures. The influx of manuscripts is good, and the editorial staff has cut down the time between receipt and acceptance of a manuscript. Some articles take a long time to publish because of extensive communications between the Co-editor and the author, or because the author has been slow to revise the manuscript after receiving the comments of reviewers. The time for such a revision has now been reduced from six to three months, and all authors are required to confirm that they have seen and accept the final version of the manuscript. Colour diagrams and photographs are published without any charge to the authors; this has been very helpful in maintaining high publication standards in the journal.

The *Short Communications* section is mainly devoted to reports of unit-cell dimensions and space groups of macromolecular crystals. 78 such articles were published in 1996. In addition, 15 full articles were published on experiments to

obtain crystals, or to improve current crystallization methods. In addition, reports on policies for deposition of macromolecular data and on a workshop on procedures for recording and validating results of three-dimensional structural studies of biological macromolecules were published.

Authors of all structural papers are required to deposit three-dimensional structural coordinates and structure factors with the Protein Data Bank before the article can be published. The author may, however, request that atomic coordinates be given a privileged status for one year and structure factors for four years.

The fine work of the Co-editors, the excellent support of the office at Chester, and the care with which the reviewers referee submitted manuscripts have each played a substantial role in the continued viability of this section of *Acta*.

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

During 1996, the *Journal of Applied Crystallography* contained its usual very varied diet, with 759 printed pages in total. The April issue contained a major Lead Article on Magnetic Compton Scattering and Measurements of Momentum Distributions of Magnetic Electrons by N. Sakai. As usual, the section on *Computer Programs/Abstracts* has been popular. We have seen this year the start of the new section on *Cryocrystallography*, and we have a few papers in the *Teaching and Education* section. In order to boost this section, a decision was taken following the Seattle Congress to appoint Å. Oskarsson to be in charge of this section. Another appointment has been made this year to start a *Software Review* section, under the charge of P. White, but, to date, no reviews have been published. In general, the journal is functioning well and the papers are of a high standard.

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

The first major review of *Journal of Synchrotron Radiation (JSR)* was published in *Nature [Nature (London)]* (1996), **383**, 42]. It is worth repeating some of the points made in this independent review. It says that 'developments in the application of synchrotron radiation research have benefited enormously from fertilization between otherwise distinct research areas, and there is no doubt that this new journal will play an important part in furthering such interdisciplinary interactions'. The review goes on to say that the 'speed, together with the quality of the contributions so far and the high standard of production, makes the journal attractive to authors and required reading for workers in what worldwide is still a rapidly expanding field'. We note that the reviewer points out that even though the quality of articles in *JSR* has been high, the issues have remained fairly slim.

Last year, we reiterated our main objectives of *JSR* becoming the focus of the whole of the synchrotron radiation community and to accept papers only of a high standard covering sources, instrumentation, methods and applications. We have strived to publish them rapidly and to a high technical standard so that the rapidly expanding community is informed of the latest developments quickly and effectively. The review cited above confirms that these objectives have been met.

Our main focus now is to increase the size of the issues without compromising the quality of the papers. Even though we are receiving a larger number of quality contributions, a number of very suitable papers are being published elsewhere. Our aim is to attract more of these.

The six issues in 1996 have covered the whole range of subjects spanning the production of synchrotron radiation and its utilization throughout the spectral region. In each of the issues, the interdisciplinary and potential for cross-fertilization has been obvious. Several 'first results' from third-generation sources have been reported.

The growth of synchrotron radiation has continued worldwide with the news that the first beam was established in the Brazilian synchrotron radiation source. This year, SPring-8, the world's highest energy synchrotron radiation source, is due to have its first beam and first results are expected to be reported at SRI-97, the refereed proceedings of which will be published in *JSR*.

The excitement of continued growth and opportunities can also be felt in new concepts emerging for the fourth-generation synchrotron radiation sources, whether these are large centralized sources such as X-ray free electron lasers or distributed 'single-user' customized synchrotron radiation sources. *JSR* will continue to play its part in providing the necessary platform for rapid communication and scientific and technical exchanges necessary for the evolution of these ideas to facilitate the development of synchrotron radiation sources, and their applications, in the next millennium.

#### *Commission on International Tables*

The major event in 1996 was the Seattle Congress. During this congress, the Commission on *International Tables* held an open meeting (12 August) and three closed meetings, in addition to numerous personal contacts between volume editors, technical editors and authors. The open Commission meeting featured six lectures on the status of the *International Tables* volumes published and in preparation. Reports about this meeting are available on the World Wide Web (WWW) Commission page (see below) and in the *Newsletter* of the British Crystallographic Association (No. 58, September 1996; No. 59, December 1996).

At Seattle, the Executive Committee approved two new *International Tables* volumes: Volume F on *Macromolecular Crystallography*, editors M. G. Rossmann and E. Arnold; Volume G on *Crystallographic Information*, editors B. McMahon and S. R. Hall.

In the second half of the year, the *International Tables* home page for the WWW was prepared. It consists of two parts:

The publication page contains information about the published volumes and how to order them. It is located in Chester as part of the IUCr home page and available at <http://www.iucr.ac.uk/>. It is presently being maintained and updated by S. E. King.

The Commission page lists the members of the Commission on *International Tables* and their editorial responsibilities. It describes the contents of all published and approved volumes and reviews their status. The Commission page is located in Tel Aviv, Israel, with U. Shmueli as Webmaster, and can be reached at <http://chemsg7.tau.ac.il/xtal/comit/comitq.html>.

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

The Fourth, Revised Edition of Volume A, published in March 1995, has sold so well that a corrected reprint became necessary which appeared in October 1996. It contains corrections of all errors and flaws known at that time. Preparations for the Fifth Edition are under way.

The Fourth, Revised Edition of the Brief Teaching Edition of Volume A appeared in October 1996. It is based on the

corrected reprint of the Fourth Edition of Volume A, mentioned above.

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

The activities related to the editing of Volume B of *International Tables*, during the tenure of this report, can be summarized as: (i) extensive interaction with authors of revised and new contributions to Volume B, by correspondence as well as in personal meetings during the Seattle Congress; and (ii) open and closed meetings of the Commission on *International Tables*, in which status reports on all volumes were presented and important discussions took place. The end of 1996 also marks the completion of most of the preparatory work that was needed in order to start the technical processing of the Second Edition of Volume B.

Details on the current status of Volume B are readily available by accessing the home page of the Commission on *International Tables* via the IUCr home page (<http://www.iucr.ac.uk/>) or directly at its primary address <http://chemsg7.tau.ac.il/xtal/comit/comitq.html>.

The details, as presented in the above home page and updated to the time of writing this report, are:

Some minor corrections that do not require repagination are included in the Corrected Reprint of the First Edition of Volume B (published 1996).

Revised and updated chapters and sections (for the Second Edition):

- 1.2. The Structure Factor (by P. Coppens)
- 1.4. Symmetry in Reciprocal Space (by U. Shmueli; Appendix B by U. Shmueli, S. R. Hall and R. W. Grosse-Kunstleve)
  - 2.1. Statistical Properties of the Weighted Reciprocal Lattice (by U. Shmueli and A. J. C. Wilson)
  - 2.5. Electron Diffraction and Electron Microscopy in Structure Determination – Foreword (by J. M. Cowley)
    - 2.5.2. Space-Group Determination by Convergent-Beam Electron Diffraction (by P. Goodman)
    - 3.3. Molecular Modelling and Graphics (by R. Diamond)
      - 4.1. Thermal Diffuse Scattering of X-rays and Neutrons (by B. T. M. Willis)
        - 5.1. Dynamical Theory of X-ray Diffraction (by A. Authier).

New contributions and their planned locations (in the Second Edition):

- 1.5. Crystallographic Viewpoints in the Classification of Space Group Representations (by M. I. Aroyo and H. Wondratschek)
  - 2.5.6. Direct Methods in Electron Crystallography (by D. L. Dorset)
  - 4.5. Polymer Crystallography (by D. L. Dorset and R. P. Millane)
  - 4.6. Reciprocal-Space Images of Aperiodic Crystals (by W. Steurer and T. Haibach)
  - 5.3. Dynamical Theory of Neutron Diffraction (by M. Schlenker and J.-P. Guigay).

Status as of January 1997: all revised chapters and sections as well as all new contributions have been received by the Editor. Most of the available material has been received by the Technical Editor.

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

Because stocks of the Corrected Reprint of Volume C, published in 1995, were projected to run out in 1997 and, in view of the fact that much of its content was becoming increasingly

outdated and a further reprinting seemed undesirable, a major effort was made during 1996 to complete the revised and expanded Second Edition so that it could be published during 1997. By the end of 1996, all except two of the revised manuscripts had been delivered to the Technical Editor, Parts 1, 2 and 3 had been typeset and preliminary proofs sent to the authors, and Part 5 had been sent to the printers for typesetting. The remaining manuscripts are expected during the first half of January 1997.

Two of the chapters of Part 2 and most of three chapters of Part 3 have been successfully typeset from  $\text{\LaTeX}$  files, either provided by the authors or converted from other word-processing systems, and much of the remaining material exists in machine-readable form, so that there are grounds for optimism that the goal of timely publication can be met, and that future corrections and revisions will be possible at minimum cost.

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

Volume D is progressing steadily, if slowly. About two thirds of the manuscripts have now been received. Only one is missing for Part I (*Tensorial Aspects of Physical Properties*); there is still quite some work to be done to coordinate the various contributions, but it is hoped that this part will be sent to the Technical Editor before the summer of 1997. Two chapters are missing for Part II (*Symmetry Aspects of Excitations*).

Several authors of Part III (*Symmetry Aspects of Structural Phase Transitions, Twinning and Domain Structures*) have met once in Prague and several times in Aachen. Their work is progressing in close cooperation. A meeting was held in Nijmegen in February 1997 to discuss the proposed accompanying software. There was a very promising demonstration of the program to determine the independent components of tensors for any rank, for spaces of  $n$  dimensions,  $n \geq 3$  (applicable to quasicrystals for instance), and for the representations of groups. A database of *Equitranslational Structural Phase Transitions* group-subgroup relations will also be included in the CD ROM. It is hoped that every manuscript will be received by the end of 1997.

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

This volume consists of two parts: Part 1, *Subperiodic Group Tables: Frieze Group, Rod Group, and Layer Group Types*; and Part 2, *Scanning of Space Groups*. Part 1 is complete and has been sent to the Technical Editor in Chester. The tables of Part 2 are complete, as is the draft of the text of Part 2. Comments to the textual guide to the tables of Part 2 are presently being incorporated and comments to the theoretical section of Part 2 are anticipated.

*Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. Arnold*

Our goal in preparing Volume F on *Macromolecular Crystallography* is to produce a comprehensive, yet relatively concise, reference work for macromolecular crystallography. This first *International Tables* volume devoted to macromolecular crystallography is intended to complement the existing volumes. This development recognizes the increasing size and vitality of the field of macromolecular crystallography. It is hoped that this volume may be particularly useful for 10–12 years; the projected timing should not interfere with other macromolecular crystallography review volumes that are currently in preparation.

Volume F will cover the theory and practice of macromolecular crystallography with an estimated total of 650 pages. In addition, there will be surveys of the principles of macromolecular structure and of commonly used macromolecular crystallographic program systems. Approximately 100 authors have accepted invitations to write articles in a total of 27 chapters. Two advisors and an Advisory Board consisting of 27 members have assisted in the planning of the volume. An Internet site at the IUCr Offices at Chester has been set up to facilitate inter-author communication during the preparation of the volume. A CD ROM version will be produced to provide electronic access to the volume and accompanying materials.

The projected publication date is 1999.

*Volume G. Crystallographic Information; Editors B. McMahon and S. R. Hall*

Volume G on *Crystallographic Information* is a reference handbook for the interchange and archival of crystallographic information, concentrating in its first edition on the IUCr standard software interchange format CIF (the Crystallographic Information File).

The volume will comprise four parts. Part 1 (*Specification*) will present a detailed description of the data interchange file format, its syntax and use. The dictionary definition language, which permits data attributes to be stored in machine-readable dictionary files, will be defined and explained. Part 2 (*Data Definition*) will discuss the proper use of definitions in the current data dictionaries. It will be largely tutorial in nature, and will explain to the practising crystallographer how to store and interpret precisely the results of crystallographic experiments. Part 3 (*Dictionaries*) will include the data dictionary files that have been published as part of the interchange standard; at present these comprise descriptions of experimental and derived results in small-molecule, inorganic, powder diffraction and macromolecular studies. Part 4 (*Applications*) will describe the practical use of CIF dictionaries and data files in inter-laboratory data exchange, database archival and publishing. This part will include chapters describing standard software libraries that define an applications programming interface for crystallographic data interchange.

The volume will include a CD ROM containing the data dictionaries in machine-readable form, together with source code and documentation for the libraries and programs described. The CD ROM will also contain hypertext links to the IUCr Web pages permitting Internet browsers to consult the most recent dictionary files and documentation at any time. Publication is anticipated in early 1998.

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

In August 1995, the Executive Committee approved this volume, which will complete data on maximal subgroups of space and plane groups. H. Wondratschek has been appointed Editor; Co-authors are M. I. Aroyo and Y. Billiet. The contents of this volume and of the form of the data can be found in *Acta Cryst* (1996), **A52**, 94.

*Contents*

Part 1. *Introduction*: List of symbols, User's guide to the tables, Coordinate transformations.

Part 2. *Tables*: Tables of all maximal subgroups and minimal supergroups for each plane and space group. Diagrams: Diagrams for *translationengleiche* and *klassengleiche* subgroups for each plane and space group.

Part 3. *Mathematical and Practical Aspects*: Group-theoretical background. Applications.

#### *Present state*

The data have been calculated completely and transferred to forms programmed in  $\text{L}^{\text{A}}\text{T}_{\text{E}}\text{X}2\epsilon$ . The forms are now being checked by the Technical Editor as to whether the tables can be printed directly from them. All diagrams have been hand drawn and sent to the Technical Editor for tests. There is a draft by G. Nebe of the mathematical section. For the section on applications of subgroups, an author still has to be found.

The year 1996 was devoted mainly to the typing of the subgroup tables. For 1997, checking of the data, adjusting of the forms and writing the missing text sections is anticipated.

#### *Commission on Aperiodic Crystals*

At the Seattle General Assembly, the new composition of the Commission was approved. The number of members was increased by one. The microsymposium on aperiodic crystals which was held during the conference was organized under the patronage of the Commission. The symposium was well attended and covered a large spectrum of current topics in the field of quasi-crystallography.

A large part of the Commission membership had the opportunity to meet in Seattle. Future activities of the Commission for the next triennium were defined. These include: (i) coordination with other IUCr Commissions to set up standards for the publication of aperiodic crystal structures; (ii) coordination with organizations responsible for the creation of structural databases dealing with aperiodic crystal structures; (iii) coordination with organizers of various international conferences specializing in the field of quasicrystals.

Members of the Commission also had the opportunity to meet during various international meetings with the purpose of coordinating or preparing conference programmes on topics dealing with aperiodic structures (Lisbon, Portugal, March 1996, for the preparation of ECM-17; Cracow, Poland, July 1996, during the Workshop on Aperiodic Structures). The Chairman of the Commission was actively involved with the organizers of Aperiodic'97 for the preparation of the meeting which will take place in Alpe d'Huez (France) in August 1997.

The work on the checklist for the publication of incommensurate crystal structures has been completed and the document published in *Acta Cryst.* (1997), A53, 95–100. Following this publication, the Commission has launched initiatives with various contact persons responsible for the structure or content of crystallographic databases in order to establish standards regarding the publication of aperiodic structures. This work will be pursued as a priority in future activities of the Commission.

#### *Commission on Biological Macromolecules*

Part of the activity of the Commission during this period has been concerned with the follow up of the initiative taken at the International Seminar-cum-School on Macromolecular Crystallographic Data held at Calcutta, India, 16–20 November 1995. In particular, a letter was addressed by a few of the leading participants to major journals on the need for enforcing the IUCr policy on deposition. The response of the journals has been encouraging, many of them publishing the letter prominently. More importantly, some journals such as *Nature* and *Nature Structural Biology* changed their policy on deposition prior to publication to comply with, to a substantial extent, the guidelines laid down by the IUCr.

During the period under review, the Commission recommended IUCr sponsorship for the meeting Direct Methods for Solving Macromolecular Structures, Erice, Italy, 22 May–2 June 1997 and the Fifth International Symposium on Protein Structure Function Relationship, Karachi, Pakistan, 6–9 January 1997.

#### *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.

It was decided to set up a World Wide Web (WWW) page (<http://www.tuwien.ac.at/theochem/iucr/csm.html>) linked to the IUCr WWW page with continuously updated information. This page contains the names of members of the Commission, their addresses (including e-mail) and their main activities. Reports and projects will be announced there.

With great sorrow, we learned of the passing away of former member E. N. Maslen in February 1997.

#### *Meetings of the Commission*

The Commission met during the Seattle Congress and General Assembly. The next Sagamore and Gordon conferences (see below) and progress of Commission projects (see below) were discussed.

#### *Conferences*

*First European Charge Density Meeting.* The meeting was organized by Claude Lecomte and was held at the Abbaye des Prémontrés (14–16 November 1996). Sessions included material sciences, maximum entropy, high-resolution synchrotron data, electrostatics, modelling of charge density and transferability, extension of experimental work to large systems and their theoretical calculations. This meeting starts a new series to be held every three years.

*Sagamore XII conference.* This conference will be held in Saskatchewan, Canada, 27 July–1 August 1997, and is organized by B. Robertson. The main areas will be electrostatic potentials, magnetization, positron annihilation and Compton scattering and thus the conference has a stronger emphasis on solids and physics.

*Gordon Research Conference.* The next Gordon Conference on Electron Densities and Chemical Bonding will take place for the first time in Europe, at Queen's College, Oxford, UK, 30 August–4 September 1998. K. Schwarz and C. Lecomte were selected as Chairman and Vice-Chairman. In this conference, chemistry and molecules play an important role, although the interdisciplinary nature of this topic will be stressed.

#### *Projects*

The Commission is carrying out five projects (the person in charge is given in parentheses). Additional information may be found on the corresponding WWW page with continuously updated information.

1. *Density Matrix Project* (W. Weyrich). A progress report is expected at the Sagamore meeting.

2. *Fermiology of High- $T_c$  Superconductors via High-Resolution Synchrotron-Based Compton Scattering* (A. Bansil). This is one of the main topics at the next Sagamore meeting.

3. *Maximum Entropy Project* (M. Sakata). This topic has led to vigorous scientific discussions during various conferences.

Therefore, independent activities are highly encouraged and should help to clarify the pros and cons for future applications.

4. *Multipole Refinement and Related Topics* (C. Lecomte). For an inorganic candidate, it was generally agreed that  $\text{Al}_2\text{O}_3$  (corundum) was the most suitable test case. A first report on corundum is planned for Sagamore XII, where suitable centrosymmetric organic systems should be discussed.

5. *Multipole Refinement Program* (T. Koritsansky). The new program *XD* has been developed by T. Koritsansky and co-workers under the auspices of the IUCr. An *XD* Users Meeting will be held in Berlin, Germany, 15–18 September 1997.

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

The activities of the Commission in 1996 were governed by the Seattle Congress and General Assembly. The following three of four microsymposia on crystal growth were organized under the responsibility and care of the Commission Chairman:

Crystal Growth II: Fundamentals. Chairpersons: A. A. Chernov (Russia), Nai-Ben Ming (China). Six invited papers were presented. Ten contributions submitted under this topic were shown as posters.

Crystal Growth III: Methods and Materials. Chairpersons: H. Klapper (Germany), I. Smol'sky (Russia). Nine contributions, partially invited and partially selected from submitted papers, were presented. Eight submitted papers were presented as posters.

Crystal Growth IV: Controlling and Predicting Crystal Morphology. Chairpersons: N. C. Seeman (USA), E. Paulus (Germany). Seven (partially invited) papers were presented.

Moreover, 18 papers submitted to the topics Crystal Growth under Microgravity, Crystal Growth from Solutions and Melts, Epitaxial Growth, Doping and Imperfections and Others were shown as posters.

Four Commission members, among them Professor T. Nishinaga (President of the IOCG), and two consultant members attended the Seattle Congress. They met during the conference in order to discuss further activities of the Commission. It was agreed that the tradition of organizing International Schools for the benefit of young scientists from economically disadvantaged countries should be continued during the forthcoming triennium 1997–1999 in cooperation with the IOCG. Two suggestions for such schools, one to be held in Nanjing (China) and the other in Trieste (Italy) (the latter in connection with the International Centre for Theoretical Physics as principal organizer and sponsor) were discussed.

#### *Commission on Crystallographic Apparatus*

This Commission has been reformed as the Commission on High Pressure.

#### *Commission on Crystallographic Computing*

The major activities of the Commission in 1996 centred around further enhancements to the Commission's Web site (<http://www.sdsc.edu/Xtal/IUCr/CC/CC.html>), the Seattle Congress and the subsequent macromolecular computing school organized by P. Bourne and K. Watenpaugh and held at Western Washington University, USA, 17–22 August.

The school was the seventh in a series of IUCr Crystallographic Computing Symposia. There were 106 attendees from 16 countries; of these, 38 were either speakers or tutors. Of the remaining 68 attendees, 29 were graduate students, 12

were postdoctoral fellows, 9 were faculty, and 18 were from industry or elsewhere. The format of the school was formal lectures in the morning, tutorials in the afternoon, and software demonstrations and more lectures in the evening.

The school covered the latest developments in macromolecular crystallographic computing starting with data collection and processing and proceeding to phasing, model building and refinement, and finally visualization. There were also sessions dealing with the quantity and quality of structures being generated and on updates of many of the common software packages being used. Finally, there were sessions on ancillary topics important to macromolecular crystallographers – for example, object oriented programming, macromolecular CIF, and the use of the Internet. Refer to the on-line editorial for details of speakers and specific topics.

Draft proceedings were distributed to attendees of the school and final papers will appear in the published proceedings. For the first time at a computing school, full proceedings are available electronically via the World Wide Web (<http://www.sdsc.edu/Xtal/IUCr/CC/School96/>) or via anonymous ftp from <ftp.sdsc.edu> in the directory </pub/sdsc/societies/IUCr/School96>. Individual papers may be downloaded as PostScript files.

At the main Congress, the Commission sponsored a session on General Advances and Application of Crystallographic Computing and this was organized by G. Kruger and P. Bourne and chaired by D. Viterbo.

The Commission Web site has been updated to include: the mandate of the Commission, a list of current members, previous annual reports, and the reports of recent schools.

The current project being undertaken by the Commission, with IUCr sponsorship, is to develop a CD ROM with standard data sets covering all areas of crystallography. What constitutes a standard data set is presently being established by discussion among Commission members.

#### *Commission on Crystallographic Data*

This Commission has been replaced by a Committee on Crystallographic Databases. The membership of this Committee is H. M. Berman (USA; Chairman), F. H. Allen (UK), H. Behrens (Germany), P. M. D. Fitzgerald (USA), G. L. Gilliland (USA), S. R. Hall (Australia), J. R. Helliwell (UK), R. Jenkins (USA), J. R. Rodgers (Canada), J. L. Sussman (Israel) and the IUCr President.

#### *Commission on Crystallographic Nomenclature*

The Commission met 8 August 1996 (shortly before the Seattle Congress) with ten members in attendance, including retiring members C. E. Bugg and J. H. Robertson, the latter serving as Secretary, *pro tem*. Membership in the Commission is entirely *ex officio*, by virtue of a primary IUCr responsibility closely related to crystallographic nomenclature. H. Wondratschek became a member of the Commission as a result of his appointment earlier in the year as Editor of *International Tables for Crystallography*, Volume H. Following appointment during the Congress, E. Arnold and M. G. Rossmann became members as Editors of Volume F, B. McMahon as an Editor of Volume G, I. D. Brown as Chair of the Committee for the Maintenance of the Crystallographic Information File Standards (COMCIFS) and P. Coppens as Chair of the IUCr/OUP Book Series Committee. In 1996, as in prior years, the work of the



Commission was shared with its Subcommittees and Working Groups.

The report by the Subcommittee on Atomic Displacement Parameter Nomenclature entitled *Atomic Displacement Parameter Nomenclature* was published in *Acta Cryst.* (1996), **A52**, 770–781. The Report considers the confusing and inconsistent terms and symbols in current use for parameters denoting dynamic or static displacements of atoms in crystals, focusing on individual atomic anisotropic displacement parameters representing atomic motion and possible static displacive disorder. It 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. U. Shmueli translated the Report into HTML for posting on the Web. It is now accessible in full on the Commission's home page, see below.

The Subcommittee on the Nomenclature of *N*-Dimensional Crystallography [see *Acta Cryst.* (1996), **A52**, 91–124 for membership] has nearly reached consensus on its first report recommending symbols and nomenclature for use in point-group transformations, families, systems and geometric classes in *N* dimensions, in which particular attention is devoted to the need for consistency with existing nomenclature in three dimensions. The Subcommittee continues working on the nomenclature of arithmetic classes, Bravais classes and space groups.

J.-C. Toledano was elected Chair of the Working Group on Phase Transition Nomenclature during the year. R. S. Roth was elected to membership replacing R. L. Snyder who resigned [see *Acta Cryst.* (1996), **A52**, 91–124 for the remaining members]. The Working Group is considering the best nomenclature for unambiguously naming a sequence of phases formed by a material as a function of temperature or pressure.

The recommendation of the Working Group on Statistical Descriptors in Crystallography [see *Acta Cryst.* (1995), **A51**, 565–569] to replace the term 'estimated standard deviation' by 'standard uncertainty' has been accepted by the Commission on Journals and incorporated into the *Notes for Authors* published by each IUCr journal.

The Commission has established, through the efforts of B. McMahon, an attractive and informative home page accessible through the IUCr home page or directly at URL <http://www.iucr.ac.uk/comm/cnom.html>. In addition to providing general information about the Commission, the page lists all members and the titles of all Commission Reports; it also includes hypertext links to each member and to the full content of five recent Commission Reports. The Reports Statistical Descriptors in Crystallography, I and II were translated into HTML by H. D. Flack.

A. Authier has been elected Commission Observer to COM-CIFS by both bodies to enhance their close cooperation on matters of nomenclature.

#### *Commission on Crystallographic Teaching*

##### *Visiting Professorships*

A Visiting Professorship to Egypt has been granted to Dr J. P. Glusker (see below).

##### *Contributions to Schools of Crystallography*

The Commission has taken an essential part in organizing the Fifth International School and Workshop of Crystallography: Teaching and Applications, which is taking place in Suez,

Egypt, 5–11 April 1997. Professor Karimat El-Sayed is the Chairman of the Organizing Committee and L. A. Aslanov, J. P. Glusker, C. Gramaccioli, Å. Oskarsson are members of the Programme and Scientific Committee and some are also teachers there.

Similarly, Professor M. Laing has taken active part in organizing a school on Practical Applications of X-ray Powder Diffraction, which is taking place in Durban, South Africa, 22–26 September 1997.

The Commission has also positively supported applications for IUCr sponsorship and financial support from some other International Schools. Among these are the Rietveld Summer School in Cieszyn, Poland (August 1997) and Schools on Direct Methods and on Electron Crystallography, which will be held in Erice, Italy, 22 May–2 June 1997.

##### *Other activities*

At the Seattle Congress, a session on Teaching Crystallography was held. It was chaired by Å. Oskarsson and L. A. Aslanov, and several members of the Commission contributed to the session.

M. B. Hursthouse and E. Makovicky, who is a member of the Commission, are organizing a session with the title Computer-Based Teaching in Crystallography at the next European Crystallographic Meeting, ECM-17, to be held in Lisbon, Portugal, 24–28 August 1997.

#### *Commission on Electron Diffraction*

The year started with a Workshop organized for the Commission by Professors M. A. van Hove and A. Ichimiya on Electron Diffraction and Imaging from Surfaces. The five microsymbiosia at the Seattle Congress with direct organizational involvement of the Commission were well attended and stimulated a good deal of interest. However, it was felt that emphasis placed on electron diffraction was not really commensurate with its growing importance and the accuracy of the results that are now being obtained. It is intended to rectify the situation in the next Congress at Glasgow.

There was a considerable change of membership of the Commission this year not only caused by retirements but also by the departure of the gas electron diffraction members from this Commission to the newly titled Commission on Structural Chemistry. It was also decided that the Commission should have a Secretary and Dr D. L. Dorset was elected to this position.

In order to communicate with its community better and to publicize meetings of particular interest in the field of electron diffraction, it was decided to create a Web site. This is accessible at <http://www.hwi.buffalo.edu/ACA/> under IUCr or at <http://hobbes.hwi.buffalo.edu/~dorset/iucr.html>.

#### *Commission on High Pressure*

At the Perth Congress in 1987, a High-Pressure Group was established within the Commission on Crystallographic Apparatus to represent and support high-pressure crystallography. The subsequent decade has seen an extraordinary growth in the range and quality of high-pressure diffraction studies – particularly using powder methods – on both synchrotron and neutron sources. This has been stimulated by the power of present-day sources, and by major developments in detectors and high-pressure technology. The High-Pressure Group maintained a high level of activity from its inception, with a series of international workshops, starting in Munich in 1989. This

culminated in a major effort by the Group for the Seattle Congress, which saw a celebration of a fertile and exciting decade in two keynote lectures and six microsymbiosia spanning the current range of science and techniques. At the same Congress, it was decided to create this new Commission. This was a very welcome development, but unexpected; it became known to members only at the Congress itself.

In the short time since the Congress, there has not yet been any other activity. However, Commission members have been engaged in advising on the format and programme of a one-day symposium, supported by the Commission, organized as part of the International Association for the Advancement of High Pressure Science and Technology Conference, to be held in Japan in August 1997; and planning has started for an international workshop to be held at the European Synchrotron Radiation Facility, in France, in the autumn of 1997. This, too, will be supported by the Commission. An active first year for the new Commission is thus already in prospect.

#### *Commission on Neutron Scattering*

The chief activities of the Commission were preparations for the Seattle Congress and General Assembly and, in particular, the two microsymbiosia and the satellite meeting to be held at the National Institute of Science and Technology (NIST), Gaithersburg, Maryland, USA, 5–7 August 1997.

The Commission also continued its work on the two projects International Standards for Neutron Elastic Scattering Cross Sections (NISC) and Internationally Agreed Exchange Format for Neutron Synchrotron Data.

The closed meeting of the Commission was held on 5 August on the first day of the Neutron Scattering Satellite Meeting. Present were: E. Prince, B. Lebeck, B. Forsyth, Y. Endoh and J. W. White (Chairman).

The meeting considered the following agenda:

1. The length of the General Assembly and Congress Meeting and the relationship to satellite meetings.
2. Arrangements for the Neutron Scattering Satellite Meeting for 1999.
3. The coordination of international neutron scattering meetings.
4. Membership of the Commission.
5. Present status of neutron scattering institutions and their funding.
6. Any other business.

#### *Abridged Minutes*

*Agenda Item 1.* In reference to past meetings and the present meeting, there is a growing concern that the length of time people have to spend away if they go to a satellite as well as the main meeting can be as long as 2 to 3 weeks. It is thought to be too long and there needs to be some discussion with the Executive Committee about other models. The relative contributions of microsymbiosia and the satellite were discussed. Different models, *e.g.* bringing the satellites into the main meeting in some way was discussed.

*Agenda Item 2.* J. W. White reported that in conjunction with the 1999 meeting in Glasgow the Commission might like to consider a Neutron Scattering Satellite meeting. The members of the Commission supported this idea after it had been formally put to them by J. W. White.

J. W. White then reported that he had had informal discussions with Dr A. Taylor (Rutherford Appleton Laboratory, UK) about the possibilities of Rutherford looking after the

arrangements locally for a 1999 satellite meeting. Dr Taylor had said that the Rutherford Laboratory would be willing to organize a local committee if the General Assembly of the IUCr agreed to a proposal for a satellite meeting in 1999.

*Agenda Item 3.* The Chairman asked the members of the Commission whether they thought there was some role for the Commission to help to coordinate and to avoid clashes between the growing number of neutron scattering meetings that were being planned worldwide. After some discussion, the Commission agreed that there was a role and individual members agreed to help in the process.

It was agreed that the Commission would assemble a calendar for the next 5 years to see where likely clashes might occur.

*Agenda Item 4.* The Chairman brought up the question of the future membership to the IUCr Commission of Neutron Scattering in the light of the suggestions from various National Committees

*Agenda Item 5.* The Commission was informed about a number of major concerns on the funding of neutron scattering institutions in Europe, Canada and the USA and the question was posed as to what action, political or otherwise, might be taken by the Commission and the IUCr to affect matters.

The concerns were:

(i) The position by AEC (Canada) to discontinue their support of the basic science aspect of neutron scattering at the Chalk River Laboratory. There were a number of moves by Canadian scientists to have this reversed as it could lead to the demise of a major facility on which many Canadian academics and industrialists depended.

(ii) Recent reports and proposals for neutron scattering facilities in the USA were discussed. Some members felt that some of the decisions were apparently likely to lead to major opportunities for USA leadership being lost. The USA was already well behind Europe in pulsed neutron source use and the recent decisions do not look as if they would quickly correct this.

In Europe, the recently reported (*Nature*, July 1996) decision by the German government to reduce its contributions to international science agencies, *e.g.* CERN, ILL and ESRF, was a grave change of policy. As concerns the ILL, the effect was multiplied by about a factor of three because the budget is made up by approximately three times the lowest figure from any of the three major countries, UK, Germany and France. ILL was just coming back into full scientific activity after a three year shutdown and had excellent plans to deal with fuel reprocessing *etc.*, which should guarantee the very long life time of the newly refurbished facility.

Members of the Commission were asked to think about these matters, to consult and to come back later in the week with any suggestions for action that the Commission might take.

*Agenda Item 6.* The Chairman raised the position of the Agenda for the open meeting at Seattle. He reported that he had not yet had a reply to his recent e-mail (4 July 1996) asking for a specific date for the open meeting. It appears that all members of the Commission had some difficulty with communications in respect of the present General Assembly and Congress arrangements.

#### *The Satellite Meeting at Gaithersburg*

The satellite meeting was a great success. The meeting attracted 101 papers (posters and oral presentations) and was attended by about that number of people. Of the 42 oral

presentations, more than half were by young scientists. The meeting not only concentrated on novel techniques, as in the past, but presentations were encouraged to show how new science was being carried out through new instrument developments. Highlights on the instrument side were novel position-sensitive detection methods, high pressure, polarization analysis, monochromator and related developments and themes which ran through the meeting related to giant magneto resistance as studied by diffraction, small-angle scattering and inelastic scattering; hot topics on high-temperature superconductivity, reflectometry and the recent developments for new neutron sources in Asia, Europe and the USA.

#### *Neutron Scattering Microsymposia at Seattle*

Two very successful microsymposia were organized for the General Assembly. In each case, there was a very good attendance throughout the microsymposium and in the case of the neutron reflectivity meeting the Nobel Laureate Cliff Shull was present throughout and expressed his gratification at the quality and content of the presentations. It is clear that recent advances in neutron techniques and the continuing power of isotope contrast variation are opening up new scientific insights.

#### *Other major meetings*

In autumn 1996, the first major neutron meeting organized by the European Neutron Scattering Association (ENSA) took place in Interlaken, Switzerland. The meeting was a resounding success with more than 800 participants. In August 1997, the National Conference on Neutron Scattering (ICNS) will be held in Toronto, Canada, which will be supported by a number of satellite meetings at the National Institute for Science and Technology, Gaithersburg, Maryland, USA (High Resolution Inelastic Scattering) and at the Intense Pulsed Neutron Source, Argonne National Laboratory, Illinois, USA (Materials Research Using Cold Neutrons at Pulsed Neutron Sources). Whilst the Commission is not directly involved in the organization of any of these meetings, a number of members of the Commission are active on the Organizing Committees.

The workshop sponsored by the European Neutron Scattering Association and the European Science Foundation has now produced a handsome volume relating to the present and future (ten year forward look) applications of neutron scattering. A number of members of the Commission took an active part in this workshop which was interesting in that it brought together neutron specialists and a large number of non-neutron specialists who contributed to the discussions.

#### *Neutron News*

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 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*

The Commission was extremely busy in 1996 with the main Seattle Congress and the combined powder diffraction satellite and XRD/XRF conference at Denver. The Commission played a major role in both events in addition to its already very ambitious programme of size/strain, quantitative analysis and Rietveld refinement evaluation. The mailing list for the Commission *Newsletter* continues to grow and a new home page on

the World Wide Web (<http://www.dl.ac.uk/SRS/XRD/IUCR/>) has been established. The twice-yearly *CPD Newsletter* reaches a substantially different audience to the main *IUCr Newsletter* and as such will continue for the next triennium. The CPD plans to make this information available in electronic form for as wide an audience as possible.

#### *Meetings/Workshops/Schools*

The preparations for the Denver and Seattle meetings dominated the first half of the year. The Commission was involved directly with sessions on materials research using powder diffraction and structure determination techniques. The Commission was represented on the main Programme Committee by D. Cox and R. J. Hill. At the combined IUCr satellite and Denver conference the Commission organized sessions on peak profile analysis, precision and accuracy in structure refinement from powder data and phase quantification. The CPD was represented on the Denver Programme Committee by D. K. Smith and D. Cox. This was in addition to participation by individual members in a large number of other microsymposia. The sessions were so well attended in Seattle that extra seats had to be provided in the lecture theatre. The CPD sessions at Denver were also very successful providing a good balance between the academic and industrial research that characterizes the Denver meetings. Professor D. Louër (Rennes, France) gave the keynote lecture at the Seattle Congress entitled *Modern Powder Diffraction in Materials Science*. This was an excellent talk covering all aspects of powder diffraction with particular emphasis on its applications. Professor Louër pointed out just how far the subject has progressed in ten years since the CPD was formed.

The Commission has been involved in the European powder diffraction meeting in Parma (EPDIC 5) through the Programme Committee (R. J. Cernik and P. Scardi) and by recommending IUCr support for students. The general relationship between the EPDIC meetings and the IUCr is becoming clearer after some discussion. The EPDIC meetings are very successful in their own right and will continue to be independent meetings. They will still attract IUCr support and the CPD will continue to look for informal ways to encourage cooperation. The EPDIC meetings will as far as possible be held 14 to 15 months apart with a break of one year during the IUCr main congress years. The CPD hopes that powder diffraction will play an increasing role in the ECM and that the current excellent relationship with EPDIC will continue. In addition to these major meetings, the Commission lent its support to the 5th School on X-ray Diffraction from Polycrystalline Materials, Frascati, Italy. The subject of the school was glancing-angle X-ray diffraction. There was also a powder diffraction course in Merida, Venezuela, and a meeting on materials structure characterization in the Czech Republic.

#### *Projects*

The CPD has continued to help the development of the Program Exchange Bank (PEB) for powder diffraction software and has provided a platform for the launch of an anonymous ftp site. The project to evaluate quantitative phase analysis is being led by R. J. Hill and D. K. Smith; this is at the stage of calling for interested parties to participate in the programme. The Commission is following up the Rietveld refinement comparison study published by Hill *et al.* in 1994 with a set of recommendations. This is being led by L. B. McCusker and R. Von Dreele and will probably appear in one of the IUCr journals this year. The CPD is also actively searching

for new standard materials with more refineable parameters for more complex Rietveld comparisons. Retired CPD member D. Cox has agreed to continue with this project. Later this year, the Commission wishes to conduct a survey of instrumentation to determine the need for laboratory-based high-resolution studies.

#### *Newsletters*

Two *Newsletters* were produced in 1996, issue 16 was edited by V. Valvoda (Prague) and issue 17 by L. B. McCusker (Zürich). The first of these contained a detailed account of powder diffraction in Prague in an imaginative style. The work described covered a wide field and included multilayers, thin films, texture, distortions, minerals, ceramic superconductors and aerosols. The latter *Newsletter* contains a feature article on powder diffraction at the ESRF by A. Fitch; the benefits of a small source size are becoming very clear. The announcement for expressions of interest in the Quantitative Phase Analysis programme was published along with a very comprehensive series of meetings reports. These covered the Venezuelan, Italian and Czech meetings described earlier as well as session descriptions from Denver and Seattle. Reports on the Denver meeting from R. J. Hill, H. Toraya, D. Cox and R. A. Young described diffraction peak profile analysis, phase quantification, detector development, thin films and accuracy in powder diffraction. Seattle reports from R. J. Cernik, R. J. Hill and R. Tellgren described D. Louër's keynote lecture and the sessions on materials (VIII) and structure determination from powder data. Both *Newsletters* give up-to-date contact points and meetings calendars and provide a vital platform for information exchange throughout this very lively Commission.

#### *Collaboration with other Commissions*

With the expansion of the number of IUCr Commissions, the CPD wishes to form new links with other Commissions in order to promote new areas of cooperation. The CPD hopes to form strong links with the Commissions for High Pressure, Electron Diffraction, Neutron Scattering, XAFS, Small-Angle Scattering and Synchrotron Radiation. At present, these collaborations are at a very early stage although there are some very promising avenues such as structural characterization with electron crystallography followed by Rietveld structure refinement. The Commission is actively pursuing the possibilities for scientific cooperation as well as ideas for shared meeting sessions.

#### *Commission on Small Molecules*

This Commission has been renamed the Commission on Structural Chemistry.

#### *Commission on Small-Angle Scattering*

The creation of a Commission on Small-Angle Scattering (SAS) was first suggested at the Annual Meeting of the American Crystallographic Association in Montreal in July 1995. At that time, a Working Group was established with Dr J. Barnes of NIST (USA) as Chair and Dr T. Sabine of ANSTO (Australia) as Co-Chair. By February of 1996, these two had recruited six additional members to the Working Group.

The Working Group sponsored, under the leadership of Drs Barnes and Sabine, two sessions on small-angle scattering at the Seattle Congress. The Working Group also drafted Terms of Reference for a permanent SAS Commission. The working group approved these and presented them to the worldwide SAS community at the X International Conference on Small-

Angle Scattering (SAS-96) in Campiñas, São Paulo, Brazil, in July 1996. The draft Terms of Reference were forwarded to the IUCr Executive Committee in time for the Seattle General Assembly to approve formation of the Commission on Small-Angle Scattering as a permanent entity.

Since that time, the Commission members have been mainly engaged in 'community building'. Dr Barnes has established a site on the World Wide Web (<http://www.nist.gov/sas>) which the worldwide SAS community can use to communicate with one another. Up-to-date details on all matters regarding the Commission's membership, its history, and its activities can be found at that address. The community's Internet listserver has in excess of 260 subscribers as of this writing. The Commission is attempting to expand this list to include as many practitioners of SAS as possible. Additional content, in the form of links to SAS laboratories and SAS literature compilations, are being sought for the Web site.

Commission member A. Craievich deserves special recognition for organizing and promoting the X International Conference on Small-Angle Scattering. This event, held in Campiñas, São Paulo, Brazil, brought together over 250 SAS practitioners from all over the world for four days of outstanding technical sessions. A visit to the newly commissioned Brazilian National Synchrotron Light Laboratory was a highlight of the meeting. The proceedings of the conference, co-edited by A. Craievich, G. Kostorz and J. Teixeira, will be published in the *Journal of Applied Crystallography* in 1997.

Preparations are under way for the XI International SAS Conference, to be held at Brookhaven National Laboratory, USA, in the spring of 1999.

A preliminary technical agenda has been drafted and the Commission is recruiting volunteers to carry out parts of that agenda. The Commission is cooperating with the Small-Angle Special Interest Group of the American Crystallographic Association to sponsor three sessions at the 1997 ACA Annual Meeting in St Louis, Missouri, USA. A series of tutorial sessions on Small-Angle Scattering for the Industrial Plastics Laboratory is planned for the 1998 Society of Plastics Engineers ANTEC meeting. These activities are part of an outreach effort aimed at bringing SAS methods into more widespread use in the world materials community. Proposals for inter-laboratory testing programs are being formulated.

#### *Commission on Structural Chemistry*

The Commission met twice during the Seattle Congress. The outgoing Commission members met before the General Assembly sessions and the new Commission members met after the General Assembly had concluded its business.

At the first meeting, the retiring Chair, Professor F. H. Herbstein, reported that he had met with the Executive Committee to discuss membership of the Commission for the next triennium and to bring them up to date on the Commission's current activities and tentative future plans. There was also discussion at the meeting concerning the request of the single-crystal electron diffractionists to split from the Commission on Electron Diffraction and join this Commission. The result of that discussion was to have one seat on the Commission occupied by an electron diffractionist and to add up to two consultants from this area. Professor Herbstein also made a suggestion to the Executive Committee that they set up a Working Group to study the "position and future of 'small

molecule' crystallography". The suggestion was taken under advisement.

Professor Y. Ohashi asked for sponsorship for a meeting in Japan on the Analysis and Design of Solid-State Organic Reactions to be held 30 September–2 October 1996. The programme included many excellent and well known crystallographers drawn from a wide variety of countries. The Commission voted to support the request for sponsorship of this meeting.

Professor J. C. A. Boeyens requested sponsorship for Indaba II, a 5 day meeting for approximately 30 people from overseas and 60–70 people of various ages from South Africa, Zimbabwe and Zambia. No details of the programme were presented but since the first meeting was very well organized with high-quality papers, it was decided to give tentative approval for sponsorship with final approval awaiting further details.

The Commission was quite active in contributing to the programme for the Seattle Congress. The Programme Chairman, Dr W. L. Duax, was a former Commission Chair and three members of the current Commission served on the Programme Committee (F. H. Herbststein, J. A. K. Howard and J. Flippen-Anderson) and there were several sessions organized by Commission members: two sessions on Hot Structures (J. A. K. Howard and J. Flippen-Anderson); Solid State Reactions (F. H. Herbststein and E. Boldyreva); and Intermolecular Interactions (Y. Ohashi). An open Commission meeting on Small Molecule Crystallography of the Future was organized by R. Boese and R. Harlow. All sessions were well attended and well received. Reviews have been published in the *IUCr Newsletter*.

The General Assembly approved the change of name of the Commission to Commission on Structural Chemistry.

At the meeting of the new Commission members, there was discussion of the possibility of expanding the programme of the Commission to include such areas as solid-state chemistry and supramolecular assemblies. Professor G. Desiraju agreed to investigate such possibilities and report back to the Commission. J. Flippen-Anderson was asked to continue as Secretary.

J. A. K. Howard, Programme Chair for the Glasgow Congress, was present and discussed her plans for the Glasgow programme. She asked for input on programme topics and the following suggestions were among those put forward by various members of the Commission: (1) concerns with the quality of data; (2) molecular modelling; (3) crystal structure prediction including the areas of molecular interactions and recognition; (4) solid-state NMR and other upcoming new methods; (5) instrumentation; (6) anomalous dispersion – usefulness in small-molecule crystallography; (7) bio-inorganic crystallography; and (8) electron diffraction. J. A. K. Howard also announced that the 1998 Erice School, Co-Chaired by F. H. Allen and herself, would be on Chemical Kinetics – Statistical and Dynamic Aspects of Crystallography.

During the meeting, more information became available concerning the programme for Indaba II and the Commission voted to give its official support. Support was also approved for the Symposium on Organic Crystal Chemistry, 17–21 August 1997, Poznan-Rydzyna, Poland.

The Commission has a Web page which can be accessed through the IUCr home page.

#### *Commission on Synchrotron Radiation*

The Commission has continued its work over the broad field of crystallography with the use of synchrotron radiation during the last year.

The Commission was heavily involved in the Seattle Congress and the Chairman (Å. Kvik of ESRF) was active on the Programme Committee. Three microsymbiosia (Synchrotron Radiation I, II and III) were successfully organized. In the microsymbiosia, topics were focused on: Instrumentation and techniques; Macromolecules; and Applications: time-resolved, microcrystal, high energy, respectively. In addition to the main Congress in Seattle, a Synchrotron Radiation Satellite Meeting at the Advanced Photon Source (APS) in Argonne was organized under the auspices of the Commission and the APS (4–7 August 1996). As many as 150 people participated in the satellite. More than 30 invited leading synchrotron-radiation scientists presented the latest developments in the field. The impact of the new third-generation sources was reviewed. The satellite consisted of seven oral sessions and four poster sessions. The oral sessions covered: Facility report; Developments at third-generation X-ray sources; Macromolecular application; Materials science and physics application; High-pressure application; and Detector, software and instrumentation.

During the Seattle Congress, a meeting of the Commission was held, and the future plans of the Commission activities were discussed. Among nine members of the Commission, four were replaced by new members. Y. Amemiya (University of Tokyo, Japan) was elected as Commission Chairman succeeding Å. Kvik (ESRF, France) who had conducted the Commission successfully during the preceding three years.

The Commission is planning to organize a scientific meeting on crystallographic application of synchrotron radiation (1–2 August 1997) at the Photon Factory as a satellite meeting of the 6th International Conference on Synchrotron Radiation Instrumentation (4–8 August 1997), which will be held at Himeji, Japan. In the satellite, particular attention will focus on Time-Resolved X-ray Experiments. The role of second-generation sources will be discussed in relation to the new third-generation sources in order to broaden experimental opportunities available and to activate further the field of synchrotron-radiation research. The Commission also started to discuss the satellite meeting of the Glasgow Congress in 1999.

#### *Commission on XAFS*

Over the last 20 years, X-ray absorption fine structure (XAFS) has developed into an extremely useful technique for obtaining local structural information for non-crystalline systems, thus making it often the structural technique of choice when crystallography cannot be used. In recognition of this natural connection between XAFS and crystallography, the Executive Committee of the International XAFS Society (IXS) proposed that a Commission on XAFS be established within the IUCr. The creation of this Commission was approved at the IUCr Congress in Seattle (August 1996). The Chair of the XAFS Commission is E. A. Stern.

One of the principal goals of the Commission on XAFS is to promote stronger links between the IUCr and the IXS. The IXS is a relatively new organization that represents all scientists that utilize the fine structure associated with inner-shell excitation (near edge and extended) by various probes (e.g. X-rays and electrons), including those who utilize related techniques for which the data are interpreted on the same physical basis (more information about the IXS can be found at <http://ixs.csrii.iit.edu/IXS/>). It currently has over 600 members. It is hoped that the creation of a Commission on XAFS will

promote closer interactions between the X-ray diffraction and the X-ray absorption communities.

Since its creation, the principal activity of the Commission on XAFS has been to develop educational materials aimed at improving the practices of XAFS. The most visible of these is the IXS home page (special thanks are due to Professors B. Bunker and G. Bunker, and the Center for Synchrotron Radiation Research and Instrumentation for development of these pages). The IXS home page serves as a clearing house for communication within the XAFS community, including information about worldwide synchrotron sources and access to a variety of XAFS databases (archived spectra, publications and software). The Commission is also working (in cooperation with the IXS Education Committee) to develop course notes that can be used for XAFS training workshops and with the IXS Standards and Criteria Committee to formalize procedures and tests for data collection and analysis and for the reporting of errors. Finally, the Commission is working with the IXS in planning for the Tenth International Conference on XAFS to be held in Chicago, 10–14 August 1998.

#### 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 1996 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 1996 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 1997, but approved in 1996, are listed below:

5th International Symposium on Protein Structure Function Relationship and Workshop on Protein Structure Elucidation, Karachi, Pakistan, 6–9 and 11–16 January 1997.

BCA/CCG Sixth Intensive Course in X-ray Structure Analysis, Durham, UK, 7–14 April 1997.

26th International School of Crystallography: Electron Crystallography, Erice, Italy, 22 May–2 June 1997.

School on Direct Methods for Solving Macromolecular Structures, Erice, Italy, 22 May–2 June 1997.

5th European Powder Diffraction Conference (EPDIC 5), Parma, Italy, 25–28 May 1997.

Sagamore XII, Wasquesiu, Canada, 27 July–1 August 1997.

International Conference on Aperiodic Crystals (Aperiodic '97), Alpe d'Huez, France, 27–31 August 1997.

Rietveld Summer School '97-PL (RSS97-PL), Cieszyn, Poland, 4–6 September 1997.

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 meeting, writing to the Chairman of the Sub-committee. The present Chairman is Professor H. Schenk, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands (e-mail: schenk@chem.uva.nl).

Applications for sponsorship of satellite meetings require the approval of the Chairman 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 Chairman of the Congress Programme Committee for his approval or otherwise.

The IUCr continues to support and uphold ICSU's policy of non-discrimination and adheres to its decisions and procedures concerning 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

It is with the deepest regret and with a profound sense of loss that we have to report the death of Professor E. N. (Ted) Maslen on 2 February 1997. In his role as Chairman of the Working Party on Crystallographic Information, then as Director of Archiving and Crystallographic Information and then as founding Chairman of this Committee, Ted guided the IUCr's publication and archiving activity into the electronic era through a tangled maze of options and opinions.

During the period 1993–1996, the EPC was comprised of over 20 members drawn from all circles with an interest in electronic publishing be it far or near. This provided an excellent discussion forum but tended to slow down practical applications. During the Seattle Congress, the IUCr Executive Committee decided to appoint a smaller and more technical committee comprised of the following people: Y. Epelboin, H. D. Flack, E. N. Maslen (deceased), B. McMahon (IUCr Research and Development Officer) and P. R. Strickland (IUCr Managing Editor). The members of the former Committee are thanked for their interest and activity which helped to put the electronic publishing activities of the IUCr on a firm footing. In the rest of this report, we give some details of the activities of the EPC during 1996.

Four members of the EPC (Y. Epelboin, H. D. Flack, S. R. Hall and B. McMahon) attended the ICSU Press/UNESCO conference on Electronic Publishing in Science held in February 1996 in Paris for which A. Authier was one of the co-organizers. The conference brought together interested parties from learned societies, publishing houses and libraries in a series of formal presentations and working groups in which the technical, economic and social effects of electronic publishing in science were discussed. The complete set of articles from the conference may be viewed at [http://www.lmcp.jussieu.fr/icsu/Information/Proc\\_0296](http://www.lmcp.jussieu.fr/icsu/Information/Proc_0296) and the impressions of one participant are available at <http://www.unige.ch/crystal/ahdf/rpt.eps.paris.html>. User communities are different from one branch of science to another and a publishing technique adopted by one may not necessarily be applicable to another. In face of the worldwide falling number of library subscriptions to journals and supplementary costs necessary to convert to electronic submission and delivery of journals and other information services, scientific publishers are presented with a very difficult problem.

The consultant's study of publishing activities of the IUCr was received in January 1996. The consultant recommends the use of SGML favouring a DTD modelled on the Elsevier Art(icle) DTD and conforming to ISO 12083. The EPC gave due consideration to this document, in particular to the desired form in which documents would be submitted and archived.

The EPC met during the Seattle Congress and was informed of the introduction of the all electronic *CIF-access* papers by *Acta Cryst. Section C*. The EPC favoured electronic delivery of individual papers in the IUCr's journals but at a fee calculated to encourage annual subscriptions. Access should be by a password system capable of being monitored. Further, a comfortable majority of those present considered that a pre-print server for journal articles was not in the interests of the IUCr.

During the Seattle Congress, a microsposium devoted to the Internet was organized by two members of the EPC and the Committee's then Chairman E. N. Maslen gave a very clear exposition of the Science, Technology and Economics of Electronic Publishing in Crystallography, and Y. Epelboin spoke on Internet Resources for Crystallography. The microsposium also presented a talk from George D. Purvis, an outsider to crystallography, on The Role of the World-Wide Web in Computational and Pharmaceutical Chemistry and finished with short presentations on two hot subjects on the Internet, Java and VRML, both likely to have impact on the area of electronic publishing. Further, a workshop on the Internet was run to give participants hands-on experience.

Considerable effort has been deployed in improving the information content of the WWW servers for crystallography. The Chester WWW server now displays the contents of the IUCr journals in a most useful and attractive format and a service for searching the Tables of Contents is rapidly approaching the beta-test state. General information on the IUCr (e.g. Annual Reports) and its Commissions is being expanded with help from student labour. Contacts have been made for other IUCr documentation to be made available over the WWW. Preliminary tests on setting up mirror sites are under way. The WWW server gives clear and up-to-date information on the preferred formats for submitting articles to the IUCr's journals. The unofficial Crystallography World Wide server based in Geneva and mirrored at approximately ten sites around the world now also benefits from IUCr financial help for document preparation assuring its longevity. The EPC will investigate the way to amalgamate these two WWW services and to constitute an IUCr WWW Editorial Board.

In November, H. D. Flack visited the Editor-in-Chief of the Union's journals in Manchester and subsequently spent three days at the Chester office in discussions with the Managing Editor, the Research and Development Officer and the Executive Secretary.

#### *World Directory of Crystallographers (WDC) – Tenth edition*

In 1995, the keyword list to be used for entries in the database of crystallographers was updated. There are now more than 2000 keywords for the 500 that existed in the previous edition. Statistics were calculated for keyword use in the previous edition to aid in establishing the new list.

Updates to the database are made on demand by the IUCr R & D Officer. Moreover, a major revision started at the beginning of 1996 and the National Editors were invited to prepare their data to be ready *before* the end of 1996. The intention was that the next printed edition should be delivered

by July 1997. To this end, national editors of WDC met during the Seattle Congress and the necessary instructions were once again distributed. A way was also sought to continuously update the data. As always, the ability to keep within the agreed time schedule depends critically not only on the activity and organization of the regional and national editors but also on the willingness of all individuals to act promptly and accurately on requests for information updates. It is clear that assembling the data has become too heavy a burden for volunteers in a number of places and it is necessary to find new ways.

A trial has been made using the Internet to collect updates to the WDC. P. Boyle has kindly designed a Web form to allow registration by individual scientists but with a system of verification left in the hands of the appropriate national editor. This has been tested in North America and France and although successful its use leads to the following conclusions: The software should be redesigned to trap errors and inconsistencies in the data input as with the present system it takes too long to correct them. No proper identification is made of the person who submits the entry. It would be useful to be able to output the data in an intermediate format so that they could be used at a national level prior to the production of the CIF needed by the IUCr.

New software will be written in Paris at the University P. M. Curie based on software for the Crystallographic Software Database maintained on the SInCris server.

#### *SInCris*

SInCris is a Web server devoted to crystallography and material sciences opened in October 1995. By agreement between H. D. Flack and Y. Epelboin, SInCris is a complement to the information available on Crystallography World Wide in Geneva and the IUCr server in Chester. SInCris has been financed by the French Higher Education Agency and the Research Agency (CNRS). SInCris is a mirror site for Crystallography World Wide and acted as a mirror for the Seattle Congress.

One of the main sections of SInCris is a database on crystallographic software. This contains more than 350 entries and received more than 60 000 queries in 1996. A forms-based interrogation and retrieval of the database allows access to the information by keywords. SInCris works in close collaboration with the IUCr Editorial Office in Chester for the software section of *Journal of Applied Crystallography*.

#### **Committee for the Maintenance of the Crystallographic Information File Standards (COMCIFS)**

Many years of COMCIFS' work came to fruition during the present year with the approval of three major dictionaries, the first since the approval of the original core dictionary by the Executive Committee in 1991. On 12 November 1996, approval was given to an extended version of the core dictionary that includes additions and clarifications resulting from experience with *Acta Cryst. Section C*. Considering the revolutionary character of the changes in production of *Acta Cryst. Section C* in which CIF played a central role, the original version of the core dictionary has performed well, but a few infelicities in the original dictionary required correction and some extra items were added, some required as a result of changes in the techniques of structure determination.

Two major new dictionaries have also been approved, the macromolecular dictionary was approved on 8 June 1997 and the powder dictionary on 9 July 1997. Both of these have been

under construction for several years and are the result of a great deal of dedicated work by a number of people, particularly Paula Fitzgerald and her team for the macromolecular dictionary and Brian Toby for the powder diffraction dictionary. It is our understanding that these dictionaries, in addition to extending the range of papers that can be submitted to *Acta Cryst. Sections C and D*, will be adopted as archival standards by the Protein Data Bank, the Nucleic Acid Data Bank and the Powder Data File.

There are other dictionaries in preparation dealing with modulated structures, symmetry and diffuse scattering, and discussions are under way with a group planning a standard for reporting measurements from image plates. For technical reasons, the latter group will probably not adopt the STAR format on which CIF is based, but they are anxious to ensure as much compatibility with CIF as possible.

In the future, COMCIFS will spend more time approving incremental changes to the three major existing dictionaries as they are brought into use by journals and databases. For this reason, COMCIFS is reviewing its current structure and mode of operation.

The membership of this Committee is I. D. Brown (Canada; Chairman) P. R. Edgington (UK), P. M. D. Fitzgerald (USA), S. R. Hall (Australia), G. Madariaga (Spain), M. Spackman (Australia), B. H. Toby (USA) and the IUCr R&D Officer.

#### Promotion Committee

A Promotion Committee has been established with the aim of marketing the products that the IUCr provides. The membership of this Committee is A. M. Glazer (UK; Chairman), F. H. Allen (UK), P. W. Coddling (Canada), W. L. Duax (USA), H. D. Flack (Switzerland), S. R. Hall (Australia), J. Harada (Japan), S. J. Maginn (UK), the Executive Secretary, the Managing Editor, the IUCr President, and the IUCr General Secretary and Treasurer.

#### Regional Associates and Scientific Associates

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

A great deal of effort by the ACA and its members was directed towards the organization of the highly successful IUCr XVII Congress and General Assembly in Seattle. The IUCr is grateful for the very positive publicity crystallography received. The Congress was attended by many scientists not directly associated with the crystallographic community, and several were outspoken in expressing positive opinions on the organization and the scientific programme.

The ACA continues to be a vibrant organization. A new SIG, the General Interest Group, was formed and will be active at the 1997 meeting to be held in St Louis in July 1997. A new award was instituted for Science Writing, for which all ACA members can submit material that has appeared in a newspaper or a popular magazine. A statement on Ethics in Crystallography was adopted by the ACA Council and published in the *ACA Newsletter*. Calls for nominations were issued for the Warren, Buerger and Patterson Awards, to be presented at the 1997 meeting.

As the North American Regional Associate of the IUCr, the ACA aims to increase its contact and collaboration with the Mexican crystallographic community. Discussions on how best to accomplish this are continuing.

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

At the Seattle Congress in August 1996, AsCA elected a new Executive Committee and Council for a three-year term with Professor Z. Zhang (China) as President, Dr C. J. Howard (Australia) as Vice-President and Dr Krishan Lal (India) as Secretary-Treasurer. At present, 17 countries are members of the Association.

The next Triennial Conference of AsCA will be held in Malaysia in 1998. Professor Shih-Lin Chang is the Chairman of the International Organizing Committee of AsCA '98 and Professor Withman the Chairman of the Local Organizing Committee. As usual, all aspects of crystallography will be covered and the programme will consist of both invited talks and contributed papers.

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

The ECC met in Seattle on 10 August with, for the first time, South Africa as an observer.

The organizers of both 1997 and 1998 European Crystallographic Meetings to be held in Lisbon and Prague, respectively, reported on the facilities and organization of their meetings. No decision was made about the ECM in 2000.

The main discussion was about the proposed change of the rather informal organization of the European Crystallographic Committee into a European Crystallographic Association with legal status. The ECC is in favour of such a change and appointed a Working Group consisting of the ECC officers H. Fuess, J. Bernstein and A. Smith, and P. Beurskens and S. Candeloro to develop the concept Statutes. The Working Group circulated the revised Statutes by e-mail to all national delegates to obtain national approval and amendments. It is expected that the ECC will take the formal decision about the Statutes of the European Crystallographic Association in 1997.

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

During 1966, the following International Conferences were sponsored and organized by the local National Crystal Growth Associations affiliated to the IOCG:

Third Korea-Japan Electronic Materials Growth Symposium, Onyang, Korea, 7 June.

Eighth International Conference on Metal-Organic Vapour Phase Epitaxy (ICMOVPE-8), Cardiff, UK, 9-13 June.

Joint International Conference on Vapour Growth and Epitaxy (ICVGE-9) and American Conference on Crystal Growth (ACCG-10), Vail, Colorado, USA, 4-9 August.

Seventh China-Japan Symposium on Science and Technology of Crystal Growth of Materials, Shanghai, China, 1-2 November.

In addition, preparations of the Twelfth International Congress on Crystal Growth (ICCG-12), of the Tenth International Conference on Vapour Growth and Epitaxy (ICVGE-10) and of the Tenth International Summer School on Crystal Growth (ISSCG-10) were started. ICCG-12 and the ICVGE-10 will jointly be held in Jerusalem, Israel, 26-31 July 1998; ISSCG-10 will be held in Rimini, Italy (different from earlier announcements), 1-6 June 1998. The Chairpersons of ICCG-12 and of ICVGE-10 are Dr A. Horowitz and Dr M. Roth, Nuclear Research Centre Negev (NRCN), Beer Sheva, Israel. The Chairpersons of ISSCG-10 are Professor Carlo Paorici (former Chairman of the IUCr Commission on Crystal Growth and Characterization of Materials), University of Parma, Italy, and Dr Roberto Fornari, MASPEC-CNR,



Parma, Italy. Information on ICCG-12 and ICVGE-10 may be found at <http://www.technion.ac.il/~iccg12> and on ISSCG-10 at [http://www.maspec.bo.cbr.it/CG/school\\_cg.html](http://www.maspec.bo.cbr.it/CG/school_cg.html).

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

ICDD meetings were held at ICDD in Newtown Square, PA, USA, 17–21 March 1997. The financial and product meetings were on Monday and Tuesday. The Technical Committee and its Sub-committees met on Wednesday and Thursday. The Board of Directors had its meetings on Tuesday and Friday. Dr R. L. Snyder is the current Chairman of the ICDD. Highlights of the meetings were technical presentations by E. Antipov (Russia), Shao-Fan Lin (China), J. Fiala (Czech Republic) and R. Allmann (Germany).

The ICDD will be issuing set 47 of the Powder Diffraction File containing 2500 new data sets in August 1997, an increase of 500 data sets compared to previous years. Also in 1997, release J of Crystal Data and a new Electron Diffraction Database will be issued. The ICDD staff are making notable efforts towards making the PDF easier to use on the PC platform. The ICDD completed the first stage of an extensive expansion of the Web page on the Internet (<http://www.icdd.com>). Considerable information about meetings, products and personnel may be found on this Web page.

ICDD is making an internal effort to expand its membership by contacting many prominent scientists using powder diffraction in their research and suggesting they apply for membership. Over 50 new members were submitted by the Membership Committee for consideration and processing. The prescribed procedure in the By-laws requires this list to be approved by the Board of Directors and the membership. This processing is almost complete.

A new Sub-committee devoted to X-ray fluorescence had its first meeting during the week. Dr M. A. Zaitz chaired the meeting and would like to hear from others interested in becoming active in this Sub-committee ([zaitz@vnet.ibm.com](mailto:zaitz@vnet.ibm.com)).

A new Sub-committee on non-ambient powder diffraction data has been formed. Dr C. Prewitt will Chair this Sub-committee ([prewitt@gl.ciw.edu](mailto:prewitt@gl.ciw.edu)). Its first meeting will be March 1998.

The Grant-in-Aid programme is very active with over 40 projects, mostly outside the US, currently approved. Proposals are now being accepted twice yearly. Proposals for new grants will be up to 31 July 1997 for consideration in the fall. Application information may be obtained by contacting Ms T. Maguire ([maguire@icdd.com](mailto:maguire@icdd.com) and on the Web page).

The ICDD awarded four Crystallography Scholarships in 1997. The recipients were: N. Audebrand, University of Rennes, France; D. M. Teter, Carnegie Institution of Washington, USA; S. Savvides, Cornell University, USA; and Hongwu Xu, Princeton University, USA. ICDD also funds two scholarships for high-school students in the Delaware Valley for students who excel in mathematics and science and plan to attend college.

Educational activities of the ICDD continue as short courses associated with meetings such as Denver and EPDIC and the clinics given every June at Newtown Square. Workshops for Grant-in-Aid projects are given in Europe and South America.

The next meeting of the ICDD will be in conjunction with the Denver X-ray Conference, DXC, to be held in Steamboat Springs, Colorado, USA, 4–8 August 1997. Many of the ICDD Sub-committees and the Technical Committee will meet at this

conference, and the meetings are all open to any attendees of the conference. Planning for the 1998 DXC has commenced. ICDD has accepted the responsibility for the continued direction of this conference. ICDD has also assisted in the preparation of the DXC proceedings on a CD ROM which contains the 40 volumes of proceedings in page image form and the most recent volumes in searchable form along with a searchable index for the full 40 volumes.

#### **Representatives on Other Bodies**

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

The annual meeting of IDCNS was held 22–23 August 1996 at the Bureau International des Poids et Mesures (BIPM) in Sèvres, France. The meeting followed so closely on the conclusion of the IUCr Seattle Congress that neither the IUCr Representative nor the Alternate were able to participate. Nevertheless, the strong objections presented by the IUCr, at earlier meetings of IDCNS, to the 1994 proposal of the Comité Consultative d'Unités (CCU) of BIPM to deprecate the ångström were set forth very effectively by the Chair of IDCNS at the April 1996 meeting of CCU. Among the resulting recommendations made by CCU to the Comité International des Poids et Mesures (CIPM) for final action on this matter was that Chapter IV (entitled *Units outside the International System*) in the next edition of the authoritative brochure *Le Système International d'Unités (SI)*, to be published in 1997, should be substantially revised in a major change of style. Table 10 in this chapter will have the revised heading 'Other units currently accepted for use with the SI. These units should be expressed in relation to the SI in every document in which they are used.' There will be no further deprecatory remarks. Table 10 will contain the following units: are, hectare, ångström, bar, barn, nautical mile and knot, and will give their relation to the SI. The practical consequence of this decision is that ångströms may continue to be used without being in breach of anything said in the SI Brochure, provided only that such authors include a footnote in every paper that makes use of ångströms along the lines: '1 Å = 10<sup>-10</sup> m'. The IUCr has interpreted this proviso by printing the statement 'Units: The International System of Units (SI) is used in all IUCr journals except that the ångström (symbol Å, defined as 10<sup>-10</sup> m) is generally preferred to the nanometre (nm) or picometre (pm) as the appropriate unit of length.' in each issue of all journals.

Authority to act in all matters between nations concerning measurement standards 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 in Sèvres of interest to the IUCr, the third edition of IUPAC's Green Book *Quantities, Units and Symbols in Physical Chemistry* is expected to be published in 1998. It will contain a new section on uncertainties, also new material on surface science, NMR and nonlinear spectroscopy. A further development in the consideration of prefixes for binary systems is the proposal by the International Electrotechnical Commission to adopt the following: 2<sup>10</sup> = kibi (kilobinary), symbol Ki; 2<sup>20</sup> = mebi (megabinary), symbol Mi; 2<sup>30</sup> = gibi (gigabinary), symbol Gi and 2<sup>40</sup> = tebi (terabinary), symbol Ti. Comment by crystallographers on this proposal is

invited and should be sent either to the Representative or the Alternate Representative.

A total of 39 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 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)*

The IUCr representative to ICSTI since 1993, E. N. Maslen, died suddenly on 2 February 1997. The current report has been compiled from information that he communicated to the IUCr Sub-Committee on Electronic Publishing and from the ICSTI WWW server at <http://www.cisti.nrc.ca/icsti/icsti.html>.

ICSTI held its General Assembly and Conference in May 1996 in Pretoria, South Africa. The General Assembly approved the 1996–1997 programme of projects which includes:

*Access to telematics facilities in the Eastern Caribbean* aimed at promoting effective and sustainable use of information services via the Internet in the sectors of health, education and the environment.

*Networking projects* aimed at developing Web services.

*A Graphics Project* aimed at developing a standard test to measure and assess the effectiveness of electronic transmission of graphical and pictorial information using existing protocols.

*International classification scheme for physics* – 19 organizations have been invited to participate in the preparation of the 4th edition of the scheme.

*Assessing the impact of full-text document delivery on subscriptions* – organizations involved include The British Library, the Canada Institute for Scientific and Technical Information and INIST.

The *ICSTI contribution to the ISSN Register* will provide information on which abstracting and indexing services cover a given serial publication in the Register.

E. N. Maslen was the prime mover in the *Graphics Project*. The graphical images of particular interest in this project are chemical structure diagrams, contour maps, histograms, line diagrams (e.g. circuit diagrams, consisting mainly of straight lines), machine drawings, pie charts and other 3D diagrams, for which the effectiveness of the representation would be measured in terms of the size of the graphics file, the faithfulness of the representation, the ease of interpretation and the ease of reconstruction of the basic data. The advantages of bit-map raster and vector graphics were under consideration. The project was designed along the following lines: (i) preparation of standard test data; (ii) selection of test formats; and (iii) bench-marking of the formats to be tested.

E. N. Maslen had formed a team of three (or four) people who were collaborating in the project.

The next ICSTI meeting will take place in Philadelphia, USA, 6–9 June 1997.

It should be recalled that E. N. Maslen had several times in his annual and triennial reports to the IUCr Executive Committee pointed out the need for a reorganization or amalgamation of the international organizations with missions in the area of scientific data and information services such as ICSTI, CODATA and ICSU Press.

*International Council of Scientific Unions (ICSU)*

The 25th General Assembly of ICSU was held in Washington DC, USA, 24–27 September 1996, hosted by the US National Scientific Member of ICSU, the National Academy of Sciences of the United States of America. The IUCr was represented by Professor M. Hart, member of the Executive Committee. The Assembly was preceded by a Symposium on Science and Human Goals in the 21st Century, which was held on 24 September. The objectives of the Symposium were to demonstrate the inherently international character of science and its contributions to knowledge and to finding practical solutions for problems facing humanity.

The General Assembly of ICSU was attended by 232 persons, which included representatives of each of the 23 Union members of ICSU, 61 National members or National Associates, 8 Scientific Associates, 21 interdisciplinary or standing ICSU bodies, and 8 partner organizations. The Assembly had three full working days, many of which included night sessions, either of the entire Assembly or of its subsidiary organs. The proposals for modifications to the Statutes and Rules of Procedure were adopted and the revised version of these was published in the 1997 Year Book. Two new Unions were admitted for ICSU membership: the International Union of Food Science and Technology (IUFoST) and the International Union of Toxicology (IUTOX) bringing the number of Scientific Union members of ICSU to 25. The Academia Nacional de Ciencias of Costa Rica was admitted as a National Scientific member, bringing the national participation in ICSU to 95.

The Assembly divided into four working groups during the afternoon of 25 September, in order to allow participants to discuss matters of common concern around the topics of the Biological Sciences; the Earth and Space Sciences, Physical, Chemical and Mathematical Sciences; Social Sciences; and National Concerns.

R. Elliot, Chair of the Conference on Electronic Publishing which took place in Paris in February 1996 [*Acta Cryst.* (1996), **A52**, 977–981], reported on the Conference which was a direct follow-up to a resolution of the 24th General Assembly of ICSU and informed participants that the Proceedings of this were available on the WWW, as well as in book form. He suggested that the future should not be based on old methods of publishing, but that the new methods should be encouraged. The IUCr made major presentations and significant inputs to the Paris Conference. The Conference on Electronic Publishing concluded that:

- material should still be peer-reviewed and authenticated;
- action must be taken to make sure that archived material is suitably preserved so that it can be read in years to come;
- the cost of electronic publishing could be as expensive as traditional publishing because of hidden costs;
- copyright should be addressed at a legal level and scientific committees should be established to protect the interests of those involved;

the nature of the networks would impact developing countries, allowing these to leap-frog difficulties, if attention was given to those who have limited access to funds.

L. Lederman, Chair of the ICSU Committee on Capacity Building in Science (CCBS), presented his Committee's report and recommendations, recalling that the Committee had been set up by a Resolution of the 24th General Assembly of ICSU and reminding the General Assembly that the Committee members brought a wide variety of cultural, scientific, and

educational experiences to ICSU. He explained in detail the three principal foci of the work of CCBS: primary level science education; public understanding of science; and the reduction of the isolation of scientists and said that these would be the first building blocks of the proposed ICSU Programme on Capacity Building in Science.

At the end of this discussion, the General Assembly expressed through a vote that it would be in favour of launching a major ICSU Programme in Capacity Building in Science. The General Assembly further approved the establishment of a Standing Committee on Responsibility and Ethics in Science.

With the retirement of Professor O. G. Tandberg, the Secretariat of the Standing Committee on Freedom in the Conduct of Sciences (SCFCS) has been moved to Switzerland, with P. Schindler taking over as Executive Secretary of the Committee.

The next meeting of the General Committee and an Extraordinary General Assembly are to be held in Vienna, Austria, 23–25 April 1998. The report of the Committee on the Assessment of ICSU and related changes to the Statutes and Rules of Procedure are to be discussed.

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

No significant meetings occurred in 1996 but the IUCr's Visiting Professorship Programme, which receives support from the ICSU/UNESCO subvention, continues.

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

Current information on CODATA activities and strategy can be found at <http://www.cisti.nrc.ca/codata/welcome.html>. CODATA works on an interdisciplinary basis to improve the quality, reliability, processing, management and accessibility of data of importance to science and technology.

From 29 September to 3 October 1996, the 15th International CODATA Conference, Scientific Data for Global Prosperity and Better Human Life was held in Tsukuba, Japan and was followed on 4 and 5 October by the General Assembly of CODATA. Amongst the associated satellite meetings, one on Electronic Publishing was co-organized by J. R. Rodgers, the former IUCr Representative to CODATA. The conference covered a very wide range of data and information activities related to science and technology and was attended by some 280 participants from 31 countries. The current CODATA President is J.-E. Dubois (France). The 16th CODATA conference and 21st General Assembly will take place in New Delhi, India, 22–28 November 1998.

CODATA is implementing a Long Range Planning Program. Included in this plan are:

- (i) Studies of Abstract Data Structure: a task group on visualization is working towards this goal;
- (ii) Collaboration with ICSU Unions on Database Efforts: this primarily concerns a task group on standardized terminology for biological data banks with an eye to cataloging the known species on the earth;
- (iii) Access to Data; and
- (iv) Outreach Activities, which aims at the expansion of educational and tutorial activities to permit the scientific community to take advantage of modern information technology.

Of the CODATA Task Groups and Commissions for 1997–1998, the following have implications for the activities of crystallographers: (1) Biological Macromolecules with emphasis on the proteome project. (2) Distributed Data Depository. This project, initially intended to be a large

centralized depository (of thermophysical data banks), evolved into a set of distributed data banks due to the growth of the Internet. (3) Commission on Access to Data, which plans small meetings looking at access issues from the point of view of the traditions and constraints in a scientific discipline. (4) A Task Group to make CODATA more visible and known by use of the World Wide Web and to act as a source of information on scientific and technical data (apparently ICSTI is doing the same thing). (5) Data/Information Technology and Visualization Task Group, which seems to have elements in common with the ICSTI graphics project.

A current theme in CODATA documents is the assessment of data quality and the costs that this incurs.

In June 1977, Chapter 1 (*Crystallography*) of the *CODATA Directory of Data Sources for Science and Technology*, edited by D. G. Watson, was published. This directory contains information arranged in sections: International Data Projects, National Data Projects, Data Centers, Major Publication Series, Other Data Sources and Bibliographies. Much of the information is now out of date and the CODATA Executive Director has suggested that it is time to consider an update to this publication. This CODATA Directory on Crystallographic Data seems to be little known to crystallographers. In 1987, the former IUCr Commission on Crystallographic Data published an excellent soft-cover book *Crystallographic Databases*, which covered the field in detail from the user's point of view giving many examples. In August 1995, the NIST Workshop on Crystallographic Databases was held in Gaithersburg, USA, and the proceedings have been published in *J. Res. Natl. Inst. Stand. Technol.* (1996), **101**(3), 205–381. Necessarily, the impact of modern information technology, especially the Internet and the World Wide Web, occupied a high place in the considerations of the participants at the NIST Workshop. It would seem that these two publications complete and bring up to date the 1977 CODATA publication in a form which is more accessible to crystallographers. Further, the advent of the World Wide Web with its global accessibility and its inherent ease of revision makes printed documents of the type of the CODATA Directory less attractive as a means of publication for this type of compendium. Although the *CODATA Bulletin* itself has now been discontinued, CODATA output is currently in the form of a book series in collaboration with Springer Verlag, collections of conference abstracts and a *Newsletter*.

Of the CODATA activities that impact on the interests and current concerns of the IUCr, the Distributed Data Depository and the question of interconnections (by Internet) of distributed and formerly independent databases is of great relevance.

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

COSTED-IBN is concerned about the threat of scientific and technological marginalization of the many poor and underdeveloped nations with little or no science and technology infrastructure. It is co-sponsored by UNESCO. Among other activities, the Committee operates a travel grant programme which in 1996 provided some small support for the Seattle Congress. The COSTED Executive Committee is to meet in Jordan, 25–27 February 1997.

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

The 31st COSPAR Scientific Assembly and Associated Events took place at the University of Birmingham, UK,

14–21 July 1996. The duration of the congress (six days) was considerably shorter than that of previous ones (ten days), in order to reduce expenses and time for the delegates. During the Assembly, the 55th COSPAR Bureau Meeting and the 31st Council Meeting were held under the Chair of President Professor G. Haerendel. The following items extracted from the agenda and reports of these meetings are of general interest:

(i) Turkey and Ukraine became members of the COSPAR community.

(ii) The 32nd COSPAR Scientific Assembly and Associated Events will be held in Nagoya, Japan 12–19 July 1998. During the associated 1998 COSPAR Council Meeting, the new COSPAR President, Vice-President, other Bureau members, Finance Committee Chair and Finance Committee members will be elected. For the preparation of this event, a Nomination Committee consisting of five members was installed.

(iii) It was decided to hold the future COSPAR Assemblies In Poland (year 2000) and in the USA (year 2002), the latter eventually in connection with a second World Space Congress.

(iv) The installation of a new category of COSPAR affiliate, called 'Supporters', was discussed and envisaged with the objective of gaining greater attention for COSPAR's work and to help bring in funds.

COSPAR has introduced a home page on the World Wide Web with the address <http://COSPAR.itodys.jussieu.fr>.

### Finances

The audited accounts for the year 1996 are given at the end of this Report. For comparison, the figures for 1995 are provided in italics. The accounts are presented in Swiss Francs (CHF).

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 CHF at 31 December 1996 have been translated into CHF in the balance sheet at the rate operative at that date. For the income and expenditure accounts, transactions have been translated into CHF by applying the rates appropriate to the individual dates of these transactions. As a consequence of the fluctuation in exchange rates, an apparent gain has arisen on the assets of the Union, in terms of the CHF, amounting to CHF 815 641. The gain attributable to investment activities has been assigned to the General Fund and the gain attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 1996. It should be noted that this gain in CHF is not a real gain of money, but rather a gain on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 1996. The total of CHF 349 173 with the banks at the end of the year was represented by USD 114 816 with Merrill Lynch, GBP 78 563 with National Westminster Bank and CHF 36 351 with the Union Bank of Switzerland.

The balance sheet shows that the assets of the Union, including the gain of CHF 815 641 resulting from fluctuations in rates of exchange, have increased during the year, from CHF 5 224 690 to CHF 6 089 600.

Transfers of CHF 175 000, CHF 85 979 and CHF 100 000 were made to the Publication and Journals Development Fund from the *Acta Crystallographica* Fund, the *Structure*

*Reports* Fund and the General Fund, respectively. Transfers of CHF 50 000 and CHF 60 000 were made to the Research and Education Fund from the *Journal of Applied Crystallography* Fund and the *International Tables* Fund, respectively. Transfers of CHF 619 and CHF 50 000 were made to the Ewald Fund from the Book Fund and the General Fund, respectively. A transfer of CHF 75 000 was made to the *Newsletter* Fund from the General Fund. A transfer of CHF 90 000 was made to the *Journal of Synchrotron Radiation* Fund from the *International Tables* Fund.

Beneath the detailed figures of the expenditure and income for each fund account, the balance at 1 January, transfers to and from other funds, 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 market value of investments in the year'.

The General Fund account shows a deficit of CHF 68 291 before the transfers totalling CHF 150 000 to the Ewald Fund and the Publication and Journals Development Fund, as compared with a profit of CHF 139 839 before transfers totalling CHF 200 000 to the *Newsletter* Fund, the President's Fund, the Ewald fund and the Publication and Journals Development Fund in 1995. The administrative expenses were CHF 220 091 in 1996 as compared with CHF 218 220 in 1995. Of this amount, CHF 77 032 was charged to the publications of the Union.

CHF 40 169 was given for general support of scientific meetings, in addition to CHF 64 409 for financial support to young scientists attending meetings, which appears in the expenses of the Research and Education Fund, and CHF 7125 in special grants from the President's Fund. CHF 63 028 was spent on the Seventeenth General Assembly and Congress and CHF 28 842 in assisting the work of the non-publishing Commissions. The expenses of the Union Representatives on other bodies were CHF 3784. The cost of the Finance Committee meetings held in 1996 was CHF 16 508, while the Executive Committee meeting cost CHF 75 374. The cost of the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 16 225. The Union received CHF 22 359 from the UNESCO subvention to ICSU. The subscriptions from Adhering Bodies were CHF 148 822. Interest on bank accounts and investments credited to the General Fund was CHF 172 973.

The President's Fund, the Publication 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 CHF 2476. Grants totalling CHF 7125 were paid from the Fund.

The *Acta Crystallographica* account for 1996 shows a surplus of CHF 77 363 before the transfer of CHF 250 000 to other fund accounts, as compared with a surplus of CHF 181 465 in 1995 before transfers of CHF 360 000.

The subscription rates were increased for 1996. In 1996, the number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 63 (67) personal subscriptions, was 687 (719) (values for 1995 are given in parentheses). The number of paid subscriptions to *Sections A+B+C*, including 12 (11) personal subscriptions, was 133 (133). The number of paid subscriptions to the separate sections of the journal were: *Section A* 255 (285 for 1995), *Section B* 202 (217), *Section C* 147 (144) and

*Section D 174 (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 CHF 756 672 (for 6596 published pages) as compared with CHF 637 345 in 1995 (5888 pages published). The journal's accounts have also been charged with administration expenses as in previous years as shown in the General Fund.

The *Journal of Applied Crystallography* account shows a surplus of CHF 79 664 before transfers of CHF 50 000 to other fund accounts, as compared with a surplus of CHF 77 743 in 1995 before transfers of CHF 100 000. In 1996, the number of paid subscriptions, including 108 (107 in 1995) personal subscriptions, was 868 (907 in 1995).

The *Journal of Synchrotron Radiation* account shows a deficit of CHF 33 600 before receiving a transfer of CHF 90 000 from the *International Tables* Fund. The number of paid subscribers, including 129 personal subscriptions, was 253. [The *Journal of Synchrotron Radiation* Fund was started in 1995 and received a transfer of CHF 200 000 from the *Acta Crystallographica* Fund. In 1995, It 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* Fund was closed in 1996 and the balance of CHF 85 979 transferred to the Publication and Journals Development Fund. Sales of *Structure Reports* are now recorded in the Book Fund.

The *International Tables* account shows a surplus of CHF 78 172 before transfers of CHF 60 000 to the Research and Education Fund and CHF 90 000 to the *Journal of Synchrotron Radiation* Fund, as compared with a surplus of CHF 156 576 in 1995 before a transfer of CHF 50 000 to the Publications and Journals Development Fund. The net sales income was CHF 120 666 in 1996 as compared with CHF 245 749 in 1995. Volume A was out of print for most of 1996 and Volume B for part of 1996.

The Book Fund is credited with the sales of the remaining publications of the Union. Sales of *Structure Reports* are now included in this fund.

The *Newsletter* Fund Account received transfers of CHF 75 000 from the General Fund in both 1996 and 1995. The cost to the Union of producing the *Newsletter* in 1996 was CHF 66 950 (CHF 69 489 in 1995).

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 CHF 196 202 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 project to develop an SGML implementation for the Union's journals are charged to this account. CHF 64 409 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.

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

We have audited the financial statements on pages 836 to 852 which have been prepared under the accounting policies set out on page 838.

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

*Opinion*

In our opinion, the financial statements give a true and fair view of the state of the Union's affairs as at 31 December 1996 and of the result for the year then ended.

Deloitte & Touche  
Chartered Accountants and Registered Auditors

Manchester, England  
29 May 1997

## Income and Expenditure Account for the year ended 31 December 1996

Income	Note	Swiss Francs		Expenditure (cont.)	Note	Swiss Francs	
		1996	1995			1996	1995
Membership subscriptions		148,822	147,991	Subscriptions paid		7,127	6,789
Sales				Visiting Professorship Programme		1,290	3,861
Journals	2,372,961	2,290,217		Administration expenses:			
Books	166,962	364,174		General Secretary and Treasurer:			
Back numbers and single issues	32,859	39,298		Honorarium to Treasurer	7,740	8,120	
		2,572,782	2,693,689	Secretarial assistance	542	94	
Investment income				Audit and accountancy charges	32,228	29,959	
Income from investments	7 221,774	259,191		Legal and professional fees	2,415	4,867	
Bank interest	8 29,739	42,266		Postage and sundries	-	(121)	
Profit on sale of investments	9 6,009	23,076		Travelling expenses	2,685	6,520	
		257,522	324,533	Bank charges	1,307	1,506	
Other income				Executive Secretary's office:		46,917	50,945
Grants	22,359	13,746		Salaries and expenses	172,634	166,879	
Royalties and copyright fees	9,446	6,434		Travel expenses of IUCr representatives on other bodies	3,784	4,601	
Advertising income	72,259	61,725		STAR/CIF	4,646	4,265	
Reimbursement for CGA-17 second circular	-	17,048		Commission expenses	28,842	8,107	
		104,054	98,953	Sponsorship of meetings	40,169	21,691	
TOTAL INCOME		3,083,190	3,265,166	President's secretary	14,322	19,161	
				IUCr/FLZ agreement	16,225	1,860	
				Bad debts - subscriptions	6,000	-	
Expenditure						286,622	226,564
Journals				Depreciation		36,894	3,581
Publication costs	1,217,659	1,236,290		TOTAL EXPENDITURE		3,299,993	3,088,796
Editorial expenses	102,709	98,133					
Technical editing	877,301	777,373		(Deficit)/excess of income over expenditure		(216,803)	176,370
		2,197,669	2,111,796	Movement in market value of investments in year	5	266,072	440,128
Books						49,269	616,498
Publication costs	63,666	192,859		Fluctuation in rates of exchange			
Editorial expenses	22,641	14,329		Trading activities	2 78,851	(119,833)	
		86,307	207,188	Investment activities	2 736,790	(624,172)	
Newsletter						815,641	(744,005)
Publication costs	95,776	107,570		General Assembly costs		65,549	18,581
Editorial expenses	35,695	25,034		Ewald Prize		36,000	-
		131,471	132,604	Committee meetings and expenses		91,883	38,324
President's Fund Grants and Young Scientists' support		71,543	96,673	Publications and Journals Development			
				General		192,602	170,246
				Electronic Publishing Committee/Section Editors meeting expenses		1,573	17,047
				Electronic publishing project		46,546	4,597
		240,721	191,890				
				Total recognised gains and losses relating to the year		864,910	(127,507)
				Opening fund accounts at 1 January		5,224,690	5,352,197
				Closing fund accounts at 31 December		6,089,600	5,224,690

All the income and expenditure related to continuing activities.

Historic cost results would only differ from above by the profit on sale of investments — see note 9.

Separate Statements of Total Recognised Gains and Losses and Reconciliation of Movements in fund accounts are not given, as the information is incorporated in the above.

**Balance Sheet as at 31 December 1996**

		Swiss Francs	
	Note	1996	1995
<b>FIXED ASSETS</b>			
Tangible fixed assets	4	173,002	69,088
<b>CURRENT ASSETS</b>			
Stock		59,274	-
Cash at bank			
Current accounts	40,093	39,755	
Deposit and savings accounts	309,080	325,404	
Cash with Union officials	19,685	34,878	
		<u>368,858</u>	<u>400,037</u>
Investments at market value	5	5,513,221	4,882,698
Debtors, accrued income and payments in advance		236,689	194,071
Subscriptions from Adhering Bodies		27,220	35,978
		<u>6,205,262</u>	<u>5,512,784</u>
<b>TOTAL CURRENT ASSETS</b>			
		6,205,262	5,512,784
<b>CREDITORS:</b>			
Amounts falling due within one year	6	(288,664)	(357,182)
		<u>5,916,598</u>	<u>5,155,602</u>
<b>NET CURRENT ASSETS</b>			
		5,916,598	5,155,602
<b>TOTAL FUNDS</b>		<u>6,089,600</u>	<u>5,224,690</u>

**Cash Flow Statement for the year ended 31 December 1996**

		Swiss Francs	
	Note	1996	1995
Net cash outflow from operating activities (see below)		(654,874)	(136,650)
<b>Returns on investments</b>			
Interest received	29,739	42,266	
Investment income	221,774	259,191	
		<u>251,513</u>	<u>301,457</u>
<b>Net cash inflow from returns on investments</b>			
		251,513	301,457
<b>Investing activities</b>			
Purchase of fixed assets		(88,569)	(65,404)
Purchase of investments	5	(725,409)	(666,238)
Disposal of investments	9	1,103,757	511,189
		<u>289,779</u>	<u>(220,453)</u>
<b>Net cash inflow/(outflow) from investing activities</b>			
		289,779	(220,453)
<b>Decrease in cash and cash equivalents</b>	11	<u>(113,582)</u>	<u>(55,646)</u>
<i>Reconciliation of (Deficit)/Excess of Income over Expenditure to Net Cash Outflow from Operating Activities</i>			
(Deficit)/excess of income over expenditure		(216,803)	176,370
Exchange rate fluctuations attributable to operating activities	10	(3,552)	(12,581)
Interest received	8	(29,739)	(42,266)
Investment income	7	(221,774)	(259,191)
Profit on disposal of investments	9	(6,009)	(23,076)
Depreciation charges		36,894	3,581
Increase in stock		(59,274)	-
Increase in debtors		(33,860)	(71,695)
(Decrease)/increase in creditors		(120,757)	92,208
		<u>(654,874)</u>	<u>(136,650)</u>
<b>Net cash outflow from operating activities (see above)</b>			
		(654,874)	(136,650)



## 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 on trading transactions 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. Profit and losses on investments are allocated to the General Fund. All profits and losses arising from exchange rate fluctuations are taken directly to reserves.

## (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

Stocks of *International Tables* are included at cost less provision for slow moving and obsolete items. Stocks of all other publications are not valued for accounts purposes as sales are unpredictable.

## (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 depreciated on a straight line basis at a rate of 33 $\frac{1}{3}$ % per annum.

(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 recognized on an accruals basis.

## (h) Investments

Investments are stated at market value. Changes in market value are taken directly to reserve movements in the General Fund.

## (i) Lease costs

Operating lease costs are charged to the income and expenditure account on a straight line basis. Where reduced rents are payable on property in the earlier years of the lease, the total costs for the period to the first rent review date are spread on a straight line basis, and the appropriate creditor balance is maintained.

## 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. Transactions in currencies other than Swiss Francs are converted into Swiss Francs at the rate of exchange ruling on the date of the transaction.

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

	1996	1995
Netherland Guilders	1.3333	1.3534
Danish Crowns	4.5581	4.7847
Pounds Sterling	0.4605	0.5618
US Dollars	0.7752	0.8621

The net assets of the Union at 1 January 1996 (SwFr 5,224,690) would have had the value of US \$4,504,205 or £2,935,231 if expressed in those currencies.

At 31 December 1996, the net assets (SwFr 6,089,600) would have had the value of US \$4,720,658 or £2,804,261 respectively, being an increase of US \$216,453 or a decrease of £130,970 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.

## 5. Investments

	Swiss Francs							
	Holding at market value 1 January 1996	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 1996	Holding at revalued cost 31 December 1996	Holding at revalued cost 31 December 1995
Held by Merrill Lynch								
GNM P146535-2016 (US\$)	5,241	-	(978)	531	19	4,813	4,336	4,741
4,232 Units								
GNM P169332-2016 (US\$)	27,552	-	(2,962)	2,887	(531)	26,946	24,261	24,924
22,247 Units								
Hausmann Holdings (US\$)	398,487	-	(147,311)	38,730	43,999	333,905	156,621	202,412
443 Units								
Global Allocation Portfolio Class A (US\$) 5,700 Units	81,129	-	-	9,803	12,378	103,310	77,574	69,757
Meridian Funds Global Government Fund (US\$)	129,643	7,648	-	14,529	(1,163)	150,657	163,520	139,898
9,503 Units								
Permal Investment Holdings NV (US\$) 77 Units	141,441	-	-	16,841	17,252	175,534	311,161	117,943
Meridian Charter Income Fund (US\$)	147,292	9,624	-	16,507	(1,848)	171,575	176,005	149,208
12,234 Units								
British Gas Finance (US\$)	92,389	-	-	10,354	(3,157)	99,586	99,470	89,453
75,000 Units								
GEC (US\$)	87,610	-	(92,897)	5,287	-	-	-	87,797
75,000 Units								
US Treasury Note 6.875% (US\$)	117,486	-	(126,601)	9,115	-	-	-	116,168
100,000 Units								
Lehman Brothers Holdings (US\$)	93,125	-	-	10,436	(289)	103,272	102,032	91,750
80,000 Units								
ECS Capital Portfolio CLB (US\$)	261,577	-	-	31,014	29,638	322,229	267,856	240,862
20,764 units								
Pacific Equity	-	164,107	-	10,849	(1,051)	173,905	174,956	-
Held by Foreign & Colonial								
Reserve Asset Fund Class D (US\$)	495,584	322,956	-	76,294	6,195	900,999	525,604	472,636
16,887 Units								
Reserve Asset Fund Class L (£)	620,344	30,020	-	150,602	73,310	874,276	771,228	508,439
21,581 Units								
Reserve Asset Fund Class X (£)	252,003	156,845	(140,456)	56,193	4,814	329,399	397,896	262,317
9,581 Units								
Reserve Asset Fund Class C (US\$)	553,162	-	(586,543)	33,381	-	-	-	545,078
25,471 Units								
Reserve Asset Fund Class M (US\$)	305,683	14,015	-	39,626	79,556	438,880	277,248	249,308
11,080 Units								
Reserve Asset Fund Class E (£)	263,778	20,062	-	57,794	(1,563)	340,071	413,124	272,356
7,937 Units								
Reserve Asset Fund Class N (Yen)	129,306	132	-	(1,258)	20,408	148,588	131,682	133,067
17,828.27 Units								
UK Treasury 7.75% 22.9.2006 (£)	679,896	-	-	147,275	(11,895)	815,276	862,004	707,082
375,000 Units								
	<u>4,882,698</u>	<u>725,409</u>	<u>(1,097,748)</u>	<u>736,790</u>	<u>266,072</u>	<u>5,513,221</u>	<u>4,936,578</u>	<u>4,485,196</u>

**4. Tangible fixed assets**

	Leasehold property improvements SwFr	Office equipment SwFr	Computer equipment SwFr	Total SwFr
<b>Cost</b>				
As at				
1 January 1996	57,790	21,934	-	79,724
Additions	68,398	25,961	46,449	140,808
As at				
31 December 1996	126,188	47,895	46,449	220,532
<b>Accumulated depreciation</b>				
As at				
1 January 1996	-	10,636	-	10,636
Charge for year	12,637	8,774	15,483	36,894
As at				
31 December 1996	12,637	19,410	15,483	47,530
<b>Net book value</b>				
31 December 1996	113,551	28,485	30,966	173,002
31 December 1995	57,790	11,298	-	69,088

**6. Creditors: amounts falling due within one year**

	Swiss Francs	
	1996	1995
Trade creditors	73,562	79,163
Accruals	167,423	116,293
Lease creditor relating to property	7,812	-
Payroll creditor including tax and social security	35,841	156,103
Other creditors	4,026	5,623
	288,664	357,182

**7. Investment income**

	Swiss Francs	
	1996	1995
GNM P146535-2016	424	456
GNM P169332-2016	1,281	2,679
ML Capital Fund/CLB	2,596	-
Hausmann Holdings	738	1,028
Meridian Funds Global - Government Fund	7,648	10,157
Meridian Charter - Income Fund	9,624	9,098
British Gas Finance	7,809	8,072
GEC	3,632	6,704
US Treasury Note 6.875% 31.10.1996	8,353	7,872
Global Allocation	884	-
Foreign and Colonial - Reserve Asset Fund Class D	34,366	32,073
Foreign and Colonial - Reserve Asset Fund Class L	30,020	34,119
Foreign and Colonial - Reserve Asset Fund Class X	14,362	15,119
Foreign and Colonial - Reserve Asset Fund Class C	-	27,540
Foreign and Colonial - Reserve Asset Fund Class M	14,015	14,914
Foreign and Colonial - Reserve Asset Fund Class E	20,062	17,408
Foreign and Colonial - Reserve Asset Fund Class N	132	933
Lehman Brothers	6,503	3,200
UK Treasury 7.75% 22.9.2006	59,325	54,889
UK Treasury 7.75% 22.9.2006 - Tax on 1994 income	-	12,930
	221,774	259,191

Allocated to:			
President's Fund		2,476	1,704
Ewald Fund		15,335	16,188
Publication and Journals Development Fund		20,313	22,112
Research and Education Fund		40,416	41,535
Balance left in General Fund		143,234	177,652
		221,774	259,191

**8. Bank interest**

	Swiss Francs	
	1996	1995
<b>National Westminster Bank PLC</b>		
Manchester Business Reserve Account	6,465	7,487
Manchester Capital Reserve Account	3,977	10,661
	10,442	18,148
<b>Merrill Lynch</b>		
CMA Account	5,775	7,055
<b>Foreign &amp; Colonial</b>		
Cash balance	474	657
Petty cash accounts	-	8
Interest from Munksgaard	13,048	16,398
	13,522	17,063
Allocated to General Fund	29,739	42,266

**9. Profit on disposal/redemption of investments**

	Swiss Francs	
	1996	1995
Proceeds	1,103,757	511,189
Book value	1,097,748	488,113
Profit allocated to General Fund	6,009	23,076

Book value represents market value at 1 January 1996.

The profit on disposal based on historic cost was Swiss Francs 81,179 (1995: SwFr 65,947). Therefore, historic cost results would be as follows:

	Swiss Francs	
	1996	1995
(Deficit)/excess of income over expenditure	(141,633)	219,941

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

	Swiss Francs	
	1996	1995
Total fluctuations in exchange rates dealt with in fund accounts	815,641	(744,005)
Adjustments for exchange differences attributable to:		
Investments	(736,790)	624,172
Cash and bank balances	(82,403)	107,252
	(3,552)	(12,581)

### 11. Analysis of changes in cash and cash equivalents during the year

	Swiss Francs	
	1996	1995
Balance at 1 January 1996	400,037	562,935
Net cash (outflow)/inflow	(113,582)	(55,646)
Fluctuations in rates of exchange on cash and bank balances	82,403	(107,252)
	<u>(31,179)</u>	<u>(162,898)</u>
Balance at 31 December 1996	<u>368,858</u>	<u>400,037</u>

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

	Swiss Francs		Change 1996	Change 1995
	1996	1995		
Cash at bank and in hand	<u>368,858</u>	<u>400,037</u>	<u>(31,179)</u>	<u>(162,898)</u>

### 13. Capital commitment

	Swiss Francs	
	1996	1995
Contracted for but not provided	<u>7,280</u>	<u>34,491</u>
Authorized but not yet contracted for	<u>25,606</u>	<u>35,600</u>

### 14. Operating lease commitments

At 31 December 1996, 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
	1996	1996
Leases which expire:		
within two to five years	6,719	5,511
after five years	78,120	64,080
	<u>84,839</u>	<u>69,591</u>

### 15. Sponsorship commitments

At 31 December 1996, the Union had authorized, but not contracted for, sponsorship grants Sw Fr 47,916 (1995: Sw Fr 4,060)

### 16. Contingencies

During the year, the Union continued to participate in an agreement to guarantee the sales of an organization selling a crystallography database. The Union guarantees to underwrite sales up to Sw Fr 190,000. For sales over this level, the Union receives a percentage of the income.

## Fund Accounts as at 31 December 1996

	Swiss Francs						Balance at 31 December 96
	As at 1 January 1996	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Gain on market value of investments	Fluctuations in exchange rates (Note 2)		
					Trading	Investments	
<b>FUND ACCOUNTS</b>							
General Fund	1,190,554	(150,000)	(68,921)	266,072	18,504	736,790	1,992,999
President's Fund	48,386	-	(4,649)	-	654	-	44,391
<i>Acta Crystallographica</i>	1,544,696	(250,000)	77,363	-	20,514	-	1,392,573
<i>Journal of Applied Crystallography</i>	342,556	(50,000)	79,664	-	5,565	-	377,785
<i>Structure Reports</i>	85,979	(85,979)	0	-	-	-	-
<i>International Tables</i>	264,045	(150,000)	78,172	-	2,874	-	195,091
Book Fund	12,522	(615)	3,640	-	1,518	-	17,065
Publications and Journals							
Development Fund	579,275	360,979	(233,045)	-	9,288	-	716,497
Research and Education Fund	739,304	110,000	(25,292)	-	12,320	-	836,332
Ewald Fund	294,098	50,615	(23,185)	-	4,807	-	326,335
Newsletter Fund	51,741	75,000	(66,950)	-	894	-	60,685
<i>Journal of Synchrotron Radiation</i>	71,534	90,000	(33,600)	-	1,913	-	129,847
	<u>5,224,690</u>	<u>-</u>	<u>(216,803)</u>	<u>266,072</u>	<u>78,851</u>	<u>736,790</u>	<u>6,089,600</u>

## General Fund Account for the year ended 31 December 1996

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Grant received from UNESCO subvention to ICSU		22,359	13,572
Subscriptions from Adhering Bodies		148,822	147,991
Income from investments	7	143,234	177,652
Interest on bank accounts	8	29,739	42,266
Profit on disposal/redemption of investments	9	6,009	23,076
Amounts charged to the following journals and publications			
<i>Acta Crystallographica</i>		66,248	63,287
<i>Journal of Applied Crystallography</i>		7,703	9,150
<i>Journal of Synchrotron Radiation</i>		3,081	3,812
		77,032	76,249
<b>TOTAL INCOME</b>		<b>427,195</b>	<b>480,806</b>
<b>Expenditure</b>			
Subscriptions to ICSU and ICSU bodies		7,127	6,789
Administrative expenses:			
General Secretary and Treasurer:			
Honorarium to Treasurer		7,740	8,120
Secretarial assistance		542	94
Audit and accountancy charges		32,228	29,959
Legal and professional fees		2,415	4,867
Postage and sundries		-	(121)
Travelling expenses		2,685	6,520
Bank charges		1,306	1,506
Executive Secretary's office:			
Salaries and expenses		172,634	166,879
Depreciation of office equipment		541	396
		220,091	218,220
Seventeenth General Assembly and Congress			
Expenses		63,028	136
Programme Committee		-	18,445
Meeting of the Executive Committee		75,374	24,822
Finance Committee expenses		16,508	12,870
Travel Expenses of IUCr Representatives			
on other bodies		3,784	4,601
STAR/CIF		4,646	4,265
Commission expenses		28,842	8,107
Sponsorship of meetings		40,169	21,691
President's secretary		14,322	19,161
IUCr/FIZ agreement		16,225	1,860
Bad debts - subscriptions		6,000	-
		268,898	115,958
<b>TOTAL EXPENDITURE</b>		<b>496,116</b>	<b>340,967</b>
<i>(Deficit)/excess of income over expenditure</i>		<b>(68,921)</b>	<b>139,839</b>
<b>Reconciliation of movements</b>			
Balance at 1 January		1,190,554	980,148
Transfers to other Funds:			
<i>Newsletter</i> Fund		-	75,000
President's Fund		-	25,000
Ewald Fund		50,000	50,000
Publications and Journals Development Fund		100,000	50,000
		(150,000)	(200,000)
(Deficit)/excess of income over expenditure		(68,921)	139,839
Movement in market value of investments in the year	5	266,072	579,967
Fluctuations in rates of exchange		755,294	(169,561)
<b>Balance at 31 December</b>		<b>1,992,999</b>	<b>1,190,554</b>

## INTERNATIONAL UNION OF CRYSTALLOGRAPHY

## President's Fund Account for the year ended 31 December 1996

	Note	1996	Swiss Francs	1995
<b>Income</b>				
Investment income	7	2,476		1,704
Donation received		-		174
<b>TOTAL INCOME</b>		<u>2,476</u>		<u>1,878</u>
<b>Expenditure</b>				
Grants		7,125		5,964
<i>Deficit of income over expenditure</i>		<u>(4,649)</u>		<u>(4,086)</u>
<b>Reconciliation of movements</b>				
Balance at 1 January		48,386		34,363
Transfers from other funds		-		25,000
Deficit of income over expenditure		(4,649)		(4,086)
Fluctuations in rates of exchange		654		(6,891)
<b>Balance at 31 December</b>		<u>44,391</u>		<u>48,386</u>

*Acta Crystallographica* Account for the year ended 31 December 1996

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Subscriptions to Volume 52 ( <i>1995 Volume 51</i> )	1,910,033		1,892,514
Sale of back numbers and single copies	28,369		15,545
Airfreight charged to subscribers	53,691		53,271
Royalties and copyright fees	5,852		5,338
	1,997,945		1,966,668
<i>Less</i> Publisher's commission on sales	135,688	1,862,257	133,952
Income from advertisements (net)		683	521
TOTAL INCOME		1,862,940	1,833,237
<b>Expenditure</b>			
Publication expenses:			
Printing and binding Volume 52 ( <i>1995 Volume 51</i> )	686,225		721,857
Distribution and postage	108,129		92,158
Airfreight costs	25,072		40,460
	819,426		854,475
Net loss on reprints	12,039		15,127
Index to Volume 51 ( <i>1995 Volume 50</i> )	459		2,380
Supplement to Volume 52	37,415		-
Microfiche costs	-	869,339	88
			872,070
Editorial expenses:			
Editorial honoraria	73,474		55,911
Secretarial assistance	6,080		6,462
Postage, travel and sundries	13,764		16,697
Technical Editing:			
Salaries and expenses	708,502		607,218
Computer expenses	27,774		27,483
Depreciation of office equipment	20,396	849,990	2,644
			716,415
Administration expenses recharged from General Fund		66,248	63,287
TOTAL EXPENDITURE		1,785,577	1,651,772
<i>Excess of income over expenditure</i>		77,363	181,465
<b>Reconciliation of movements</b>			
Balance at 1 January		1,544,696	1,943,228
Transfers to other Funds:			
Publications and Journals			
Development Fund	175,000		100,000
Research and Education Fund	-		60,000
<i>Journal of Synchrotron Radiation</i>	-		200,000
<i>Newsletter</i> Fund	75,000	(250,000)	-
			(360,000)
Excess of income over expenditure		77,363	181,465
Fluctuations in rates of exchange		20,514	(219,997)
Balance at 31 December		1,392,573	1,544,696



*Journal of Applied Crystallography* Account for the year ended 31 December 1996

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Subscriptions to Volume 29 (1995 Volume 28)	320,069		325,547
Sale of back numbers and single copies	2,805		4,306
Airfreight charged to subscribers	7,958		8,241
Royalties and copyright fees	2,406		1,096
	<u>333,238</u>		<u>339,190</u>
Less Publisher's commission on sales	22,601	310,637	23,159
			<u>316,031</u>
Income from advertisements		-	825
TOTAL INCOME		<u>310,637</u>	<u>316,856</u>
<b>Expenditure</b>			
Publication expenses:			
Printing and binding Volume 29 (1995 Volume 28)	88,512		94,911
Distribution and postage	14,262		13,377
Airfreight costs	3,157		5,514
	<u>105,931</u>		<u>113,802</u>
Net loss on reprints	10,987	116,918	7,524
			<u>121,326</u>
Editorial expenses:			
Editorial honoraria	6,784		4,639
Secretarial assistance	2,140		1,814
Postage, travel and sundries	2,444		1,092
Technical Editing:			
Salaries and expenses	89,383		96,736
Computer expenses	3,229		3,974
Depreciation of office equipment	2,372	106,352	382
			<u>108,637</u>
Administration expenses recharged from General Fund		7,703	9,150
TOTAL EXPENDITURE		<u>230,973</u>	<u>239,113</u>
<i>Excess of income over expenditure</i>		<u>79,664</u>	<u>77,743</u>
<b>Reconciliation of movements</b>			
Balance at 1 January		342,556	413,600
Transfers to other funds:			
Publications and Journals			
Development Fund	-		50,000
Research and Education Fund	50,000	(50,000)	50,000
			<u>(100,000)</u>
Excess of income over expenditure		79,664	77,743
Fluctuations in rates of exchange		5,565	(48,787)
Balance at 31 December		<u>377,785</u>	<u>342,556</u>

**Journal of Synchrotron Radiation Account for the year ended 31 December 1996**

	Note	Swiss Francs		
		1996		1995
<b>Income</b>				
Subscriptions to Volume 3 (1995 Volume 2)	77,945		10,031	
Sales of back numbers and single issues	1,684		-	
Airfreight charged to subscribers	2,393		613	
	82,022		10,644	
Less Publisher's commission on sales	5,574	76,448	1,770	8,874
Income from advertisements		6,055		14,312
Income from copyrights		30		-
<b>TOTAL INCOME</b>		<b>82,533</b>		<b>23,186</b>
<b>Expenditure</b>				
Publication expenses:				
Printing and binding Volume 3 (1995 Volume 2)	60,164		62,622	
Distribution and postage	4,276		12,306	
Airfreight costs	760		8,977	
	65,200		83,905	
Net loss on reprints	1,427	66,627	108	84,013
Editorial expenses:				
Editorial honoraria	3,827		6,317	
Secretarial assistance	3,784		2,760	
Postage, travel and sundries	821		2,441	
Technical editing:				
Salaries and expenses	35,753		40,306	
Computer expenses	1,292		1,656	
Depreciation of office equipment	948	46,425	159	53,639
Administration expenses recharged from General Fund		3,081		3,812
<b>TOTAL EXPENDITURE</b>		<b>116,133</b>		<b>141,464</b>
<i>Deficit of income over expenditure</i>		<u><u>(33,600)</u></u>		<u><u>(118,278)</u></u>
<b>Reconciliation of movements</b>				
Balance at 1 January		71,534		-
Transfers from other funds:				
Acta Crystallographica Fund		-		200,000
International Tables Fund		90,000		-
Deficit of income over expenditure		(33,600)		(118,278)
Fluctuations in rates of exchange		1,913		(10,188)
<b>Balance at 31 December</b>		<u><u>129,847</u></u>		<u><u>71,534</u></u>

**Structure Reports Account for the year ended 31 December 1996**

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Sale of copies			
Earlier volumes and indexes		-	19,447
Less Publisher's commission on sales		-	5,056
TOTAL INCOME		-	14,391
<b>Expenditure</b>			
Printing and binding		-	-
Excess of income over expenditure		-	14,391
<b>Reconciliation of movements</b>			
Balance at 1 January		85,979	108,833
Transfers to other funds:			
Publications and Journals Development Fund	85,979	(85,979)	(25,000)
Excess of income over expenditure		-	14,391
Fluctuations in rates of exchange		-	(12,245)
Balance at 31 December		-	85,979

**International Tables Account for the year ended 31 December 1996**

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Sale of copies			
Volume A	60,078		175,068
Volume B	53,349		32,248
Teaching Edition of Volume A	3,562		4,711
Volumes II, III and IV	55		4,362
Volume C	46,016		118,185
		<u>163,060</u>	<u>334,574</u>
Less Publisher's commission on sales	42,394		88,825
<b>TOTAL INCOME</b>		<b>120,666</b>	<b>245,749</b>
<b>Expenditure</b>			
Publication expenses:			
Printing and Typesetting Volume A	11,646		36,619
Printing and Typesetting Volume C	7,779		38,225
Printing and Typesetting Volume B	(5,379)		-
Printing and Typesetting Teaching Edition of Volume A	6,296	20,342	-
		<u>22,152</u>	<u>78,844</u>
Editorial expenses:			
Editorial honoraria	10,449		3,085
Secretarial assistance, postage and office equipment	11,703		7,619
Technical Editing	-	22,152	3,625
		<u>42,494</u>	<u>89,173</u>
<b>TOTAL EXPENDITURE</b>		<b>42,494</b>	<b>89,173</b>
<i>Excess of income over expenditure</i>		<u>78,172</u>	<u>156,576</u>
<b>Reconciliation of movements</b>			
Balance at 1 January		264,045	195,075
Transfers to other funds:			
Research and Education Fund	60,000		-
Publications and Journals			50,000
Development Fund	-		-
<i>Journal of Synchrotron Radiation</i> Fund	90,000	(150,000)	(50,000)
		<u>78,172</u>	<u>156,576</u>
Excess of income over expenditure		78,172	156,576
Fluctuations in rates of exchange		2,874	(37,606)
<b>Balance at 31 December</b>		<u><u>195,091</u></u>	<u><u>264,045</u></u>

**Book Fund Account for the year ended 31 December 1996**

	Note	1996	Swiss Francs 1995
<b>Income</b>			
Sales of copies, net of Publisher's commission on sales			
<i>Atlas of Crystallography</i> (1995 net)		332	857
<i>World Directory of Crystallographers</i> 9th Edition		1,267	25,548
Sundry Publications		182	1,178
<i>Structure Reports</i>		2,120	-
Royalties			
IUCr/OUP Book series		1,158	2,017
		<hr/>	<hr/>
TOTAL INCOME		5,059	29,600
<b>Expenditure</b>			
Publication expenses:			
<i>World Directory of Crystallographers</i> 9th Edition		1,419	24,134
		<hr/>	<hr/>
TOTAL EXPENDITURE		1,149	24,134
		<hr/>	<hr/>
<i>Excess of income over expenditure</i>		3,640	5,466
		<hr/> <hr/>	<hr/> <hr/>
<b>Reconciliation of movements</b>			
Balance at 1 January		12,522	8,839
Transfers between funds:			
to Ewald Fund		(615)	-
Excess of income over expenditure		3,640	5,466
Fluctuations in rates of exchange		1,518	(1,783)
		<hr/>	<hr/>
Balance at 31 December		17,065	12,522
		<hr/> <hr/>	<hr/> <hr/>

**Publications and Journals Development Fund Account for the year ended 31 December 1996**

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Investment income	7	20,313	22,112
<b>Expenses</b>			
Computer expenses:			
Purchase of computer equipment and software	17,722		57,462
Programming and development	174,880	192,602	112,784
		<u>192,602</u>	<u>170,246</u>
Electronic Publishing Committee/Section			
Editors Meeting		1,573	17,047
Electronic Publishing Project		46,546	4,597
Depreciation on leasehold property		12,637	-
		<u>60,756</u>	<u>21,644</u>
<b>TOTAL EXPENDITURE</b>		<b>253,358</b>	<b>191,890</b>
<i>Deficit of income over expenditure</i>		<u><u>(233,045)</u></u>	<u><u>(169,778)</u></u>
<b>Reconciliation of movements</b>			
Balance at 1 January		579,275	556,554
Transfers from other Funds:			
<i>Journal of Applied Crystallography</i> Fund	-		50,000
<i>Structure Reports</i> Fund	85,979		25,000
<i>International Tables</i> Fund	-		50,000
General Fund	100,000		50,000
<i>Acta Crystallographica</i> Fund	175,000	360,979	100,000
		<u>360,979</u>	<u>275,000</u>
Deficit of income over expenditure		(233,045)	(169,778)
Fluctuations in rates of exchange		9,288	(82,501)
Balance at 31 December		<u><u>716,497</u></u>	<u><u>579,275</u></u>

**Research and Education Fund Account for the year ended 31 December 1996**

	Note	Swiss Francs	
		1996	1995
Investment income	7	40,416	41,535
<b>Expenses:</b>			
Young Scientists' Support	64,409		90,709
Moscow ECM Funds	9		-
Visiting Professorship Programme	1,290		3,861
		<u>65,708</u>	<u>94,570</u>
<b>TOTAL EXPENDITURE</b>		<b>65,708</b>	<b>94,570</b>
<i>Deficit of income over expenditure</i>		<u><u>(25,292)</u></u>	<u><u>(53,035)</u></u>
<b>Reconciliation of movements</b>			
Balance at 1 January		739,304	787,530
Transfers from other Funds:			
<i>Acta Crystallographica</i> Fund	-		60,000
<i>Journal of Applied Crystallography</i> Fund	50,000		50,000
<i>International Tables</i> Fund	60,000	110,000	-
		<u>110,000</u>	<u>110,000</u>
Deficit of income over expenditure		(25,292)	(53,035)
Fluctuation in rates of exchange		12,320	(105,191)
Balance at 31 December		<u><u>836,332</u></u>	<u><u>739,304</u></u>

**Ewald Fund Account for the year ended 31 December 1996**

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Investment income	7	15,335	16,188
<b>Expenditures</b>			
Selection Committee and expenses		2,520	632
Ewald Prize		36,000	-
<i>(Deficit)/excess of income over expenditure</i>		<u>(23,185)</u>	<u>15,556</u>
<b>Reconciliation of Movements</b>			
Balance at 1 January		294,098	270,428
Transfers from other Funds:			
Book Fund	615	-	-
General Fund	50,000	50,615	50,000
<i>(Deficit)/excess of income over expenditure</i>		<u>(23,185)</u>	<u>15,556</u>
Fluctuations in rates of exchange		4,807	(41,886)
Balance at 31 December		<u>326,335</u>	<u>294,098</u>

**Newsletter Fund Account for the year ended 31 December 1995**

	Note	Swiss Francs	
		1996	1995
<b>Income</b>			
Income from advertisements		65,521	46,067
Reimbursement for CGA-17 second circular		-	17,048
<b>TOTAL INCOME</b>		<u>65,521</u>	<u>63,115</u>
<b>Expenditure</b>			
Editorial honoraria		4,585	4,060
Editorial expenses		32,110	20,974
Newsletter printing and distribution		79,396	96,053
Advertising costs		16,380	11,517
<b>TOTAL EXPENDITURE</b>		<u>132,471</u>	<u>132,604</u>
<i>Deficit of income over expenditure</i>		<u>(66,950)</u>	<u>(69,489)</u>
<b>Reconciliation of movements</b>			
Balance at 1 January		51,741	53,599
Transfers from other Funds:			
General Fund		75,000	75,000
Deficit of income over expenditure		(66,950)	(69,489)
Fluctuation in rates of exchange		894	(7,369)
Balance at 31 December		<u>60,685</u>	<u>51,741</u>