

### 1. Nineteenth General Assembly and International Congress of Crystallography

The Nineteenth General Assembly and International Congress of Crystallography were held at the Palexpo Conference Center, Geneva, Switzerland, 6–15 August 2002, by invitation of the Israeli Crystallographic Society. A report, including a detailed report of the General Assembly, has been published [*Acta Cryst.* (2003), **A59**, 374–433].

The General Assembly and Congress were attended by 1,835 scientists, 120 accompanying members and 35 exhibitors from 56 countries. The Sixth Ewald Medal and prize were accepted by Professor M. M. Woolfson at the Opening Ceremony. There were 31 Keynote Lectures, 95 Microsymposia and 14 Open Commission Meetings. The early afternoon sessions were reserved for poster sessions. The abstracts in the published book of Collected Abstracts were prepared from electronic submissions and were also provided on a CD-ROM. A commercial exhibition comprising 35 companies and booksellers was organized. Computer terminals to enable e-mail access for all attendees were provided.

The General Assembly met on the evenings of Wednesday 7 August, Thursday 8 August and Tuesday 13 August. Changes in the names of the Adhering Bodies of Belgium and South Africa were accepted. The change in Category of Adherence of the Adhering Body for the Czech and Slovak Republics from Category I to Category II was accepted. The Minutes of the Eighteenth General Assembly in 1999 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 Eighteenth General Assembly in 1999. New officers of the Union, Chairs and members of Commissions and Union Representatives were elected; the full list of these people is given as an Annex to the report of the Nineteenth General Assembly and Congress. The formation of a new Commission on Inorganic and Mineral Structures was approved. Reports of the Chair of the Sub-committee on the Union Calendar, of the Chair of the Committee on Electronic Publishing, Dissemination and Storage of Information, of the Chair of the Committee for the Maintenance of the CIF Standard, of the Chair of the Promotion Committee, of the Chair of the Committee on Crystallographic Databases and of the Editor of the *IUCr Newsletter* were received. 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 1,000 for the years 2003–2005 inclusive. It reaffirmed its decision to hold the Twentieth General Assembly and Congress in Florence, Italy, in 2005. It also provisionally accepted an invitation from the Science Council of Japan and the Crystallographic Society of Japan to hold the Twenty-First General Assembly and Congress in Osaka, Japan, in 2008.

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.

### 2. Other meetings

Other meetings held in 2002 and sponsored by the Union were:

International School on Powder Diffraction, Calcutta, India, 20–23 January (moved from 12–14 November 2001).

First Moroccan School of Crystallography, Marrakesh, Morocco, 29 January–1 February.

School on Computer-Based Crystallographic Teaching Methods, Ismailia, Egypt, 2–7 February (moved from 3–8 November 2001).

European Powder Diffraction Conference (EPDIC-8), Uppsala, Sweden, 23–26 May.

From Genes to Drugs *via* Crystallography, Erice, Italy, 23 May–2 June.

XII International Conference on Small-Angle Scattering, Venice, Italy, 25–29 August.

XII International Symposium on Supramolecular Chemistry (ISSC-XII), Eilat, Israel, 6–11 October.

### 3. Executive Committee

The membership of the Executive Committee, including new members elected at the General Assembly in 2002, is as follows:

President: Professor W. L. Duax (USA); Vice-President: Professor L. A. Aslanov (Russia); General Secretary and Treasurer: Professor S. Larsen (Denmark); Immediate Past President: Professor H. Schenk (The Netherlands); Ordinary members: Professor M. A. Carrondo (Portugal), Professor G. Heger (Germany), Professor Y. Ohashi (Japan), Professor I. L. Torriani (Brazil), Professor D. Viterbo (Italy), Professor Z. Zhang (People's Republic of China).

### 4. Publications

Volume 58 of *Acta Crystallographica*, Volume 35 of *Journal of Applied Crystallography* and Volume 9 of *Journal of Synchrotron Radiation* were published.

### 5. 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 Nineteenth General Assembly and International Congress of Crystallography [*Acta Cryst.* (2003), **A59**, 374–433].

## 6. Work of the Commissions

### 6.1. Commission on Journals

**6.1.1. Overview.** The year saw the publication of a total of 9,078 pages and 2,369 articles compared with 9,215 pages and 2,464 articles in 2001; the distribution across the IUCr journal titles has been buoyant. Last year concern was flagged with respect to the considerable variations in published pages in the *Journal of Synchrotron Radiation (JSR)*. As a result of initiatives taken, for example with Special Issues on focused topics, the variations have been smoothed out and the number of pages increased to the benefit of readers and authors in the synchrotron-radiation field. 2002 was also the first year in which the complete back catalogue of IUCr journals became available from **Crystallography Journals Online**. There have been many favourable comments on its utility. Benchmarks must also include the impact on journal subscriptions and on the journal rankings as readers and authors alike are hopefully attracted in expanding numbers to the IUCr journals as a vehicle for crystallographic science publications. We are now in a position to compete fully in the e-publications era. The promotion of the journals is also vital, and 2002 marked the third year of such activity by the Journals Working Group. In consultation with relevant Editors, we have so far designed and distributed a general publicity leaflet for the journals, as well as leaflets for *Acta Cryst.* Section D (in combination with Volume F of *International Tables for Crystallography*), *Acta Cryst.* Section E and the *Journal of Applied Crystallography (JAC)*. The Journals Working Group also spearheaded the compilation of the IUCr's first themed CD-ROM: Selected papers on X-ray diffraction physics, edited by A. Authier and M. Hart. In addition, highlighting of articles from our journals has continued in the *IUCr Newsletter*. We gratefully acknowledge the co-operation of the Editor of the *Newsletter* (Professor W. L. Duax) with that activity. At the Geneva Congress, in discussion with the Executive Committee, it has been agreed to highlight more articles per issue of the *Newsletter* by moving instead to a press release style statement of important results.

Last year's report thanked several retiring Editors, namely Professor A. Authier (Section Editor of *Acta Cryst.* Section A), Dr F. H. Allen (Section Editor of *Acta Cryst.* Section B), as well as Professor S. S. Hasnain and Dr H. Kamitsubo (two of the Main Editors of *JSR*). I welcome now their successors: Professor D. Schwarzenbach (Editor of *Acta Cryst.* Section A), Professor C. P. Brock (Editor of *Acta Cryst.* Section B), Professors Å. Kvik and T. Ohta (Main Editors of *JSR*, joining Dr D. M. Mills). The year end of 2002 also saw the retirement, after 10 years, of Dr J. P. Glusker as Editor of *Acta Cryst.* Section D. Jenny had magnificently steered *Acta Cryst.* Section D through its establishment phase and finally into being a very buoyant monthly journal of many pages per issue. On behalf of all biological crystallographers I extend a heartfelt thanks to her. Jenny, in fact, has two successors, Professor E. N. Baker and Dr Z. Dauter, a measure in itself of the success in depth and breadth of *Acta Cryst.* Section D.

I wish to make a hearty thank you to the retiring President, Professor Henk Schenk. Henk's contribution to the development of the journals has been important with the many useful ideas he has given, for example, at the IUCr Finance Committee meetings. Especially vital, but not exclusively, has been his input to the *Acta Cryst.* Section E initiative and to *JSR*. Finally, as ever, I have greatly appreciated the high professional interactions and knowledge of the IUCr Chester staff, notably Peter Strickland (Managing Editor), Brian McMahon (Research and Development Officer), Andrea Sharpe (Promotions Officer) and Mike Dacombe (Executive Secretary), and indeed all the IUCr staff at Abbey Square, Chester, UK.

A survey of the contents of the IUCr journals is given in Table 1. Details of each journal can be found in the reports below.

#### J. R. Helliwell, Chair

**6.1.2. *Acta Crystallographica* Section A.** Section A published 630 pages in 2002, its content comprising 65 Research Papers, 14 Short Communications, as well as Obituaries, Letters to the Editor and Book Reviews. These numbers are comparable to those of 2000, but lower than those of 2001 by 173 pages or 10 Research Papers. We conclude that some of the decrease is due to a smaller average number of pages per publication. In addition, Section A comprises 372 pages, plus indexes, of abstracts of contributions presented at the IUCr's Geneva Congress. A special issue on Phase Transitions is planned for 2003.

The very diverse topics of the papers touched on all aspects of crystallography, ranging from materials science and biology to mathematics, including geometry of structures, symmetry, structure determination, computation, charge distribution, diffraction theory, electron microscopy, real structure and imperfections. The authorship was truly international. Roughly one half of the submitting authors were from Europe, one quarter from North America and one quarter from Asia and Australia. Co-editors show roughly the same geographical distribution.

The average handling time is stable at 2.6 months. Several Co-editors are handling electronically the bulk of the submissions for which they are responsible. The distribution of submissions by Chester in the form of pdf files should further improve handling times in 2003. The rejection and withdrawal rate is 25%.

#### D. Schwarzenbach, Editor of Section A

**6.1.3. *Acta Crystallographica* Section B.** The 2002 statistics for Section B show significant growth relative to previous years, mainly because of the publication of a special issue. If the counts for that issue are removed (13 articles; 106 pages) then the growth is more modest (877 pages in 2001 to 982 pages in 2002). The number of regular articles was about the same as in 2001 but the average length increased slightly. The special database issue, which appeared in June as Number 1 of Part 3, was a joint issue with Section D. The intent was to document the databases, their associated software, and their applications. It is expected that these articles will be referenced widely; the issue is being marketed independently. Pages appropriate to Sections B and D were numbered separately. Subscribers to Section B received an issue with a Section B cover and the B pages printed first, while subscribers to Section D received an issue with a Section D cover and the D pages printed first. The distribution of articles among the classifications inorganic, metal-organic and organic fluctuates over the years, but it appears that papers about molecular crystals are becoming more frequent relative to papers about inorganic crystals. The impact factor of Section B rose again, this time from 1.73 to 1.96. The impact factor has risen each year since 1997, when it was 1.46. The Chester staff discussed the new electronic submission system at some length with the new Section Editor. The first version of that system will be implemented in early 2003. Discussions about the numerical values that should appear in the printed version (for example, in Table 1) and about some aspects of the checking procedure continue. Colour figures became increasingly common in 2002 and will be even more common in 2003. The colour enhances the visual appeal of the journal pages. At the end of September 2002, Frank Allen retired as Editor of Section B after nine years of exceptional service. He set a high standard for others to

**Table 1**  
Survey of the contents of IUCr journals.

*Acta Crystallographica*

Vol.	Year	Number of pages§	Number of papers	Full Articles†		Short Communications‡	
				Number	Average length	Number	Average length
A54	1998	1049	113	103	9.7	10	1.7
B54		943	106	103	8.8	3	2.3
C54		2026	884	874	3.1	10	1.2
D54		1500	229	213	6.3	26	3.5
A55	1999	1073	122	99	9.7	23	4.3
B55		1128	126	113	9.6	13	1.6
C55		2192	929	924	2.4	5	4.4
D55		2079	394	394	5.4	39	3.1
A56	2000	649	82	68	8.2	14	6.0
B56		1127	137	124	8.6	13	1.2
C56		2179	943	591	2.8	352	1.3
D56		1723	339	300	5.3	39	2.4
A57	2001	803	103	78	8.9	25	5.6
B57		877	110	100	8.6	10	1.6
C57		1504	545	541	2.7	4	2.8
D57		1980	390	349	5.2	41	3.3
E57		1998	800	795	2.5	5	1.7
A58	2002	630	102	65	8.0	37	2.8
B58		1088	132	115	8.9	17	1.1
C58		1570	535	531	2.6	4	1.8
D58		2243	457	425	5.0	32	2.3
E58		2374	922	918	2.3	4	2.4

*Journal of Applied Crystallography*

Vol.	Year	Number of pages§	Number of papers	Full Articles		Short Communications††		Short items‡‡	
				Number	Average length	Number	Average length	Number	Average length
31	1998	988	162	104	7.7	33	3.4	25	2.2
32	1999	1208	192	126	7.9	28	4.5	38	1.9
33	2000	1468	259	190	6.1	43	4.1	26	1.3
34	2001	798	140	93	7.1	21	3.5	26	1.5
35	2002	760	128	83	7.2	25	4.0	20	1.6

*Journal of Synchrotron Radiation*

Vol.	Year	Number of pages§	Number of papers	Full Articles		Short Communications		Short items‡‡	
				Number	Average length	Number	Average length	Number	Average length
5	1998	1431	371	86	6.0	285	3.0	0	0
6	1999	1209	69	57	8.1	2	2.0	10	2.2
7	2000	419	65	58	6.6	4	2.8	3	1.3
8	2001	1255	376	70	5.4	280	2.9	26	1.1
9	2002	413	93	68	5.5	2	4.0	23	0.7

§ Numbered pages excluding contents pages. † Including Lead Articles and Topical Reviews for Sections A, B and D, and Crystallization Papers for Section D. ‡ Including Addenda & Errata, Letters to the Editor, IUCr Notices, Notes & News, Book Reviews, Books Received, Obituaries, Scientific Comments, Abstracts, Current Events and Editorials. †† Including Addenda & Errata, Computer Programs and CIF Applications. ‡‡ Including Letters to the Editor, Laboratory Notes, Meeting Reports, Cryocrystallography Papers, Computer Program Abstracts, IUCr Notices, Notes & News, Book Reviews, Books Received, Obituaries, Crystallographers, Commission Reports, New Products, Abstracts, Current Events and Editorials.

follow. The assistance provided by the fine staff in Chester during the transitional period is gratefully acknowledged.

**C. P. Brock**, Editor of Section B

**6.1.4. Acta Crystallographica Section C.** Section C published 1,570 pages in 2002 comprising 531 Full Papers compared with 1,504 pages (541 Full Papers) in 2001. Meetings of the Section C editorial group prior to the Geneva Congress concentrated on how to make easier

the submission process for *Acta Cryst.* Sections C and E. To this end, there has been a thorough revision of the checkcif process that authors are required to use prior to submission. Section C publication times have continued to improve and are now under a month from submission to publication for the majority of papers. Proofed papers are posted on the web on a weekly basis and receive an online publication date when they appear on the web site. As before, at the end of a month, the online papers are collected and published as the

next month's issue of Section C. Diagrams in the printed version of Section C continue to be in black and white, but diagrams submitted in colour appear in colour in the HTML and PDF format versions of the papers *via* the web. It is a pleasure to thank the Co-editors, anonymous referees and the dedicated Chester staff for their invaluable assistance in the preparation of Section C. New Co-editors and members of the Section C Editorial Board this year include J. Barbier (McMaster University, Canada), L. R. Falvello (Universidad de Zaragoza, Spain), G. J. Gainsford (Industrial Research Limited, New Zealand), J. A. Krause-Bauer (University of Cincinnati, USA), P. J. Squattrito (Central Michigan University, USA) and M. Tremayne (University of Birmingham, UK). I also acknowledge and warmly thank C. P. Brock (University of Kentucky, USA), I. D. Brown (McMaster University, Canada) and M. Vijayan (Indian Institute of Science, India), who have now retired from the Section C Editorial Board, for their services to Section C and to the crystallographic community.

#### G. Ferguson, Editor of Section C

**6.1.5. Acta Crystallographica Section D.** There were fourteen issues of Section D in 2002 and, of these, three were special issues. One, jointly with Section B (with editors F. H. Allen and J. P. Glusker), was published on current crystallographic structural databases and examples of their use. Databases described in this issue included the Cambridge Structural Database, the Protein Data Bank, the Nucleic Acid Database, the Biological Macromolecule Crystallization Database, the Metals Data File, the Powder Diffraction File, the NIST Surface Structure Database, and the Inorganic Crystal Structure Database. In October, we published the Proceedings of the Ninth International Conference on the Crystallization of Biological Macromolecules, which was held in Jena, Germany, 23–28 March 2002. This issue, with Guest Editors M. Riès-Kautt and R. Hilgenfeld from Paris and Jena, respectively, consisted of 52 research papers and reports on 10 new commercial products. The conference, with 420 participants, saw the creation of the International Organization for Biological Crystallization with Professor Hilgenfeld as President. We were also fortunate to be able to publish the Proceedings of the CCP4 study weekend on High-Throughput Structure Determination, comprising 12 research papers. The Organizers were A. Ashton, P. Broadhurst, and M. H. Eales and the Guest Editors were R. Esnouf, D. Stuart and K. Wilson. They noted that 'A tidal wave of high throughput technology is sweeping through biology revolutionizing research methods, and structural biology will not be spared. Crystallographers have traditionally been at home with technology and sophisticated software so it is perhaps not surprising that improvements in software for phasing and refinement and steps towards beamline automation lead the way, but new techniques and ideas for protein production and crystallization are now catching up'. This highlights the changes in technology that Section D is currently addressing, evident, for example, in a lead article describing the 'automation of crystal optimization techniques for adaptation to high-throughput techniques'.

In 2002, Section D contained 456 scientific articles. Three-dimensional coordinates and structure factors of a total of 155 macromolecular crystal structures of biological interest reported in this journal were deposited in the Protein Databank (three currently 'on hold'), and four oligonucleotide structures were deposited in the Nucleic Acid Database. The resolution of these reported structures, covering a wide range of molecular weight, continues to improve; three had a resolution better than 1 Å and 20 had a resolution better than 1.3 Å. Three 'crystallization Co-editors', N. Chayen, M. Pusey

and A. Zagari, were in charge of the crystallization papers, of which there were 219 in 2002. Illustrations continue to be essential to the success of this journal; colour figures are free to the authors. The cover of each monthly journal portrays an interesting structure or item of information from the scientific contents of that month. Table 2 lists structure determinations (with resolution) published during 2002.

Research articles, in addition to structure reports and analyses, covered a wide range of subjects. Several involved phase determination and extension, including phasing *via* SAD, MAD, SIRAS and MIRAS, the use of noble gases to improve phase determination and the estimation of triplet phases from three-beam diffraction. Articles on the preparation and handling of crystals, twinning, and solvent and detergent effects, and on experimental methods of data collection (including small-angle scattering for macromolecules) will be useful for readers. Other articles involved structure refinement, model building, precision assessment, and the fitting of electron density (including electron-microscopy reconstruction maps and the use of noncrystallographic symmetry). Structural results were accessed in articles on conformational analysis, interactions of macromolecules with ligands and applications of structural conclusions to the World Wide Web.

The invaluable assistance of reviewers who comment in detail on each submitted article is again acknowledged and they, together with the staff at Chester, ensure that this is a high-quality journal. The editorship of the journal is now passed on to the excellent team of Z. Dauter and E. N. Baker. My thanks to all, particularly Louise Jones in Chester, for support during my ten years as editor.

#### J. P. Glusker, Editor of Section D

**6.1.6. Acta Crystallographica Section E.** The IUCr's purely electronic journal continues to flourish. In its second year of operation, 922 papers were published, an increase of 15% over the previous year; the August issue contained 102 papers and the December issue 100. The contributions were distributed as follows: inorganic 5%, metal-organic 32% and organic 63%. It is interesting to note that, as in 2001, there has been a very large proportion of papers originating from laboratories in India, South-East Asia and the People's Republic of China. Publication continues to be extremely rapid.

Efforts have been made to rationalize the checking of CIF files by a combination of *checkcif* and *PLATON*. A number of people have had an opportunity to test the new scheme, with the intention of making it fully available in 2003. The CIF editor, *enCIFer*, provided by the Cambridge Crystallographic Data Centre, has also made progress into  $\beta$  testing, and should shortly be released to the public, making the production of manuscripts significantly easier.

To cope with the increasing workload, three more Co-editors have been appointed, *viz* J. L. Flippen-Anderson (RCSB Rutgers, USA), A. Lough (University of Toronto, Canada) and H. Stoeckli-Evans (University of Neuchâtel, Switzerland), bringing to 17 the total number of Co-editors. Their dedicated work, and that of the Chester editorial staff, continues to promote the success of the journal.

#### W. Clegg and D. G. Watson, Editors of Section E

**6.1.7. Journal of Applied Crystallography.** *JAC* published 760 pages in 2002 (about 5% less than in 2001). This included 98 full research papers and 40 shorter papers. The new leaflet aiming at convincing biologists, chemists, physicists and materials scientists to place their crystallography-based work in *JAC* was widely distributed. Seven Co-editors retired in 2002 after nine and sometimes even more years of dedicated service; H. Hashizume (Japan), C. Howard

**Table 2**

Some of the macromolecular crystal structures reported in 2002 in Section D

Structure	Resolution
<b>With PDB entries</b>	
<i>0.8–1.0 Å and better</i>	
High-potential iron–sulfur protein	0.8 Å
Catalase	0.88 Å
Human type VI collagen	0.9 Å
<i>1.0–1.5 Å</i>	
Nitric oxide reductase	1.0, 1.05 Å
Endoglucanase A	1.0 Å
NH <sub>2</sub> -dependent NAD <sup>+</sup> synthetase	1.0 Å
RNase Sa	1.0 Å
Trypsin inhibitor	1.0 Å
Ribonuclease A at 6 pH values	1.05–1.15 Å
Rhamnolacturonan acetyltransferase	1.12 Å
Modified photoactive yellow protein plus caffeic acid	1.16 Å
Arginine kinase	1.2 Å
Maltodextrin-binding protein	1.2 Å
Thaumatococcus crystallized with glycerol	1.25 Å
Lipase	1.3 Å
RhoGDI	1.3 Å
Snake-venom metalloproteinase	1.35 Å
Thaumatococcus crystallized with glycerol	1.36 Å
Endoglucanase	1.4 Å
Lysozyme structure: temperature dependence	1.4 Å
Mutant chitinase beta	1.45 Å
Phytotoxic cryptogein plus cholesterol	1.45 Å
<i>1.5–2.0 Å</i>	
Catalase	1.5, 1.74, 1.96 Å
N-Acetyl-L-glutamate kinase	1.5 Å
Xenon-derivatized halide-soaked proteins	1.5 Å
Endoglucanase	1.55 Å
Thymidylate kinase plus caged ATP	1.55, 1.6 Å
Xylose isomerase (triiodide)	1.55 Å
Concanavalin A	1.56 Å
Endoglucanase	1.6 Å
Platinated decanucleotide	1.6 Å
Thymidylate kinase plus caged ATP	1.6 Å
Oligonucleotide (hexamer)	1.64 Å
Ribonuclease binase	1.65 Å
P3 from bacteriophage PRD1	1.65 Å
apo-S100A3	1.7 Å
Barnase mutants	1.7 Å
Elastase	1.7, 1.85 Å
Gd-HPD03A	1.7 Å
Glucosamine-6-phosphate deaminase	1.73 Å
TRAP–RNA complexes	1.75 Å
Lysozyme	1.77 Å
3-Dehydroquinase	1.78 Å
Barnase mutants	1.8 Å
$\beta$ -Cinnamomin	1.8 Å
Cytochrome <i>b<sub>5</sub></i> mutants	1.8, 1.9 Å
FERM domain of merlin	1.8 Å
Lysozyme and stabilizing additives	1.8 Å
Nudix protein	1.8, 1.85 Å
Pectate lyase	1.8 Å
Phosphatidyl ethanolamine-binding protein	1.8 Å
Trematode hemoglobin	1.85 Å
Allosteric effectors of hemoglobin	1.87 Å
Glucosamine-6-phosphate deaminase	1.9 Å
Acetate CoA-transferase $\alpha$ -subunit	1.9 Å
Cellulohydrolase Ce16A mutant	1.9 Å
Dihydrofolate reductase ternary complex	1.9 Å
Lysozyme and stabilizing additives	1.9, 1.95 Å
Mucosal addressin cell-adhesion molecule	1.9 Å
Mutant plasmepsin II	1.9 Å
Ovotransferrin	1.9, 1.95 Å
Immunoglobulin light-chain dimer	1.94 Å
Type III secretion chaperone SycE	1.95 Å
<i>2.0–2.5 Å</i>	
Barnase mutants	2.0, 2.03 Å
Carbonmonoxyhemoglobin C	2.0 Å
Grass pollen allergen Phlp 5b	2.0 Å
Lysozyme and stabilizing additives	2.0, 2.1 Å
Phospholipase A2 plus ligand	2.0 Å
Ribonuclease binase	2.0 Å
Space- versus earth-grown aminoacyl-tRNA synthetase	2.0 Å
Apoferitin	2.01 Å

**Table 2 (continued)**

Structure	Resolution
RNase-related protein	2.05 Å
3-Dehydroquinase	2.1 Å
Dihydrofolate reductase ternary complex	2.1 Å
Endoglucanase	2.1 Å
Pectate lyase	2.1 Å
Lactamase	2.13 Å
Transferrin	2.15 Å
Carbonmonoxyhemoglobin	2.16 Å
Glucosamine-6-phosphate deaminase	2.2 Å
Mutant cathepsin S	2.2 Å
P3 from bacteriophage PRD1	2.2 Å
Periplasmic chaperone SfaE	2.2 Å
Phosphoglycerate kinase	2.3 Å
Thermolysin	2.3 Å
Four-way Holliday junction oligonucleotide (decamer)	2.35 Å
$\beta$ -Lactoglobulin	2.4 Å
Dihydrofolate reductase ternary complex	2.4 Å
Methyltransferase with trefoil knot	2.4 Å
Netropsin-decamer complex	2.4 Å
Nudix protein	2.4 Å
Triose phosphate isomerase	2.4 Å
<i>2.5–3.0 Å</i>	
Endoglucanase	2.5 Å
Inhibited aldose reductase	2.5 Å
Matrix metalloproteinase MMP9	2.5 Å
Peroxidase C	2.5 Å
TRAP–RNA complexes	2.5 Å
Venom acidic phospholipase A <sub>2</sub>	2.5 Å
Cyclized green fluorescent protein	2.6 Å
Oxy- and deoxyhemoglobin	2.6, 2.7, 2.8 Å
Transferrin	2.6 Å
Bacterioferritin	2.6 Å
AhrC, arginine repressor/activator protein	2.7 Å
Creatine amidinohydrolase	2.7 Å
Hexameric S100A12	2.7 Å
Pyruvate formate-lyase	2.7 Å
Ribosomal protein L1	2.7 Å
Rhamnolose-1-phosphate aldolase (class II)	2.7 Å
Garlic lectin	2.8 Å
Glyceraldehyde-3-phosphate dehydrogenase	2.8 Å
Acetylcholinesterase	2.85 Å
Uracil DNA glycosylase	2.9 Å
<i>3.0–3.5 Å</i>	
3-Carboxy- <i>cis,cis</i> -muconate lactonizing enzyme	3.0 Å
Glyceraldehyde-3-phosphate dehydrogenase	3.0 Å
Lactoferrin N-lobe	3.0 Å
Uracil phosphoribosyltransferase	3.0 Å
Oxy- and deoxyhemoglobin	3.1, 3.3 Å
C-Reactive protein	3.15 Å
Apolactoferrin	3.2 Å
Uracil DNA glycosylase	3.2, 3.35 Å
Chaperonin-10	3.5 Å
Cytochrome <i>c<sub>6</sub></i>	3.5 Å
<b>No PDB entry</b>	
Copper nitrite reductase	1.0 Å
Thaumatococcus crystals in space	1.28 Å
Flavodoxin	1.34, 1.44 Å
Typaredoxin II	1.5, 2.5 Å
Cocaine hydrolytic antibody	2.35 Å
<b>Theoretical model</b>	
Xenon-derivatized halide-soaked proteins	

(Australia), T. C. Huang (USA), K. Moffat (USA), O. Nittono (Japan), J. S. Pedersen (Denmark) and J. Vicat (France) deserve our gratitude for their input to the well being of the journal. Seven new Co-editors – A. J. Allen (USA), D. Chateigner (France), E. Dodson (UK), S. E. Ealick (USA), J. L. Hodeau (France), K.-I. Ohshima (Japan) and T. R. Welberry (Australia) – started their work with great enthusiasm during the past year. Another small-angle scattering conference took place (in Venice, Italy) in August 2002, and more than 100 accepted manuscripts are now in the production stage as a

special issue of *JAC*. I join the Commission Chair in expressing my gratitude to the Chester staff for handling ordinary and extraordinary matters with admirable professionalism.

**G. Kosterz**, Editor of *JAC*

**6.1.8. Journal of Synchrotron Radiation.** *JSR* published 68 full articles and a total of 413 pages in the six issues produced in the 2002 calendar year. We expect these numbers to increase next year as the number of manuscripts submitted in 2002 was up by 17% over the previous year. Selected papers from two international workshops, the 5th Harima International Forum on New Aspects of X-ray Imaging Technology with Synchrotron Radiation – Present Status and Future Possibilities, held at SPring-8, Hyogo, Japan, in July 2001, and the 2nd International Workshop on X-ray Damage to Crystalline Biological Samples, held at the Advanced Photon Source, Argonne, USA, in December 2001, were published in *JSR* in 2002. We believe that the publication of selected papers from workshops is an important service to the synchrotron-radiation community and we plan to continue to do so in the future. Two new Main Editors were appointed in 2002, Å. Kvick (ESRF, France) and T. Ohta (University of Tokyo, Japan), to replace S. S. Hasnain and H. Kamitsubo, who retired as Main Editors. In addition, seven new Co-editors [L. Berman (NSLS, Brookhaven, USA), A. Freund and H. Graafsma (ESRF, Grenoble, France), S. S. Hasnain (SRS, Daresbury, UK), G. Ice (ORNL, Oak Ridge, USA), A. Iida (Photon Factory, Tsukuba, Japan) and H. Kitamura (SPring-8, Hyogo, Japan)] were added to replace retiring Co-editors (Y. Amemiya, M. Ando, D. H. Bilderback, P. Elleaume, R. Fourme, T. Matsushita, S. Mobilio, K. Moffat, I. H. Munro, V. Saile, M. Sauvage-Simkin and H. B. Stuhmann). We would like to take this opportunity to welcome the new Co-editors and thank the outgoing Main Editors and Co-editors, some of whom have served from the inception of the journal, for their dedication and hard work to make *JSR* a success.

Å. Kvick, D. M. Mills and T. Ohta, Editors of *JSR*

## 6.2. Commission on International Tables

The years 2001 and 2002 were rather successful for the series *International Tables for Crystallography*. Whereas in 2001 two volumes, B and F, appeared, in the year 2002 three volumes, A, E and the Brief Teaching Edition of Volume A, have been published. The remaining three volumes, D, G and A1, are scheduled for publication in 2003. All volumes are now computer-produced, which has involved extensive and time-consuming programming and proof-reading work.

With this rather positive state of *International Tables*, the work of the present Chair of the Commission (Th. Hahn) is completed, and he resigned during the Geneva Congress and General Assembly, but has agreed to prepare the present report for 2002. He presented to the Executive Committee his ideas for the future of the *International Tables* project, which were very favourably received. In a Closed Commission Meeting in Geneva, names of potential Chairs were collected and transmitted to the Executive Committee. No appointment of a new Chair has been made at the time of writing this report.

At Geneva, the possibility of electronic versions of volumes of *International Tables* was discussed extensively. The Executive Committee has established a working group to develop proposals for electronic versions of *International Tables*. This working group comprises S. R. Hall (Australia, Chair) and H. D. Flack (Switzerland) as well as B. McMahon and P. R. Strickland from the IUCr office in Chester.

During the Geneva Congress, some members of the Chester staff arranged for an '*International Tables* wine party' (instead of an Open Commission Meeting), which featured an exhibition of all volumes published as well as selected parts of volumes in preparation. The party was very well attended and appreciated by all participants.

The *International Tables* home page was throughout the year updated by U. Shmueli in Tel Aviv, Israel, and B. McMahon at the IUCr office in Chester, with the following URL addresses: <http://crystal.tau.ac.il/xtal/comit/promot.html>, <http://www.iucr.ac.uk/iucr-top/it/index.html>.

**6.2.1. Volume A. Space-Group Symmetry; Editor Th. Hahn.** The Fifth Edition of Volume A was published in April 2002. It is now completely computer-produced and printed from an electronic file, as described in the Section *Computer Production of Volume A*. The volume consists of 911 pages and sold more than 1,100 copies in 2002.

In the same month, April 2002, the Fifth, revised Edition of the Brief Teaching Edition of Volume A also appeared (164 pages). It sold nearly 700 copies in 2002.

**6.2.2. Volume B. Reciprocal Space; Editor U. Shmueli.** The Second Edition of Volume B was published in the spring of 2001 and has sold more than 500 copies since. The editorial activities during the year 2002 dealt mainly with editor–author correspondence regarding possible changes and updates to be introduced in the next edition or revision of the volume. Several informal discussions were held by the Editor with authors of various chapters and sections of Volume B who attended the Geneva Congress. It is planned to summarize the correspondence during the spring of 2003.

Professor M. Tanaka was invited to contribute a section on convergent-beam electron diffraction, based on the corresponding section by the late Professor P. Goodman plus new developments in this field.

**6.2.3. Volume C. Mathematical, Physical and Chemical Tables; Editor E. Prince.** Because the stock of the Second Edition of Volume C, which was published in 1999 and has sold about 1,000 copies so far, is projected to run out during 2003, an effort was made to collect necessary and desirable revisions in preparation for a reprinting. The Second Edition was the first of the *International Tables* volumes to be published entirely by electronic typesetting. Because the technology of publication has continued to advance rapidly, an unfortunate result of this is that the existing files are in an obsolete format, and it will be more difficult than we had hoped to make extensive revisions. We anticipate that there will be a Third Edition in 2003/2004.

**6.2.4. Volume D. Physical Properties of Crystals; Editor A. Authier.** The proofs are being sent out to the authors and it is expected that the volume will be printed in the course of 2003.

**6.2.5. Volume E. Subperiodic Groups; Editors V. Kopsky and D. B. Litvin.** Volume E was published in December 2002. It contains 562 + ix pages. In the few remaining days of 2002, 62 copies had already been sold.

**6.2.6. Volume F. Macromolecular Crystallography; Editors M. G. Rossmann and E. A. Arnold.** Volume F was published in July 2001 and has sold more than 900 copies. Two reviews of the volume have appeared, one in *Structure* [(2002), **10**, 289], the other in *Z. Kristallogr.* [(2002), No. 217, pp. 627–628].

**6.2.7. Volume G. Definition and Exchange of Crystallographic Data; Editors B. McMahon and S. R. Hall.** At the request of the Executive Committee, the title of Volume G has been revised to reflect its specific role as a reference handbook for CIF, the current data exchange standard within crystallography. By the start of 2003, drafts of all chapters in the first three Parts of the volume were in hand; a small number are still undergoing active revision. Some chapters are also in hand for Part 4, which deals with software

libraries and applications, but some others have yet to be delivered. Nevertheless, we hope to deliver the complete manuscript to the editorial office by the middle of 2003.

**6.2.8. Volume A1. Maximal Subgroups of Space and Plane Groups; Editors H. Wondratschek and U. Müller.** Volume A1 is now a combination of the data on maximal subgroups of space and plane groups by M. Aroyo, Y. Billiet & H. Wondratschek with the data on Wyckoff positions of group-subgroup related space groups by U. Müller. The volume is nearly completed and under thorough and detailed revision of the text parts. Its completion and delivery to the editorial office is expected for the spring of 2003.

The retiring Chair wishes to extend his sincere thanks to all editors and authors for their capable and loyal co-operation and to the editorial staff at the Chester office for their competent and dedicated work.

**Th. Hahn**, Chair

### 6.3. Commission on Aperiodic Crystals

The activities of the Commission were focused on the organization of international conferences and the coordination of activities between the different communities working on quasicrystals and incommensurate structures.

The organization of the congress Aperiodic 2003 by N. Speziali proceeded. The dates for this meeting have been fixed at 8–13 September 2003 and it will take place at the Federal University of Minas Gerais in Belo Horizonte (Brazil). The web site of Aperiodic 2003 is [http://agora.grude.ufmg.br/QuickPlace/aperiodic2003/Main.nsf/h\\_Toc/](http://agora.grude.ufmg.br/QuickPlace/aperiodic2003/Main.nsf/h_Toc/).

The Commission continued to promote activities on the crystallography of aperiodic crystals at national and international meetings. Two microsymbiosia on aperiodic crystals were organized at the Geneva Congress. One microsymposium on Diffraction and Symmetry Aspects of Aperiodic Crystals was chaired by M. Ohmasa and M. De Boissieu. The second microsymposium on Diffraction by Non-Periodic Structures was chaired by G. Chapuis and T. Janssen. A hot topic was the still unsolved problem of the atomic structures of quasicrystals. Presentations included discussions on diffuse scattering, dynamics and non-ordered aspects of the structures of quasicrystals. The crystal structures of modulated compounds were discussed in the non-harmonic regime.

At the Geneva Congress, an Open Commission Meeting was organized around the question 'What is a crystal?' Although seemingly a simple question, it requires careful consideration of the properties we wish to assign to crystalline materials. One property that does not characterize the crystalline state is a periodic atomic structure. Aperiodic crystals are crystals that lack three-dimensional (3D) translational symmetry. A property that can be assigned to an ideal crystal structure is that it will have infinitely sharp Bragg peaks in the diffraction. For aperiodic crystals, these Bragg reflections cannot be indexed on the basis of a 3D reciprocal lattice. In 1993 'an essentially discrete diffraction diagram' was used by the IUCr as the definition of the crystalline state – see the 1991 Annual Report of the Executive Committee [*Acta Cryst.* (1992), **A48**, 922–946]. A problem with this definition is that it requires the understanding of diffraction. Thus, a motivation for the discussion was to try to develop a definition that generalizes the notion of a periodic array of atoms towards aperiodic crystals, and that can be made easily understandable for non-specialists.

At the Open Commission Meeting, these questions were introduced by S. van Smaalen, W. Steurer and D. Pandey. Subsequently,

they were discussed with many contributions from the audience. An agreement on one particular definition was not obtained, but the discussion led to three statements, that each by itself might characterize the crystalline state:

1. A solid with an essentially discrete diffraction diagram;
2. A solid with an atomic structure with long-range order;
3. A solid with an atomic structure that can be obtained as a section of an  $n$ -dimensional periodic structure ( $n = 3, 4, \dots$ ).

The  $n$ -dimensional periodic structure refers to the superspace description of the crystal structures of aperiodic crystals. Long-range order is defined through the autocorrelation function of the electron or atomic density function. It can be simplified to the statement that crystalline structures are structures for which knowledge of the positions of a few atoms enables one to compute exactly the positions of all atoms, including those at large separations, e.g. 1 m. Advantages of and problems with each of these definitions were discussed.

Following previous work, the CIF dictionary for modulated structures was completed in February 2002. Based on this new CIF dictionary, a database of incommensurately modulated structures and composite crystals was developed. Both projects evolved under the direction of G. Madariaga (Bilbao, Spain), in co-operation with the Committee for the Maintenance of the CIF standard. The CIF standard is available at the IUCr web site. The database is available at the Bilbao Crystallography Server at <http://www.cryst.ehu.es/icsdb/index.html>.

The Commission maintains internet pages at the web site of the IUCr at <http://www.iucr.org/iucr-top/comm/capd/index.html>. A web site on all aspects of the crystallography of aperiodic crystals is maintained by the special interest group (SIG) on aperiodic crystals of the European Crystallographic Association. It is maintained by M. Dusek (Prague, Czech Republic), and may be found at <http://www-xray.fzu.cz/sgip/aphome.html>.

**S. van Smaalen**, Chair

### 6.4. Commission on Biological Macromolecules

The most significant activity of the Commission in 2002 related to the Geneva Congress. The Commission provided pre-meeting support to the Programme Committee in the form of advice on speakers, microsymposium Chairs and topics and on the membership of the Committee itself. Despite the difficulties arising from relocating the meeting from Jerusalem to Geneva, the Congress was very successful. Following the trends of recent years, the macromolecular community was strongly represented with 13 of the Keynote Lectures and 29 of the microsymbiosia in the area of macromolecular crystallography in addition to the hundreds of posters. Spurred on to some degree by the requirements for high throughput generated by structural genomics initiatives, the Congress highlighted new and improved methods ranging from protein crystallization to applications of direct methods and automated structure refinement.

The major activity of the Commission at the Congress was a Joint Open Meeting of the Commissions on Journals and Biological Macromolecules. The purpose of the meeting was to bring to the attention of the community initiatives by the IUCr to provide for high throughput electronic publication of macromolecular structures. These structures might result from structural genomics or, for example, from studies of complexes arising from drug screening. The meeting discussed the need for close liaison with the Protein Data Bank (PDB) to coordinate data deposition and publication. H. M. Berman, from the PDB, outlined procedures being developed jointly with the Editorial staff of *Acta Crystallographica* to provide details

required by the journal directly to the author for incorporation in the electronic publication. It is also envisaged that referees will be provided with copies of the structure verification data compiled by the PDB for every submission.

The Chair had the opportunity in Geneva to meet with the Executive Committee of the IUCr to discuss plans for the Commission and its achievements in the preceding three years. These achievements included the support of a very successful Workshop on Structural Biology held in Bangalore, India, in conjunction with a meeting of the Asian Crystallographic Association (AsCA). The question of the revised requirements for the deposition of coordinates and diffraction data was resolved early in the three-year term of the Commission. Letters were written to the editors of all journals that publish macromolecular crystal structures with generally positive responses. Most journals now enforce the minimum recommendations of the IUCr although some, for commercial reasons, have not enforced the deposition of structure-factor data despite the arguments that these data need to be properly curated to prevent loss. All members of the community should deposit such data and encourage their colleagues to do so.

Members of the Commission have been actively engaged in the planning of national crystallographic meetings and of the meetings of the Regional Associates of the IUCr. There was also a strong representation from the Commission at the inaugural meeting of the International Structural Genomics Organisation held in Berlin, Germany, in November 2002. This new body seeks to provide a forum for the discussion and planning of structural genomics initiatives and has by its nature a large crystallographic membership.

The future plans for the Commission include support of a Workshop on Structural Biology to be held in conjunction with the joint meeting of the Society for Crystallographers in Australia and New Zealand and AsCA in Broome, Western Australia, in August 2003 and a School for Protein Crystallography to be sponsored jointly with the American Crystallographic Association in Brazil in 2004.

**J. M. Guss**, Chair

#### 6.5. Commission on Charge, Spin and Momentum Densities

The main activity of the Commission was the preparation of the Sagamore conference to be held in Broome, Australia, 14–18 August 2003. The Chair will be M. A. Spackman and 90 participants are expected to attend.

**C. Lecomte**, Chair

#### 6.6. Commission on Crystal Growth and Characterization of Materials

2002 has been a transition time for the Commission because of the Geneva Congress and consequent election of Chair and members. As no sponsorships could be given for events falling in the months preceding and following the Congress, there was little chance to promote schools and/or workshops and the activity was necessarily reduced.

Nevertheless, the Commission decided to support the Latin-American Summer School on Crystal Growth, chaired by E. Dieguez, which took place 3–7 July 2002 at the Universidad Autonoma de Madrid (Spain). Two members of our Commission were enrolled as lecturers at the school.

The Commission was partly renewed in August, with inclusion of three new members and three new consultants.

The last months of 2002 were essentially dedicated to the organization of the International School on Crystal Growth of Technologically Important Electronic Materials, co-Chaired by K. Byrappa and R. Fornari. The school will be held in January 2003 in Mysore (India). Ten members and consultants of our Commission will participate in the school as lecturers, which will provide an excellent opportunity for open discussion about future Commission activities.

**R. Fornari**, Chair

#### 6.7. Commission on Crystallographic Computing

The main efforts of the Commission during 2002 were related to the Geneva Congress. It was rather disappointing to see that virtually none of the proposals for computing-related microsymbiosia put forward by the Commission were accepted by the Programme Committee. In contrast, the lunchtime Open Commission meetings were well attended with excellent presentations that would have merited an even wider audience as part of a microsymbiosium.

During the Geneva Congress, a new Commission membership was appointed. An important focus of this Commission will be the realization of several computing-related microsymbiosia as part of the forthcoming Florence Congress. In parallel, work is under way to organize a satellite computing school.

The Commission also started a *Newsletter* (<http://www.iucr.org/iucr-top/ccom/newsletters/>), edited by Commission member L. M. D. Cranswick.

**A. L. Spek**, Chair

#### 6.8. Commission on Crystallographic Nomenclature

The Commission met in closed session at the Geneva Congress. Three working groups are presently active:

(1) Working Group on Co-Crystal Nomenclature [F. H. Allen (Chair), J. L. Atwood, J. D. Dunitz, U. Griesser, F. H. Herbststein, L. R. Nassimbeni, A. Authier]. The group has been established to examine the nomenclature of co-crystals, for which a wide variety of terminologies currently exists, *e.g.* inclusion compound, clathrate, molecular complex, adduct *etc.* An initial meeting was held in Geneva in August 2002, and views are being sought from a range of relevant experts.

(2) Working Group on Phase Identifiers [I. D. Brown (Chair), S. C. Abrahams, M. Berndt, J. Faber, V. L. Karen, W. D. S. Motherwell, J.-C. Toledano, P. Villars, J. Westbrook, B. McMahon (consultant)]. The group is looking for those properties of a condensed phase that can be uniquely assigned and that provide maximum discrimination between different materials and phases. Since phases can only be fully identified if they are completely characterized, it is impossible to generate an identifier that will work in all situations, but the identifier we will propose should be able to retrieve the same phases in different data collections though probably with some false matches. We have not yet given serious consideration to the problems of identifying an agency that could assign a registry number to well characterized phases.

(3) Working Group on Synchrotron Radiation Nomenclature [D. Mills (Chair), Å. Kvik, T. Ohta, I. Robinson, A. Authier]. The group is presently consulting various experts on suitable recommendations regarding the uses of the terms 'brilliance' and 'brightness'.

The web page of the Commission at the IUCr web site has been revamped, <http://www.iucr.org/iucr-top/iucr/cnom.html>.

The IUCr representative on the IUPAC Interdivisional Committee on Nomenclature and Symbols, S. C. Abrahams, reports that the

Committee has been restructured and renamed Interdivisional Committee on Terminology, Nomenclature and Symbols, thus recognizing the importance of terminology.

**A. Authier**, Chair

## 6.9. Commission on Crystallographic Teaching

No report has been received from the Chair.

**R. B. Neder**, Chair

## 6.10. Commission on Electron Diffraction

The past year has seen considerable activity in the field of electron diffraction and microscopy. At the Geneva Congress, several sessions were devoted to electron diffraction. One treated the combination of X-ray crystallography and electron microscopy, chaired by H. Saibil and A. Engel. Another, on electron diffraction, was chaired by H. Zandbergen and Li Fang-hua. Finally, a session on high-resolution electron microscopy was chaired by D. Van Dyck and Y. Matsui. D. L. Dorset, winner of the Patterson Award of the ACA, presented a keynote address on electron diffraction. Since then we have seen sessions on electron diffraction at the ICEM-15 Congress in Durban, South Africa (September 2002) and at the Microscopy Society of America (MSA) meeting in Quebec, Canada (August 2002); another session will be held at the MSA meeting in San Antonio, USA (August 2003). A workshop will be held in Delft, The Netherlands, on electron diffraction (January 2003) and a conference on related matters honouring J. M. Cowley will be held at Arizona State University in January 2003, and a summer school was held at Tampere, Finland in June 2002. A special issue of *Microscopy and Microanalysis* will appear shortly devoted to electron diffraction (J. C. H. Spence, Editor). A special issue of *Zeitschrift für Kristallographie* is similarly planned for 2003 (U. Kolb, Editor). The Commission met at the Geneva Congress and J. C. H. Spence was elected to replace D. L. Dorset as Chair, to whom, with S. Hovmöller, we express our gratitude. The Commission gave the strongest support to biologists in cryomicroscopy to make this forum their home.

A new web page has been established by the Chair, whose temporary site address is <http://www.public.asu.edu/~jspence/ElectrnDiffn.html>. This will be moved to a permanent home at the Chester facility soon, as recommended by the Executive Committee. This site now contains a list of pedagogically sound texts for newcomers to the field, a list of sources for software, a list of recent and forthcoming conferences, and links to many active research groups. The address has been widely circulated by e-mail to active researchers around the world, and may be useful for guiding students to practical texts in the subject.

**J. C. H. Spence**, Chair

## 6.11. Commission on High Pressure

High-pressure crystallography remains a rapidly evolving and expanding field impacting many of the subdisciplines of the IUCr. For this reason, this Commission has organized annual workshops in non-Congress years. These workshops have sometimes emphasized particular specialities, for example synchrotron-based techniques and results, and at other times have attempted to cover the complete breadth of disciplines and techniques. All have emphasized the free exchange of new ideas. The common format of lectures and posters is followed. We have found over several workshops that an emphasis on

devoting considerable time for both formal and informal discussions has been very effective in involving young scientists, especially students. We feel that this active motivation of young scientists is an effective recipe for sustained progress in the field.

### *Geneva Congress*

In 2002, the Commission's activities were embedded in the general Geneva Congress and four microsymbiosia and two Open Commission meetings were organized. This turned out to be at or below the lower level in terms of size in order to be able to represent properly the broad range of interests covered in high-pressure crystallography.

The topics of the microsymbiosia covered purely structural aspects of high-pressure science (Structures and Phase Transitions at High Pressure, Chairs J. Loveday and S. Desgrenier; Extremes of Pressure and Temperature, Chairs R. Hemley and G. Fiquet), but extended also into physical properties (Novel Materials and Physical Properties at High Pressure, Chairs P. McMillan and Y. Fuji) and non-crystalline matter (Liquids and Amorphous Materials at High Pressure, Chairs C. Benmore and O. Shimomura). Reports on these sessions can be found at <http://www.iucr.org/iucr-top/comm/chp/index.html>.

The two Open Commission meetings focused on new technical developments (Experimental Challenges at High Pressure, Chairs M. Kunz and N. Ross) and a very challenging new field, namely the combination of protein crystallography and high pressure (High-Pressure Biology and Soft Matter under Pressure, Chairs R. Winter and K. Heremans). In addition, there were three well attended plenary lectures related to high-pressure crystallography: What High-Pressure Can Do For Us, J. Parise; Pressure-Tuned Crystal Chemistry: H-Bonds *versus* Central Forces in Polymorphs, A. Katrusiak; and High-Pressure Effects on the Structure and Behaviour of Proteins, K. Heremans.

### *New Commission members*

At the Geneva Congress, the Commission held two meetings, which were attended by eleven members and two consultants. Central to the first meeting was a thorough change in the members of the Commission. Most notably, the former Chair and driving force behind the re-establishment of the Commission, R. J. Nelmes, stepped down as Chair and Commission member. At the urging of the IUCr Executive Committee and the Commission at Geneva, he agreed to serve the community as a consultant. Other new members of the commission are M. Mezouar (France), S. Tolbert (USA), N. Hamaya (Japan), J. Loveday (UK), R. Winter (Germany) and J. Tse (Canada). R. J. Nelmes (UK) and A. Katrusiak (Poland) were elected as new consultants. Subsequent to these deliberations by the Commission, S. K. Sikka (India) was added as a consultant. Further topics discussed during the meetings were the Commission's home page, forthcoming meetings as well as the idea to publish a text-book (*e.g.* an *International Tables* volume) with important information with respect to high-pressure crystallography.

### *Home page*

The home page <http://www.iucr.org/iucr-top/iucr/chp.html> is prepared and updated by J. Loveday. It is expanded to include various sources of information (software, reports of previous meetings and announcement of forthcoming meetings, central facilities) relevant to structural high-pressure science.

### *Future Meetings*

The most prominent activity of the Commission, namely the organization of workshops and meetings, occupied most of the business of the Commission's meeting in Geneva. In 2003, the 34th Crystallographic Course in Erice, 4–15 June (<http://hpc.amu.edu.pl/erice/copy/m12.html>) will be devoted to high-pressure crystallography. This meeting is being coordinated and co-Chaired by

Commission consultant A. Katrusiak. The meeting reflects the broad range of disciplines now involved in high-pressure crystallography. Furthermore, it was agreed that in 2003 a small specialized workshop, focusing on new materials at high pressure, should be organized on the west coast of the USA. S. Tolbert, a new member of the Commission, was asked and agreed to take over the coordination and organization. The meeting will take place in Berkeley at the Advanced Light Source.

Longer term, in 2004, a workshop is planned at the new Canadian synchrotron in Saskatoon and in 2005 we hope to be involved as a Commission in planning and presenting exciting high-pressure crystallography at the Florence Congress. The Commission and several of the attendees at high-pressure meetings have urged the organization of a high-pressure programme similar in size and scope to the popular programme in high-pressure science presented at the Seattle Congress in 1996.

**M. Kunz**, Chair

## 6.12. Commission on Inorganic and Mineral Structures

The formation of the Commission on Inorganic and Mineral Structures (CIMS) was approved by the General Assembly at the Geneva Congress. Consequently, the only activity for the year ending 31 December 2002 has been to plan future activity. Some members of the freshly appointed Commission met during the Congress and on the occasion of the 18th General Meeting of the International Mineralogical Association (Edinburgh, UK, 1–6 September 2002). Further contacts have been maintained *via* e-mail and the web site of CIMS at <http://www.iucr.org/iucr-top/iucr/cims.html>, which is maintained by consultant member M. Nespolo (Université de Nancy, France).

The initial plan of activity was agreed as follows:

- a symposium during 2003;
- a school during 2004; and
- a strong presence with CIMS symposia (and possibly a satellite meeting) at the Florence Congress in 2005.

So far the participation of CIMS is assured *via* its support of the following meetings:

9th European Conference on Solid State Chemistry [3–6 September 2003, Stuttgart, Germany (<http://www.mpi-stuttgart.mpg.de/conf/ecssc9/>)];

XV International Conference on X-ray Diffraction and Crystal Chemistry of Minerals [St Petersburg, Russia, 15–19 September 2003 ([http://crystal.pu.ru/engl/info\\_E.shtml](http://crystal.pu.ru/engl/info_E.shtml))]; and

Satellite Meeting on Mathematical and Symmetry Aspects (Budapest, Hungary, 22–24 August 2004) in association with ECM-22.

**G. Ferraris**, Chair

## 6.13. Commission on Neutron Scattering

During the Geneva Congress, the Commission held two business meetings, including both the former (1999–2002) and the new (2002–2005) members; one meeting was closed and the other open. We discussed the global situation of neutron sources. Two important reports were introduced.

One was on the ‘Status and Needs of Major Neutron Scattering Facilities and Instruments in the United States’ issued by the Office of Science and Technology Policy Interagency Working Group on Neutron Science under the Executive Office of the President of the USA. This report recommends that neutron scattering is an essential tool of modern science; therefore, the way to maximize the impact

and effectiveness of all US facilities has been sketched. (See <http://www.ostp.gov/html/NeutronIWGReport.pdf>.)

The other report was on the recent developments around the ESS (European Spallation Source). This project has been under way in recent years and in 2002 reached a status such that a decision about its future was hoped for after a very successful public presentation in Bonn (Germany). This being a European Project, a decision at the European level would have been needed. However, since there is no formal procedure for this, decisions have been prepared at the national level: in Germany, the German Science Council has evaluated several large projects, such as the ESS in 2001/2002, and came to the conclusion in summer 2002 that the ESS was not a high-priority project. This recommendation sparked a public discussion not only in Germany, but without a significant result. In the second half of 2002, the ESFRI (European Strategy Forum for Research Infrastructure) Group worked on a strategy paper, which was published at the end of 2002. This stated that, while a new neutron source like the ESS was considered necessary for the European Research Infrastructure in the future, the time was not right for a decision to build ESS now. Following this, the German government in February did not see the possibility to support the start of the realization of the ESS at that time. This situation, certainly strongly biased by the difficult financial situation, leaves the European neutron scatterers without a perspective for a new horizon in neutron scattering. We have to make best use of the existing facilities, in particular that at the ILL, still the most powerful neutron source in the world. We will work very hard to obtain the necessary funding for the possible use of the ILL. In Germany, we have hope that the FRM II will get its licence soon, giving the German neutron scatterers new possibilities on the national scene (see also below). (Web page <http://www.neutron-eu.net/>.)

The current status of neutron sources was reported. The SNS (Spallation Neutron Source, 2 MW) in USA and JSNS (Japanese Spallation Neutron Source, 1 MW) are under construction as scheduled towards their completion in 2006 and 2007, respectively. The FRM II reactor at Munich in Germany (20 MW) has been completed and is waiting for government approval for its start. The RRR (Replacement Research Reactor, 20 MW) in Australia is under construction and will be completed in 2005. The Millennium Programme of ILL at Grenoble in France started to upgrade its facilities and instruments significantly. At ISIS in the UK, the first allocation for site preparation of the second target station project has been approved.

Our Commission’s project to compile a ‘Catalogue of Neutron Sources’ all over the world was also discussed and its page layout was decided. This project is now going to be followed in collaboration with major neutron facilities and users’ communities. We also discussed a possible satellite meeting (where, when) linked to the Florence Congress in 2005.

By taking the opportunity of the 3rd ECNS (European Conference on Neutron Scattering) at Montpellier, France, 3–6 September 2003, our Commission business meeting is planned to be held there. This will give us the possibility to discuss details of the planning for the Florence Congress

**M. Steiner**, Chair

## 6.14. Commission on Powder Diffraction

Commission on Powder Diffraction (CPD) round robins and the *Newsletter* are still the main pillars of CPD activity. As the new Chair, it is my pleasure to express my deepest thanks to the previous Chair,

P. Scardi, who has put in a tremendous amount of highly successful work for the Commission, and in particular regarding the improvement of our *Newsletter*, which has considerably increased in size, quality and number of subscribers. Support was given to a variety of conferences, schools and workshops and several projects such as the development of Rietveld guidelines, the QPA, and the size-strain round robin were accomplished. Our new members (J. M. Delgado, C. R. Hubbard, I. C. Madsen and N. Masciocchi) are cordially welcomed. Following our tradition, they all will be guest editors of upcoming CPD *Newsletters*. In turn, several members have left the CPD and we are grateful to S. P. Sen Gupta, R. Von Dreele and H. Fjellvåg for their valuable contributions during the past triennium.

**6.14.1. Newsletters.** During 2002, two issues of the CPD *Newsletter* were published (see also the url <http://www.iucr.org/iucr-top/comm/cpd/index.html> for downloading). The summer issue (No. 27) was edited by L. M. D. Cranswick and G. J. Kruger and was entitled 'Powder Diffraction in Mining and Minerals'. The winter issue (No. 28) was edited by P. Scardi and was entitled 'XRD Line Profile Analysis'. These two issues can both be considered as state-of-the-art contributions and important references. *Newsletter* No. 27 also included as an annex the second paper on the QPA round robin: 'Outcomes of the International Union of Crystallography Commission on Powder Diffraction Round Robin on Quantitative Phase Analysis: Samples 2, 3, 4, Synthetic Bauxite, Natural Granodiorite and Pharmaceuticals' by N. V. Y. Scarlett, I. C. Madsen, L. M. D. Cranswick, T. Lwin, E. Groleau, G. Stephenson, M. Aylmoree and N. Agron-Olshina [*J. Appl. Cryst.* (2002), **35**, 383–400].

The *Newsletter* has now reached a size that creates some logistical and financial problems. In an attempt to keep production costs as low as possible, following *Newsletters* will be printed and distributed from Venezuela. Special thanks go to M. Delgado who voluntarily offered his help in this matter. P. Scardi has almost finished his task of transferring all CPD *Newsletters* from paper to electronic format, which will be made available online and distributed on CD-ROMs soon.

The popularity of the computer software pages by L. M. D. Cranswick is still very high. These pages are very much appreciated by readers for their informative content and their effective presentation. News from ICDD and from the IXAS are also present in all issues, together with news on forthcoming events.

#### **6.14.2. Projects.** (i) *Quantitative phase analysis*

The first part of the study is reported in a publication by I. C. Madsen *et al.* [*J. Appl. Cryst.* (2001), **34**, 409–426], distributed as a free offprint with CPD *Newsletter* No. 25. The second part was published later by N. V. Y. Scarlett *et al.* [*J. Appl. Cryst.* (2002), **35**, 383–400] and was distributed as an offprint with *Newsletter* No. 27. Readers can refer to these papers for an exhaustive discussion on the outcomes of the QPA round robin. Both parts may be freely downloaded from the CPD web site (<http://www.iucr.org/iucr-top/comm/cpd/>), where additional information and original data files may be found.

#### (ii) *Size-strain analysis*

The preliminary report and analysis of results are still available at <http://www.boulder.nist.gov/div853/balzar>, and the CPD and CCP14 web sites. A paper has been recently submitted for publication in *Journal of Applied Crystallography*. The most recent issue of the *Newsletter* (No. 28) includes a summary of this work, presented by D. Balzar and N. C. Popa.

**6.14.3. Meetings/workshops/schools.** 2002 was dominated by the Geneva Congress, a real success in terms of attendance and scientific quality. Powder diffraction (PD) was very well represented with more than 11 microsymbiosia directly related to PD. Meetings of interest for

the CPD in 2002 included the 8th European Powder Diffraction Conference in Uppsala, Sweden (May 2002, Chair R. Tellgren). After the establishment of the EPDIC committee ECA-SIG, the CPD takes part in the planning activity for the EPDIC conference. The CPD also gave support to the II International School on Powder Diffraction, organized by the Indian Association for the Cultivation of Science (Jadavpur, Calcutta, India, January 2002).

**6.14.4. Web site.** The CPD web site is still the reference point for powder diffractionists around the world and is in the process of undergoing a major reorganization. Besides links and information on events related to PD (including the CPD round robins), the web site gives free access to the CPD *Newsletter* archive, from which recent and past issues maybe downloaded in pdf (Acrobat) format, which has greatly expanded the number of readers.

**R. E. Dinnebier**, Chair

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

The Commission wishes to recognize the contributions of J. D. Barnes and G. Kostorz, who have retired from the Commission after six years of service (they continue as consultants to the Commission).

**6.15.1. Commission Meetings.** During 2002, various members of the Commission were able to meet in connection with meetings and conferences around the world. These opportunities were important with respect to exchange of ideas and opinions, and to plan the future directions of the Commission's work.

In the course of these meetings, the Commission dealt with the following topics.

(1) Commemoration of the passing of H. Brumberger. G. Kostorz delivered a very moving tribute to Harry at a session of the XIIth International Conference on Small-Angle Scattering, Venice, Italy, 25–29 August 2002 (SAS 2002).

(2) The Commission has worked actively towards establishing a satisfactory relationship between the IUCr Congress and the future SAS conferences (SAS 2002+). This could be achieved either by obtaining a regular satellite status or by moving the future meeting one year out of phase with the IUCr Congress. The members of the Commission who are also members of the International Science Advisory Board of the SAS meeting took the initiative for a meeting of the Board during the SAS 2002 conference and participated very actively in the discussions about future SAS conferences. The result was that the Board recommended moving the next SAS meeting to 2007 (to take place in Japan, as decided *in plenum* at the SAS 2002 conferences). The plan is then to continue the SAS meetings on a triennial basis beyond 2007, so that future conflict is avoided.

(3) The Commission decided to take an active role in supporting the future SAS conferences and to provide guidance as well as 'institutional memory' for future organizers. A good first contact has already been established with the organizers of the SAS 2007 conference.

(4) The Commission has decided to take responsibility for the SAS prizes (administration, funding and support for prizes – especially the Guinier Award) at future SAS conferences (see also below).

(5) The Commission has decided to provide 'moral support' for future canSAS and NOBUGS conferences related to software, data handling and analysis. J. D. Barnes was a co-organizer of the 4th edition of NOBUGS held at NIST, Maryland, USA, in November 2002.

(6) For technical issues, the Commission will organize the work by forming 'task groups'. The various groups will have one main person

responsible for the work being carried out and for reporting to the Commission.

(7) The Commission will work towards having a one-day workshop and three microsymbiosia during the Florence Congress in 2005.

**6.15.2. SAS prizes.** At the SAS 2002 conference, the Commission together with the organizers took an initiative to award SAS prizes. There were three Young Scientist Prizes, named after O. Kratky, P. W. Schmidt and H. Brumberger, which were given for the best contributions related to experimental aspects, theory and applications, respectively. The prizes were sponsored by companies related to SAS instrumentation (Bruker AXS, Anton Paar and Osmics). In addition, a prize, named after A. Guinier, was given to a scientist for a significant (breakthrough or life-long) contribution to the advancement of the SAS technique. This prize was sponsored by the IUCr from the President's Fund.

The A. Guinier prize was awarded to M. Agamalian (Oak Ridge National Laboratory, USA), the O. Kratky Prize to G. Pabst (Austrian Academy of Science, Graz, Austria), the P. W. Schmidt prize to B. Goderis (Catholic University of Leuven, Heverlee, Belgium) and the H. Brumberger prize to D. Pontoni (ESRF, Grenoble, France).

The Prize Committee consisted of representatives of the SAS Commission (P. Fratzl, J. S. Pedersen), of the organizers (A. Benedetti, R. Triolo) and of the former recipient of the SAS prize at the SAS 99 conference in Brookhaven, USA (G. Wignall). The Commission has the impression that the prize initiative was well received by the SAS community.

**6.15.3. Workshop and microsymbiosia during the Geneva Congress.** (1) J. D. Barnes organized a one-day workshop on 'Scattering Methods for Nanoscale Structure Characterization'. The workshop was attended by about 30 scientists, most of them newcomers to the field. Lectures were presented by K. Erlacher, A. Allen, J. S. Pedersen and J. D. Barnes.

(2) A microsymbiosium on 'Nanostructural Characterization by Small-Angle Scattering' was organized by J. S. Pedersen and I. L. Torriani. The programme comprised six lectures on topics at the forefront of SAS research in materials science.

(3) A microsymbiosium on 'Soft Matter Studied by Small-Angle Scattering' was organized by T. Zemb and J. S. Pedersen. The programme consisted of lectures on very diverse and active fields of soft matter: aggregates of surfactants, liquid crystals, polyelectrolyte polymers and semicrystalline polymers.

**6.15.4. Education.** I. Torriani has been very active in organizing educational activities as well as in teaching during these events. In July 2002, she organized a three day course at the National Synchrotron Laboratory (LNLS) in Brazil on the use of the SAXS technique using synchrotron radiation. In September 2002, she alone gave a one-week course on the SAXS theory and applications at the Balseiro Institute of the Atomic Energy Commission, in Bariloche, Argentina. This was part of a graduate course on experimental physics and had students from several Latin American countries. In December 2002, she organized the Interamerican Workshop on the Applications of Synchrotron Radiation, sponsored by the American Physical Society, which took place at the LNLS. SAXS was one important topic. S. Doniach, B. Chu, S. Gruner, and several Brazilian speakers included SAXS results in their lectures. The workshop had 123 participants from the USA and Latin American countries.

J. S. Pedersen has been co-organizer of the 6th European School on Scattering Methods Applied to Soft Condensed Matter, which took place in Bombannes, Gironde, France, 26 May–1 June 2002. The school lasted for a full week and was attended by 40 participants and 15 teachers.

As mentioned elsewhere in this report, J. D. Barnes organized a one-day workshop on 'Scattering Methods for Nanoscale Structure Characterization' in connection with the Geneva Congress. P. Fratzl's group in Leoben contributed to this workshop with lectures by K. Erlacher.

**6.15.5. Other activities.** (1) The Commission is collecting information on standards that are currently used for calibration of the absolute intensity as well as the scattering-vector values. The plan is to publish some recommendations on the Commission's web pages.

(2) Round Robin. The initiative of the Commission to perform an inter-laboratory calibration/check will be re-initiated. The aim is still to circulate a set of samples to the participating laboratories and to have intensities *versus* scattering vectors reported on an absolute scale, in order to establish the degree of agreement that exists among SAS laboratories. The results of this activity may serve to motivate the community towards a better appreciation of the needs for standardization of procedures and it is of course closely related to point (1). A 'zeroth' round of the round robin has already taken place but with modest success as only a few laboratories reported back to the Commission. The samples were semi-crystalline polymers, polyethylene (PE), which are relatively strongly scattering, when using high-intensity synchrotron radiation and this caused some problems. The participants were asked to report both actual experimental results as well as the results of some limited data analysis. In the next round, we will avoid the data analysis, as many laboratories are not familiar with the analysis of scattering data from semi-crystalline polymers. However, compared to solutions of, for example, polymers of surfactants, the PE samples have the advantage that they are easy to handle and do not require any special sample container. It is not yet decided whether the same samples should be used in the next round or whether more weakly scattering samples should be used.

**6.15.6. Communication.** The Commission's web pages are maintained by J. D. Barnes. The Commission (D. I. Svergun and J. S. Pedersen) has made a call through the SAS list server for SAS related links to web pages on hardware and software. The material will be edited by D. I. Svergun and J. S. Pedersen and placed on the Commission's web pages during 2003.

**J. S. Pedersen, Chair**

## 6.16. Commission on Structural Chemistry

The main activity of 2002 was of course the Geneva Congress. The meeting contained numerous microsymbiosia of interest to the structural chemistry community. As noted in last year's report, two Commission members (G. Punte and L. Brammer) served as microsymbiosia organizers and four others (V. Belsky, J. L. Flippen-Anderson, T. W. Hambley and D. C. Levendis) served as co-organizers for microsymbiosia.

The Commission met during the Congress and discussed the scope of what we define as 'structural chemistry' as well as where the interests of the Commission overlap or intersect with other Commissions, such as (i) Inorganic/Mineralogical Crystallography, (ii) Charge, Spin and Momentum Density, (iii) Crystal Growth and Characterization of Materials, and (iv) Powder Diffraction. Thinking ahead to planning for the Florence Congress in 2005, there is clearly scope for collaboration with these neighbouring Commissions in terms of planning microsymbiosia.

With regards to other meetings, the Commission discussed the possibility of providing input in the area of structural chemistry to the organization of the AsCA regional meeting, and possibly also the ECM meeting.

*Acta Crystallographica* Section B, the IUCr journal which is perhaps most closely associated with the Commission, is planning to organize a series of special issues in areas such as drug design and polymorphism. The Commission will endeavour to provide useful input into these and similar initiatives.

The Commission endorsed the 3rd National Russian Crystal Chemistry Conference to be held 19–23 May 2002 in suburban Moscow and funds were subsequently committed by the IUCr in support of the meeting. The Programme Chair was Commission member V. Belsky. The Commission also endorsed the Indaba IV meeting, entitled 'Patterns in Nature', to be held in Skukuza in the Kruger National Park, South Africa, 18–23 August 2003, as a satellite of the European Crystallography Meeting in Durban, South Africa. Commission members L. Brammer, G. R. Desiraju and D. C. Levendis will serve on the Programme and/or Organizing Committees. In this regard, Commission members felt that the current requirement for meeting organizers to apply for IUCr support nine months in advance of a meeting was too long a lead time. L. Brammer has requested that the Sub-Committee on the Union Calendar consider reducing this period to six months.

#### *Agenda items for previous year*

(1) CIFs – the need for new dictionary items. There had been previous discussion in the Commission about the inclusion of new data items (for example, for twinning) in the CIFs generated for small-molecule structures. L. Brammer contacted B. McMahon (IUCr Research and Development Officer and Secretary of COMCIFS) to ascertain the current status of any developments. An informal working party has been established to look into this. L. Brammer will check on future progress. There was also discussion of the possible need to include more data entries on area detectors in the small-molecule CIF.

(2) Archiving of structure factors. There had been previous discussion in the Commission of the value of providing a mechanism for archiving structure factors. L. Brammer checked with B. McMahon regarding the status of this idea. The IUCr appear to be open to considering some form of repository for structure factors from other journals or database depositions, but would need to be convinced that there was genuine scientific need. It is likely also that any costs for such a project would need to be recovered.

**L. Brammer**, Chair

## 6.17. Commission on Synchrotron Radiation

The assumed mission of the Commission is to promote access of crystallographers worldwide to the world's synchrotron-radiation facilities. A subcharge is to promote the development of crystallographic instrumentation technology and standards, particularly in the direction of X-ray detectors. To foster communication, we endorse (and sometimes sponsor) international meetings as the best means to achieve these goals.

(1) The Commission helped sponsor a detector workshop at the ESRF users meeting, which was very successful. A verbal summary was provided by the organizer, H. Graafsma (ESRF, France). A US–European collaboration on new thin phosphors was established. Alternative materials for sensor layers, such as CdSe, were discussed. Detector development of the popular FRELON CCD readout system is advancing well at ESRF, but there is no easy way to commercialize it so that it can be adopted by other sources. Four components are generally required for a CCD: phosphor, coupling, sensor and readout.

The future looks very bright for a new detector technology, called a pixel detector, which should ultimately replace CCDs. The technology offers photon counting and energy resolution at high count rate in every pixel. The ESRF pixel detector project is benefiting strongly by tying in development efforts of CERN and the medical imaging industry. A  $256 \times 256$  prototype, called 'Medipix', is being tested at BM05 (ESRF) in April 2003. A low-doped  $300 \mu\text{m}$  Si drift detector array of  $55 \mu\text{m}$  square pixels is biased to about 300 V. The bottom electrode is bump-bonded to a readout circuit occupying the same area as each pixel. Each circuit contains the amplifiers, discriminators and 13 bit scaler needed to obtain four decades of dynamic range. The design is a prototype that would partially satisfy the potential needs of two communities: for medical imaging applications, the sensitivity at high energies is insufficient, while the dynamic range is rather poor for crystallographic uses. Both applications will eventually need considerably larger arrays, which might be available in about five years' time, according to ESRF detector group leader H. Graafsma.

A summary of the workshop programme was abstracted from the <http://www.esrf.fr> web site. 'X-ray Detectors: The Way to Get More Out of Your Beamline!' will be held 13–14 February 2003 with a Scientific Organizing Committee comprising H. Graafsma (Chair), M. Kocsis, T. Martin and C. Ponchut. The objectives of the meeting are to review the current status of detectors, how they are used, what is needed and what is coming. The workshop intends to bring the synchrotron user community and the detector developers together, with an explicit goal to inform the detector developers of the forthcoming needs and requirements and to inform the user community of the worldwide state of the art as well as future perspectives.

A special topical issue on X-ray detectors for synchrotron radiation will be published in *Journal of Synchrotron Radiation*. All workshop attendees were sponsored by the IUCr to receive a free copy. Meanwhile presentation materials from most of the talks are available at the web site <http://www.esrf.fr/Conferences/UsersMeeting2003/Detectors/Speakers/>.

(2) An American detector workshop was held in Washington, DC, USA, 30–31 October 2000. The workshop resulted in a white paper entitled 'A Program in Detector Development for the US Synchrotron Radiation Community' by A. Thompson (ALS, LBNL), D. Mills (APS, ANL), S. Naday (ANL), J. Hormes (Center for Advanced Microstructures and Devices, CAMD), S. Gruner (Cornell High Energy Synchrotron Source, CHESS), P. Siddons (NSLS, BNL), J. Arthur (SSRL), R. Wehlitz (University of Wisconsin Synchrotron Research Center, SRC) and H. Padmore (ALS, LBNL). S. M. Gruner attended the meeting and forwarded the document. The summary page is included here for information:

There is a clear gulf between the capabilities of modern synchrotrons to deliver high photon fluxes, and the capabilities of detectors to measure the resulting photon, electron or ion signals. While a huge investment has been made in storage ring technology, there has not to date been a commensurate investment in detector systems. With appropriate detector technology, gains in data rates could be 3 to 4 orders of magnitude in some cases. The US community working in detector technology is under-funded and fragmented and works without the long-term funding commitment required for development of the most advanced detector systems. It is becoming apparent that the US is falling behind its international competitors in provision of state-of-the-art detector technology for cutting-edge synchrotron-radiation-based experiments.

There is thus an urgent need for a coordinated national programme in detector research and development for synchrotron-radiation research. Several new technologies are becoming avail-

able that could revolutionize the capabilities of detectors. One of the most important advances is the massive integration of parallel electronics into detectors on a pixel by pixel basis. Such detectors have the capability not only to work at very high rates, in some cases approaching 1 THz, but to include 'smart processing' of information on a chip. Other important areas include the revolution in low-temperature X-ray detectors capable of high-energy resolution and, if used in the form of arrays, potentially high counting rates. The science enabled by such detectors will be spread across the whole spectrum of synchrotron-radiation research. For example, the study of the 3D structure of systems with short-range order using X-ray fluorescence holography (XFH), microsecond dynamics in polymers and magnetic systems studied using photon correlation spectroscopy, environmental chemistry studied using fluorescence yield micro-XAS, the study of chemical and electronic structure *via* photoemission and X-ray emission, and many more areas will be revolutionized by the use of advanced detectors.

The principal conclusions of the above national Workshop were that:

(i) Funding of advanced detectors is the most cost effective way of increasing the effectiveness of both existing and planned future synchrotron facilities.

(ii) Funding agencies should make provision for use of the most advanced present-day detectors on existing facilities; there are examples of multi-million dollar third-generation beamline facilities with first-generation detectors.

(iii) There should be a nationally coordinated programme to provide funding of long-range strategic research in a number of highlight areas.

(iv) An organization modelled after the successful BioSync dealing with biological applications of synchrotron radiation, 'DetectorSync' should be formed to coordinate the area of detector research, and to represent the communities needs to funding agencies.

In this document, we point out general areas that should be targeted and, in coming months, these will be refined into definitions of specific programmes with delineated targets. We urge that a major funding initiative and associated call for proposals be focused on these areas, with the aim of setting up large programmes to serve the needs of the whole community. Key elements will be provision of information and resources to the research community, as well as wherever possible promotion of technology transfer to the industrial sectors associated with synchrotron radiation and other fields. A detailed cost estimate of such a programme has not been made, but based on the expected number of areas of research and the size of each group required for an aggressive and efficient operation, an initial estimate would be approximately USD 25M/year.

(3) An Indo-US Workshop on Radiation Physics with Synchrotrons and Other New Sources will be held at Argonne National Laboratory, Argonne, Illinois, USA, 13-16 May 2003. It is sponsored by the Indo-US Forum (a joint venture of the National Academy of Sciences and the Department of Science and Technology of India), with 12 participants from India, 12 from around the United States and about 20 from the local institutions. The aim of the workshop is to foster closer scientific ties between Indian and US scientists and to identify new opportunities resulting from the synchrotron and high-power laser sources in both countries. These include the behaviour of correlated many-particle systems in intense fields and other environments. The meeting is organized by L. Young and S. Roy.

**I. Robinson**, Chair

#### 6.18. Commission on XAFS

No report has been received from the Chair.

**D. Arvanitis**, Chair

#### 7. 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 2002 the Executive Committee approved sponsorship of several schools and meetings, mostly with financial support. Those held in 2002 are listed at the beginning of this Report of the Executive Committee. Those scheduled for 2003, but approved in 2002, are listed below:

International School on Crystal Growth of Technologically Important Electronic Materials, Mysore, India, 20-27 January 2003.

VI Latin American Workshop on Magnetism, Magnetic Materials and Their Applications, Chihuahua, Mexico, 7-11 April 2003.

BCA/CCG Ninth Intensive Course in X-ray Structure Analysis, Durham, UK, 7-14 April 2003.

School on X-ray Charge Density Analysis and the XD Programming Package, Buffalo, USA, 13-17 May 2003.

Third National Crystal Chemical Conference, Chernogolovka, Russia, 19-23 May 2003.

School on High-Pressure Crystallography, Erice, Italy, 4-15 June 2003.

Third European Charge Density Meeting, Aarhus, Denmark, 24-29 June 2003.

ACA Annual Meeting, Covington, Kentucky, USA, 26-31 July 2003.

AsCA '03 and Crystal-23 Combined Conference, Broome, Australia, 10-13 August 2003.

Biological Structure Workshop, Broome, Australia, 13-15 August 2003.

Sagamore XIV Meeting on Charge, Spin and Momentum Densities, Broome, Australia, 13-18 August 2003.

Organizers of meetings wishing to seek IUCr sponsorship should submit applications at least nine months in advance of the meeting, writing to the Chair of the Sub-committee. The present Chair is Professor M. A. Carrondo. For up-to-date contact information, see <http://www.iucr.org/iucr-top/iucr/calendar.html>.

Applications for sponsorship of satellite meetings require the approval of the Chair 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 Chair of the Congress Programme Committee for approval, or otherwise.

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

## 8. Sub-committee on Electronic Publishing, Dissemination and Storage of Information (CEP)

### 8.1. Meeting attendance

In 2002, members of the CEP attended the following meetings:

B. McMahon attended a meeting 'XML Use in Chemistry' in Cambridge, UK, January 2002.

Y. Epelboin attended the seminar on 'Digital Preservation of the Record of Science – State of the Art', UNESCO, Paris, France, 14–15 February 2002. H. D. Flack also attended as ICSTI representative and participated in the ICSTI winter committee meetings 16–17 February 2002 at ICSU, Paris.

P. R. Strickland gave a short presentation on the IUCr's experience in selling journals to library consortia at a meeting of the Association of Learned and Professional Society Publishers in London, UK, 19 February 2002.

H. D. Flack gave a short presentation entitled 'FORTRAN Archaeology: an Issue for a Knowledge Organization like the IUCr?' to the Open Meeting of the Commission on Crystallographic Computing 'The Problems Facing Crystallographic Computing' at the Geneva Congress, August 2002.

B. McMahon and H. D. Flack attended the 2nd Workshop on the Open Archives Initiative (OAI): Gaining Independence with e-prints Archives and OAI, 17–19 October 2002, CERN, Geneva, Switzerland.

H. D. Flack was unable to visit the IUCr editorial offices, Chester, UK, during 2002.

The meeting attendances of the CODATA and ICSTI representatives, whose work is so closely related to that of the CEP, are recorded in their individual reports.

### 8.2. Information services

The CEP has continued its task as editorial body for the on-line information services of the IUCr. The task of day-to-day maintenance of **Crystallography Online** is performed under the responsibility of S. Parsons. No action on the restyling and restructuring of **Crystallography Online** took place in 2002 owing to other commitments. It is definitely intended to put this high on the action plan of the CEP in 2003.

### 8.3. World Directory of Crystallographers (WDC)

By way of the online interface of *WDC* 11, entries are gradually being updated by individuals. However, more publicity is necessary to encourage crystallographers to keep their own record up to date. It is expected that when *WDC* is integrated with the journals electronic submission procedure individual updating of *WDC* will be more regular and reliable.

### 8.4. NeXus CD-ROM

Under the continued leadership of L. M. D. Cranswick, 1,000 copies of a new version of the *Xtal* NeXus: Virtual Crystallographic Internet on CD-ROM version 8.56 were produced in November 2002. All of these CD-ROMs have now been distributed and at present individual CD-ROMs are being made on request. The CD-ROM is made available to laboratories and scientists with an interest in crystallography lacking adequate connection to the internet. The CD-ROMs contain public domain software and copies of web sites of interest to crystallographers. The CD-ROMs were publicized through many channels in such a way that scientists have to apply to receive a copy. We propose to continue this project and make further batches of CD-ROMs. The European Crystallographic Meeting in South

Africa in August 2003 will be an ideal opportunity to find further markets for this popular product.

### 8.5. Crystallography Journals Online

Attention continues to be given to ways of improving the sale of the IUCr journals to consortia of libraries. Moreover, the CEP is particularly attentive to developments in the scientific community at large concerned with access to scientific literature and data. Currently 'Open Access' and the 'Open Archive Initiative' are attracting wide attention, and the CEP is seeking to understand how these interesting initiatives can be turned into viable and sustainable operations of use to the crystallographic community.

### H. D. Flack, Chair

## 9. Committee for the Maintenance of the Crystallographic Information File Standard (COMCIFS)

Twelve years after being officially adopted by the IUCr, the CIF standard is now in regular use by the major crystallographic journals and structural databases, with the Union journals setting the pace. CIF is also increasingly working itself into the fabric of crystallographic software. It suffers, however, from a lack of basic software in the form of editors and browsers that can be used to prepare and validate CIFs, though these are gradually becoming available. Of more serious concern to COMCIFS is the role CIF will play in the coming genomics revolution. It is a well established standard for the archiving of macromolecular structures, and compatible file structures also based on STAR have been adopted by a number of related disciplines. However, the information technology community is developing and supporting a different, though similar, file structure, XML, whose design makes it more flexible than CIF. XML has more available software, though CIF has a more fully developed and integrated suite of dictionaries and is better adapted to a mature discipline such as crystallography where XML's flexibility can be something of a liability. CIF and XML will therefore coexist for the foreseeable future and COMCIFS is working to ensure that the interface between them is as transparent as possible so that crystallographers will be able to exploit the advantages of both systems.

CIF software is, however, slowly being developed, and in response to requests from the people doing this work, COMCIFS has prepared and approved a detailed definition of the CIF standard, designed to remove ambiguities from the CIF syntax. Copies of this specification can be found on the COMCIFS page of the IUCr web site, <http://www.iucr.org/iucr-top/iucr/comcifs.html>.

COMCIFS organized both open and closed meetings at the Geneva Congress in August. Those attending the open meeting heard about the 'methods' extensions that we hope eventually to incorporate into the CIF dictionary language, as well as several assessments of the technical problems of interfacing CIF and XML. The closed COMCIFS meeting established two committees, one to make recommendations for defining metadata within CIF and interfacing CIF with XML, and the other to look at ways in which COMCIFS might obtain the full-time services of a person to encourage and coordinate the development of CIF software.

Publicity remains an important part of COMCIFS' activities. In the rapidly changing field of information technology, which impacts the work of all crystallographers, one of COMCIFS roles is to assist the users in adapting to the technology as it now exists, while at the same time preparing them for the changes that still lie ahead. The CIF page on the IUCr web site and a regular column in the *IUCr Newsletter*

provide both specific and general information about CIF and the activities of COMCIFS and its committees.

As this year marks the beginning of a new triennium, the membership of COMCIFS was reviewed and the following members were appointed by the Executive Committee to serve as voting members for the next three years: I. D. Brown (Chair), B. McMahon (Secretary), H. M. Berman, H. J. Bernstein, R. Grosse-Kunstleve, S. R. Hall, G. Madariaga, J. Westbrook.

In addition to the voting members, there are many others who have joined the COMCIFS discussion list but do not vote on matters brought before COMCIFS for approval.

Following the approval of the Modulated Structures and Symmetry CIF Dictionaries in 2001, COMCIFS approved the following Dictionary Maintenance Groups:

Modulated Structures: G. Madariaga (Chair), G. Chapuis, V. Petricek, M. Onada, J. Zuñiga.

Symmetry: I. D. Brown (Chair), M. Aroyo, R. Grosse-Kunstleve, V. Kopsky, D. B. Litvin, G. Madariaga.

A decade of experience in the submission of papers to *Acta Crystallographica*, and the extension of CIF use to other areas, has shown that the time has arrived for a major review of the Core CIF Dictionary. This review is already under way and will result in the incorporation of many new requested items into the dictionary, and the tightening of some existing definitions. The latter are needed to make the dictionary conform to current practice which has undergone a number of significant changes since the first version of the Core Dictionary was approved.

The Magnetic, Electron Density (RHO) and Small-Angle Scattering CIF Dictionaries are still in development and COMCIFS is awaiting their formal submission for approval.

**I. D. Brown**, Chair

## 10. Committee on Crystallographic Databases

The major activity during 2002 was the preparation, editing and publication of a Joint Special Issue of Sections B and D of *Acta Crystallographica* devoted to the crystallographic databases. The issue contained current descriptions of the major databases and their access software systems, together with a number of papers that reviewed their research applications across a very broad range of science. A total of 18 papers were published, 13 in Section B and 5 in Section D. These papers were bound together to form a single Special Issue for sale to individuals, and the Issue was available at the Geneva Congress and was promoted at various other conferences during the year.

By the end of 2002, the structural databases (PDB, NDB, CSD, ICSD, CRYSTMET) contained details of nearly 450,000 crystal structures, with an overall accession rate of about 35,000 new structures predicted for 2003. The PDB, with an accession rate of 18% during 2002, remains the major growth area, with other databases showing growth rates ranging from 3 to 8% during the year.

**F. H. Allen**, Chair

## 11. IUCr Newsletter

Three issues of the *IUCr Newsletter* were printed in 2002. Two contained 32 pages and the third 24 pages. The content covered activities of the IUCr and its Regional Associates, news concerning crystallographers and crystallography, notices, awards, elections,

resources, obituaries, meeting reports, future meeting announcements, and a general calendar.

Each issue devoted two or three pages to brief summaries of selected articles recently published in IUCr journals. Articles of particular interest in Volume 10 (2002) were the reports of the Regional Associates (ECM-20 in Krakow, Poland, and ACA in San Antonio, USA) and the Geneva Congress, and reports of the activities of the IUCr Commission on Crystallographic Nomenclature, COMCIFS, and the Protein Data Bank. Twelve meeting reports from six countries, announcements of twelve future meetings in ten countries, and five obituaries of prominent crystallographers in four countries were published.

The mailing list was maintained with little change in total circulation. Eighteen countries continue to assist in the effective and economic distribution of the *Newsletter*. Sustained advertising volume coupled with efficient production has kept the cost to the IUCr below USD 30,000 for the year.

**W. L. Duax**, Editor

## 12. IUCr/Oxford University Press (OUP) Book Series

The Book Series Committee continued its activities during 2002 in close cooperation with the OUP. In the series *IUCr Texts on Crystallography*, the book *Crystal Structure Analysis – Principles and Practice*, by W. Clegg, A. J. Blake and R. O. Gould was published. In the same series also the second edition of *Fundamentals of Crystallography* by C. Giacovazzo, H. L. Monaco, G. Artioli, D. Viterbo, G. Ferraris, G. Gilli, and others, was published. In the Series *IUCr Monographs on Crystallography*, two more titles appeared: Monograph 13 *Structure Determination from Powder Diffraction Data*, edited by W. I. F. David, K. Shankland, L. B. McCusker and Ch. Baerlocher, and Monograph 14 *Polymorphism in Molecular Crystals* by J. Bernstein, both in Spring 2002.

Several other manuscripts have been considered by the Committee or are in the negotiating stage. Prospective authors are encouraged to contact the Chair of the Committee. Manuscripts covering specific aspects of crystallography and related fields are most welcome. In addition, suggestions for topics or potential authors are solicited.

**H. Schenk**, Chair of Book Series Committee

## 13. Regional Associates and Scientific Associates

### 13.1. American Crystallographic Association (ACA)

This year of activities of the ACA reflects the dynamic and ever growing structure of the Society and the efforts to combine a proficient management of local affairs and to open new space for international and regional activities. The publication of the *Newsletter* continues to be a successful way of reaching the crystallographic community.

As on previous occasions, during the year in which the IUCr Meeting was taking place, the 2002 Annual Meeting of the ACA was held in the spring (25–30 May) at San Antonio, Texas. The Lindo Patterson Award, established in 1980 and given every three years, was awarded to D. L. Dorset (the entire contents of his award conference was published in the Winter 2002 *Newsletter* of the ACA). This motivated the inclusion of two symposia on Electron Crystallography and Electron Microscopy of Biological Macromolecules in the scientific programme. The Elizabeth A. Wood award was granted to the science reporter I. Flatow, host of of NPR's 'Talk of the Nation.'

Science Friday'. Several posters were awarded the Oxford and Pauling prizes.

The creation of two new special interest groups (SIGs) has been announced, one on Structure Determination by Powder Diffraction and another on Electron Crystallography; the first has already been approved by the Council of the ACA.

The ACA has continued the efforts of recent years in trying to extend its activities to Central and South America. To encourage participation of young crystallographers from Latin American countries and make possible their attendance at the ACA meeting, travel awards were granted to several PhD students and researchers. A previous proposal for the creation of a SIG was not successful, but a fund was established to extend financial support for Pan-American participation.

**I. L. Torriani**, IUCr Representative

### 13.2. Asian Crystallographic Association (AsCA)

Following the AsCA '01 meeting held in Bangalore, India, in November 2001, a few changes in the Association were initiated by the Past President, Y. Ohashi. The formal discussion was executed during the 10th council meeting held in Geneva during the 19th IUCr Congress. Election of AsCA executives was also held then. A few conclusions were reached, as follows.

*New AsCA Meetings.* In order to increase the regional activities, new interim AsCA meetings (in addition to the established meetings) every three years would be initiated and, for economic reasons, these would be held in conjunction with annual meetings of various crystallographic societies in different countries. The first such meeting will be in conjunction with the Society of Crystallographers in Australia and New Zealand (SCANZ): AsCA '03/Crystal-23 will take place in Broome, Australia, in August 2003. The second such meeting will be in conjunction with the Crystallographic Society of Japan (CrSJ) and will be held in Japan in 2006, AsCA '06/CrSJ '06. Presidents of both SCANZ and CrSJ have approved the idea of such joint meetings.

*Location of AsCA '04.* The next normal AsCA meeting, AsCA '04, will be held in Hong Kong, People's Republic of China; Professor I. D. Williams (Hong Kong) was elected Chair of the organizing committee (IOC/AsCA '04) and Professor M. Sakata (Japan) was elected Programme Chair (IPC/AsCA '04).

*Election of AsCA Executive.* The newly elected officers are: President: Yu Wang (Taiwan), Vice President: M. Vijayan (India), Secretary/Treasurer: B. Skelton (Australia).

*Timing of AsCA Elections.* Following the minutes of the ninth Council Meeting, it was agreed by the council members that the timing of the election of officers and selection of the venue for forthcoming AsCA meetings would not be done at the triennial IUCr Congress but at the normal AsCA meetings. Accordingly, item 4 of the constitution should be updated accordingly.

**Y. Ohashi**, IUCr Representative

### 13.3. European Crystallographic Association (ECA)

In 2002, there was no ECA meeting because of the Geneva Congress. The main activity was the preparation for the European Crystallographic Meeting, ECM-21, to be held in Durban, South Africa, in August 2003, in collaboration with the local coordinators A. Roodt and D. C. Levendis. The ECA Council and Executive Committee met in Geneva and several important decisions were taken. Preliminary steps for the organization of ECM-22 in August

2004 in Budapest, Hungary, were discussed with Professor A. Kálmán, and it was decided to hold ECM-23 in 2006 in Leuven, Belgium.

**D. Viterbo**, IUCr Representative

### 13.4. International Organization of Crystal Growth (IOCG)

During 2002, the International Organization of Crystal Growth was very quiet. No particular initiatives were undertaken by the President and Executive Committee.

The main activities were carried out by the Organizing Committees of the next conference in Grenoble, France (ICCG-14, <http://iccg14.inpg.fr/introICCG14.htm>) and of the Summer School on Crystal Growth in Berlin, Germany (ISSCG-12, <http://isscg12.ikz-berlin.de/index.phtml>). These two events will see the involvement of the IUCr Commission on Crystal Growth and Characterization of Materials as the main organizers are also Commission members. Additional members of the Commission have been included in the Advisory committee of ICCG-14.

**R. Fornari**, IUCr Representative

### 13.5. International Centre for Diffraction Data

As for the previous year, R. L. Snyder represented the ICDD at the CPD meetings, and now also the International X-ray Analysis Society (IXAS) (information is available *via* the ICDD web site: <http://www.icdd.com/>; and the IXAS web site: <http://www.ixas.org/>). It is still a main target of the CPD to maintain active collaborations and positive relationships with these organizations.

**R. E. Dinnebier**, IUCr Representative

## 14. Representatives on Other Bodies

### 14.1. IUPAC Interdivisional Committee on Terminology, Nomenclature and Symbols (ICTNS)

The Interdivisional Committee on Nomenclature and Symbols was renamed and restructured at the last General Assembly of the International Union of Pure and Applied Chemistry (IUPAC), with effect as of January 2002. Renaming recognizes the importance of 'terminology' in the Committee's charge, restructuring adds titular and associate members and provides a clearer connection between it and each Division Committee. ICTNS is responsible for ensuring that all recommendations concerned with terminology, nomenclature and symbols made on behalf of IUPAC are consistent with its own and other international standards. The IUCr, the Bureau International des Poids et Mesures (BIPM), the International Organization for Standardization (ISO) and five other International Unions are represented on ICTNS.

Restructuring includes a meeting schedule change from annual to biennial, hence the Committee has not met since the 41st IUPAC General Assembly in Brisbane, August 2001. It was accompanied by the appointment of a new Chairman and a new Secretary. For reasons still undetermined, subsequent activities of ICTNS have been minimal. With the next meeting due August 2003 in Ottawa, Canada, and a dearth of circulated information, members have requested IUPAC to appoint provisional leaders in the near future so that the ICTNS meeting in Ottawa can be productive.

**S. C. Abrahams**, IUCr Representative

#### 14.2. International Council for Scientific and Technical Information (ICSTI)

The IUCr Representative attended the following ICSTI meeting:

General Assembly held in the Royal Institute of Technology Library, Stockholm, Sweden, 15–19 June 2002. This included a one-day public conference entitled ‘Scientific Information: the Challenges of Creating and Maintaining Access’.

In addition, H. D. Flack represented/will represent the IUCr at the following meetings:

Winter committee and discussion meeting held at ICSU, Paris, France, 16–17 February 2002.

ICSTI Seminar on ‘Digital Preservation of the Record of Science – State of the Art’, 14–15 February 2003, UNESCO, Paris, France.

During 2002, an ICSTI Statement on ‘Maintaining the Permanent Availability of the Digital Records of Science’ was prepared and published. As part of this statement, ICSTI urged ICSU and its Scientific Unions to undertake for each of the scientific disciplines a high-level audit of digital preservation policies and practices that are now in place. ICSTI are to undertake a prototype audit and are investigating whether crystallography would be an appropriate area for this audit.

ICSTI maintains a public web site at <http://www.icsti.org/>, where the newsletter *ICSTI Forum* and other general information are made available. A private section is available only to members, the IUCr Representative sharing this opportunity with the IUCr’s Sub-Committee on Electronic Publishing, Dissemination and Storage of Information (CEP). A distribution list operates where the ICSTI Executive Director distributes news clips and other information.

During 2002, ICSTI was under pressure from ICSU to free its office space in Paris, but this matter has now been resolved.

In 2003, the ICSTI annual meeting will take place in Ottawa, Canada, 8–12 May, organized and sponsored by CISTI (Canadian Institute of Scientific and Technical Information). The meeting includes a one-day public conference entitled ‘The Information Imperative: Impacts of STM Information and STM Information Organizations’. In 2004, the winter meeting will probably take place in Paris, France, and the annual meeting in London, UK.

ICSTI is composed of a large spectrum of professionals from the STM and library sectors but with few scientists present. IUCr membership of ICSTI continues to fulfil its expectations by providing a source of current documentation and personal contacts in the field of scientific and technical information (electronic publishing).

Finally, following the AGM in Stockholm, Sweden, H. D. Flack received and accepted an invitation to become an *ad hoc* member of the ICSTI Executive Board. In practice, this means that H. D. Flack will continue to represent the IUCr at the winter committee meetings in Paris.

**P. R. Strickland**, IUCr Representative

#### 14.3. International Council for Science (ICSU)

The 27th General Assembly of ICSU was held in Rio de Janeiro, Brazil, 24–28 September 2002, hosted by the Brazilian Academy of Sciences. The IUCr was represented by H. Schenk, the Immediate Past President of the IUCr. The format of the General Assembly was again different in the sense that on the first day the Scientific Unions and the National Scientific Members met in separate business meetings, the second day was devoted to Scientific Fora and a symposium on Science in Brazil, and the General Assembly itself took place from 26 to 28 September.

Firstly ICSU reformulated its mission into:

“To identify and address major issues of importance to science and society, by mobilizing the resources and knowledge of the international scientific community; to promote the participation of all scientists, irrespective of race, citizenship, language, political stance or gender, in the international scientific endeavour; to facilitate interactions between different scientific disciplines and between scientists from ‘developing’ and ‘developed’ countries; to stimulate constructive debate by acting as an authoritative independent voice for international science and scientists.”

The Fora specialized in the following subjects: Science for Sustainable Development; Energy and Sustainable Societies; Ensuring Global Access to Scientific Data and Information; and Capacity Building for Science or Strengthening Science in Developing Countries. In particular, the last two are of interest to the IUCr.

Data issues are becoming more and more important. Research is increasingly being financed by the private sector, and data access is often difficult. In many cases, governments wish data collected by public funds to be sold. At the same time, there is no consensus on how the international and global monitoring systems should be financed. Often it is difficult to exchange data, and there is an EU directive for the legal protection of databases. The digital divide is increasing, making it even more difficult for scientists from developing countries to access data. These issues will be addressed by ICSU in the World Summit on the Information Society (December 2003). The IUCr is actively involved in some of these fields. Capacity Building for Science should be high on the agenda. All countries experience declining interest among young students to major in natural sciences disciplines. A large proportion of the current generation of scientists are approaching retirement. The demands on scientists pull them in two opposite directions: more specialized to be competitive in cutting-edge disciplinary research and broader approaches to deal with problems relevant for society. A compendium of ICSU activities in the area of capacity building shows a wealth of different initiatives, including projects of the IUCr.

In the business meeting of Scientific Union Representatives, it was stressed again that greater contact and coordination between the Unions is necessary now their role in ICSU is less pronounced. The inter-General Assembly (GA) meeting of the Union Representatives has proved to be very important in this respect.

In the General Assembly, major subjects were the activities of the Committee on Scientific Planning and Review (CSPR). The aim of the ICSU grants programme is to provide ‘seed-corn’ funding, which is often difficult to obtain from other sources, to support the initial stages of development of a project. The CSPR refined the Grants Programme to ensure that this is a fully competitive programme, where awards are made uniquely on the scientific merit of the projects. Some of the sponsored projects were: Inter-Union Bioinformatics Group IUPAB/IUCr/IUBMB), International Biodiversity Observation Year (DIVERSITAS), Standardization and Dissemination (Internet) of Physico-Chemical Property Electronic Datafiles (CODATA/ICSTI), and Foods for Development. Priority Area Assessments, which are already planned (Environment/Sustainable Development/Capacity Building/Data/Information), will solicit input from all interested ICSU bodies and any further assessments will be conducted in a similarly inclusive manner.

The GA followed a proposal of CSPR and decided to dissolve COSTED/IBN after many years of excellent work and establish ICSU Regional Offices for Developing Countries in Africa, Asia, the Arab Region and Latin America. ICSU adopted a procedure (developing, approving and distributing) to produce a formal ICSU position statement. Also the supporting role ICSU may play in

statements from individual ICSU bodies or groups of bodies was agreed upon.

ICSU sent a strong delegation to the World Summit on Sustainable Development (September 2002, Johannesburg) and organized a series of meetings around the summit entitled Forum on Science, Technology, and Innovation for Sustainable Development. The delegation received much attention for its contributions and statements, and operated successfully.

On the last day, the elections took place. The Executive Board now comprises the following officers: President J. Lubchenco, Past President H. Yoshikawa, President-Elect G. Mehta, Vice-President for Scientific Planning & Review D. A. D. Parry, Vice-President for External Relations P. D. Tyson, Secretary-General A.-M. Cetto, and Treasurer R. Elliott; Union members are G. Berlucchi, B. Richter, R. Brett and M. Denis. The elections were followed by the decision to hold the 28th General Assembly of ICSU in the People's Republic of China.

**H. Schenk**, IUCr Representative

#### 14.4. ICSU Programme on Capacity Building in Science (PCBS)

No report has been received.

**R. B. Neder**, IUCr Representative

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

The major event for CODATA during 2002 was the biennial conference and General Assembly held in Montreal, Canada, 29 September–5 October. The CODATA 2002 meeting explored six cross-disciplinary themes relating to scientific and technical data:

- preservation and archiving;
- legal issues in using and sharing data;
- interoperability and data integration;
- information economics;
- emerging tools and techniques for data handling;
- ethics in the creation and use of data.

The following notes highlight some of the presentations; a fuller meeting report is available at <http://www.iucr.org/iucr-top/data/docs/>.

In a keynote lecture on preservation and archiving, K. Ashley (University of London, UK) struck some encouraging notes. The technical problems of archiving digital data are well understood; challenges are economic, social and managerial. Growth in bulk storage capacity will be able to handle the growing volume of data, but the difficulty will become locating the desired data within a collection. One cannot store everything; selection is important. Collectors of raw data often lack the necessary selection skills to maximize future usefulness. Hence funding bodies should support the digital archiving and libraries communities; but these are not always attuned to the requirements of scientific data management, and collaboration is needed to safeguard essential information when scientific data are transferred to non-specialized repositories.

The Open Archival Information System (OAIS) reference model has been well accepted. Where it has been adopted, it has proven effective, whether in the generation of code from a formal UML representation (Jet Propulsion Laboratories, USA), or as a more traditional blueprint for software engineering using XML, SOAP and other web services tools (Centre National d'Etudes Spatiales, France). The CNES experience showed how OAIS promoted interoperability between different databases: its level of abstraction makes it effective across disciplines. In other contributions related

to archiving, the point was repeatedly made that original data must be retained, whatever subsequent processing it might undergo. The distinction was made between 'migration' of data to different physical media, and 'transcription' into different formats required for subsequent reprocessing or storage. A difficulty with large-scale transcription projects is that the lifetime of the target format may be short compared with the time taken for the transcription operation.

The interoperability thread was introduced by a keynote talk by R. Robbins (Hutchinson Cancer Research Centre, Seattle, USA). He believed that interoperability between databases in the life/molecular biology sciences was hampered, partly by scale, but also by technical, semantic and social obstacles. The trend is to tackle semantic and social obstacles on the back of technical improvements. Technical problems arise from the fact that relational database management systems are optimized for business databases, and are not ideally suited to the scientific open universe of observations with inductive logic. However, relational database systems have a sound theoretical basis and are amenable to set-theoretic analysis. Object-oriented databases can be efficient but are often designed to solve the problem in hand. The difficulties of integrating several such *ad hoc* solutions are severe. Biological databases will form at best a 'loosely coupled federation' and never a fully integrated distributed database. One thing essential to achieve this was a resource registry able to direct structure queries to an appropriate WWW server.

Other talks in this thread illustrated how interoperability starts at the technical level. The oceanographic OpENDAP protocol has been successful in bringing together data sets in many different formats behind a common front-end. It is an open-source network data access protocol that sits like a format translation layer on top of TCP/IP. Mechanical procedures for translating between formats are employed, and the amount of semantic metadata required by search and retrieval applications is rather low. It was pointed out that one can get a lot of functionality out of 'smart' clients, but the more intelligent the client, the lower (in general) its capability for interoperability. The OpenGIS Consortium demonstrated the overlaying of map-based information from different geography sources using a number of web-compatible services. Among the tools used in XML-based data transfer applications, UDDI (Universal Description, Discovery and Integration) was mentioned by a number of speakers, and may go some way towards fulfilling the role of the resource registry mentioned in the keynote presentation. C. Lagoze (Cornell University, USA) discussed the Open Archives Initiative (OAI) protocol for metadata harvesting (PMH) that is designed to collect metadata across disciplines. It is based on Dublin Core metadata, but may provide a way to aggregate disparate metadata from different sources.

The keynote talk in the 'Emerging Tools' thread was on Text Mining by S. Matwin (University of Ottawa, Canada). This is the process of mechanically analysing natural-language text to extract structured information from an unstructured source. Text mining projects combine linguistic analysis (word stemming, tagging and rule-based parsing of grammatical structures) with machine learning. The objective is to work towards a semantic analysis, which for scientific texts is imaginable because the formal language of scientific discourse uses relatively direct mappings between syntax and semantics. The machine-learning component involves a preliminary feeding into the system of text tagged by experts as relevant or not relevant to a particular type of query. This is an effective way to generate thesauri relevant to a topic area. It was claimed that early projects concerned with the automatic categorization of documents in genomics and the detection of e-mail spam were showing promise.

Among the contributions to this thread, H. Kehiaian (Université de Paris VII, France) presented the standard file format SELF for physicochemical data as a technique for publishing, retrieving and exchanging such data. X. R. Lopez (Oracle Corporation, USA) discussed innovations within Oracle databases for storing spatial data, extending the database query language to include operations on spatial data types and introducing optimized spatial indexing. In collaboration with the San Diego Supercomputing Center, there are plans to provide biospatial types compliant with mmCIF.

P. Samuelson (University of California, Berkeley, USA) discussed some topical legal concerns and emphasized the need for the scientific community to uphold the value of the public domain in safeguarding access to information and ideas, fertilizing new ideas and upholding the general principles of scientific openness. Current legislation on intellectual property rights provides strong safeguards for the owners of data, but at the potential cost of eroding the doctrine of 'fair use' for educational and research purposes.

Among the contributions to the discussion section on the handling of physicochemical data, the undersigned presented a summary of CIF-based procedures within the crystallographic community.

**14.5.1. General Assembly.** Beyond the administrative affairs of CODATA, the main function of the General Assembly is the appointment or re-confirmation of Task Groups or Working Groups charged with furthering the objectives of CODATA. The Task Groups approved by the 23rd General Assembly for the period 2002–2004 are as follows (those marked with an asterisk are continuations of existing Task Groups):

- Fundamental Constants\*
- Global Species Data Networks\*
- Data Sources in Asian–Oceanic Countries\*
- Data, Information and Visualization\*
- Natural Gas Hydrates\*
- Data Management and Virtual Laboratories\*
- Biological Collection Data Access
- Preservation and Archiving of Scientific and Technical Data

The Preservation and Archiving Task Group is a continuation of the Working Group established at the last General Assembly, which has specific concerns about preservation and access in the developing world. A proposal was advanced for a new Working Group on ethics, and continued work arising from the Task Group on standardization of physicochemical property electronic datafiles was invited within the structure of a Working Group.

The new President of CODATA is S. Iwata (Japan; 2002–2006), and two Vice-Presidents were elected: A. Gvishiani (Russia; 2002–2006) and H. Sun (China; 2002–2006). Names of other officers are posted on the CODATA web site <http://www.codata.org>.

Thailand, Ukraine and the Czech Republic were welcomed as new National Members of CODATA. The successful launch of the peer-reviewed *Data Science Journal* was noted.

**14.5.2. Other activities.** The CODATA Representative attended, with the Chair of the Electronic Publishing Committee (H. D. Flack), a workshop at CERN, Switzerland, on the open archives initiative. While the OAI is designed primarily to facilitate self-publication of technical reports and grey literature, and thus to complement (or compete against) conventional scholarly periodical publications, the harvesting protocol is equally applicable for harvesting of database content. This, and the parallel development of openURL, a distributed query protocol, offer the potential for database interoperability and the provision of portal services allowing the simultaneous querying of a number of databases. These possibilities will be considered further in the course of providing links to database records from IUCr journal articles.

The CODATA representative is also *ex officio* a member of the IUCr Committee on Crystallographic Databases, and has undertaken responsibility for a new web page on data activities (<http://www.iucr.org/iucr-top/data>), designed to increase visibility of the activities of the Committee, of the major and secondary crystallographic database organizations, and of superdisciplinary data activities through CODATA and other relevant bodies. Discussions are under way to explore how best among the crystallographic databases to approach concerns such as long-term preservation and access, and interoperability.

**B. McMahon**, IUCr Representative

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

This Committee was dissolved in 2002.

**H. Schenk**, IUCr Representative

#### 14.7. ICSU Committee on Space Research (COSPAR)

The past year was not particularly significant from the point of view of materials science in space research. COSPAR was more concentrated on traditional space topics: new satellites, climate studies, new pulsars, gravitational lensing *etc.* The most important event for COSPAR in 2002 was the 34th General Assembly and 2nd World Space Congress, which took place in Houston (USA), 10–19 October 2002. A new Bureau was elected by the assembly: President: R. M. Bonnet (France); Vice-Presidents: W. Hermsen (The Netherlands), E. C. Stone (USA); Bureau members: J. Audouze (France), G. Horneck (Germany), T. Kosugi (Japan), M. E. Machado (Argentina), G. G. Shepherd (Canada), J. B. Zielinski (Poland); Finance Committee: D. Kendall (Canada, Chair), L. Sehnal (Czech Republic), E. Thrane (Norway).

Six Awards were presented during the Scientific Assembly. All were presented to eminent scientists working in the area of pure/applied astrophysics with the exception of the Zeldovich Medal given to P. Colinet for his contributions in the field of surface-tension-driven instabilities and fluid mechanics in microgravity conditions.

**J. M. Garcia-Ruiz**, IUCr Representative

### 15. Finances

The audited accounts of the year 2002 are given at the end of this Report. For comparison, the figures for 2001 are provided in italics. The accounts are presented in 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 2002 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 loss has arisen on the assets of the Union, in terms of CHF, amounting to CHF 278,387. The loss attributable to investment activities has been assigned to the General Fund and the loss attributable to trading activities has been divided amongst the fund accounts in direct proportion to the balances on these accounts at 31 December 2002. It

should be noted that this loss in CHF is not a real loss of money, but rather a loss on paper resulting from the accounts being expressed in CHF.

Investments are noted in the balance sheet at their market value at 31 December 2002.

The balance sheet shows that the assets of the Union, including the loss of CHF 278,387 resulting from fluctuations in rates of exchange, have decreased during the year, from CHF 5,553,575 to CHF 4,483,185. The decrease in assets is largely attributable to the poor performance of the stock markets in 2002 and to the investments made in developing **Crystallography Journals Online**, the digitization of all back issues of the journals and in producing the new and revised volumes of *International Tables for Crystallography*. The movement in market value of the investments was CHF -751,472 in 2002 (CHF -563,263 in 2001).

A transfer of CHF 120,000 was made to the Book Fund from the *Acta Crystallographica* Fund. A transfer of CHF 270,000 was made to the Publication and Journals Development Fund from the *Acta Crystallographica* Fund. A transfer of CHF 130,000 was made to the Research and Education Fund from the *Acta Crystallographica* Fund. A transfer of CHF 30,000 was made to the President's Fund from the *Acta Crystallographica* Fund. Transfers of CHF 25,000 and CHF 25,000 were made to the *Newsletter* Fund from the *Acta Crystallographica* Fund and the *Journal of Applied Crystallography* Fund. A transfer of CHF 50,000 was made to the *Journal of Synchrotron Radiation* Fund from the *Acta Crystallographica* Fund.

Beneath the detailed figures of the expenditure and income for each fund account, the balance at 1 January, 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 401,439, as compared with a deficit in 2001 of CHF 329,961 (before a transfer of CHF 25,000). The administrative expenses were CHF 472,764 in 2002 as compared with CHF 405,597 in 2001. Of this amount, CHF 208,110 was charged to the publications of the Union.

The expenses of the Union Representatives on other bodies were CHF 3,379. The cost of the Finance Committee meeting held in 2002 was CHF 12,019, while the Executive Committee meeting cost CHF 92,439. The income from the IUCr/Fachinformationszentrum agreement (to provide low-cost copies of the Inorganic Crystal Structure Database) was CHF 14,874. The subscriptions from Adhering Bodies were CHF 148,000. Interest on bank accounts and investments credited to the General Fund was CHF 35,871.

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 2,215. Grants totalling CHF 19,891 were paid from the fund.

The *Acta Crystallographica* account for 2002 shows a surplus of CHF 577,436 before the transfer of CHF 625,000 to other fund accounts, as compared with a surplus of CHF 420,646 in 2001 before transfers of CHF 575,000.

The subscription rates were increased for 2002. In 2002, the number of paid subscriptions to *Sections A+B+C+D* of *Acta*, including 33 (43) personal subscriptions, was 468 (497) (values for

2001 are given in parentheses). The number of paid subscriptions to *Sections A+B+C*, including 16 (17) personal subscriptions, was 130 (127). The number of paid subscriptions to the separate sections of the journal were: *Section A* 221 (232 for 2001), *Section B* 170 (170), *Section C* 136 (144) and *Section D* 256 (254). The cost of the technical editing office has been divided between the *Acta Crystallographica*, the *Journal of Applied Crystallography*, the *Journal of Synchrotron Radiation*, the *International Tables* and the Book Fund accounts in percentages based on the staff time spent on each publication. The technical editing costs for *Acta Crystallographica* were CHF 1,092,762 (for 7,905 published pages) as compared with CHF 1,013,651 in 2001 (7,162 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 152,190, as compared with a surplus of CHF 91,148 in 2001. In 2002, the number of paid subscriptions, including 113 (114 in 2001) personal subscriptions, was 696 (708 in 2001).

The *Journal of Synchrotron Radiation* account shows a deficit of CHF 27,235 before receiving a transfer of CHF 50,000 from the *Acta Crystallographica* Fund, as compared with a surplus of CHF 9,977 in 2001 before receiving a transfer of CHF 75,000. In 2002, the number of paid subscriptions, including 90 (108 in 2001) personal subscriptions, was 243 (259 in 2001).

The *International Tables* account shows a deficit of CHF 22,445, as compared with a deficit of CHF 271,046 in 2001. The net sales income was CHF 355,715 in 2002 as compared with CHF 167,706 in 2001. The deficits in 2001 and 2002 are a result of significant expenses being incurred in connection with production of revised editions of the four existing volumes and production costs for the five new volumes.

The Book Fund is credited with the sales of the remaining publications of the Union. The deficit of CHF 63,071 is attributable to the significant amount of programming time involved in the restructuring and updating of the *World Database of Crystallographers*, which is used to produce the *World Directory of Crystallographers*.

The *Newsletter* Fund account received transfers of CHF 25,000 from the *Acta Crystallographica* Fund and CHF 25,000 from the *Journal of Applied Crystallography* Fund in 2002 (CHF 25,000 from the General Fund and CHF 25,000 from the *Journal of Applied Crystallography* Fund in 2001). The cost to the Union of producing the *Newsletter* in 2002 was CHF 87,795 (CHF 36,429 in 2001).

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 computer and promotion expenses are divided between the General Fund, the *Acta Crystallographica* Fund, the *Journal of Applied Crystallography* Fund, the *Journal of Synchrotron Radiation* Fund and the *International Tables* Fund. STAR/CIF costs, Special Issue costs, journal grants and web input costs are also charged to the Publication and Journals Development account. From 2000, costs associated with the Crystallographic neXus Project to provide CD-ROMs (containing crystallographic software and web material) free of charge to developing countries has been charged to this Fund. CHF 111,983 for financial support to young scientists, to enable them to attend scientific meetings sponsored by the Union, and CHF 8,570 for the Visiting Professorship Programme were charged to the Research and Education Fund.

## 16. Auditor's Report to the International Union of Crystallography

We have audited the financial statements of the International Union of Crystallography for the year ended 31 December 2002 which comprise the income and expenditure account, the balance sheet, the cash flow statement and the related notes 17.1 to 17.15. These financial statements have been prepared under the accounting policies set out therein.

This report is made solely to the Union's members, as a body, in accordance with Section 11.1 of the Statutes of the Union. Our audit work has been undertaken so that we might state to the Union's members those matters we are required to state to them in an auditor's report and for no other purpose. To the fullest extent permitted by law, we do not accept or assume responsibility to anyone other than the Union and the Union's members as a body, for our audit work, for this report, or for the opinions we have formed.

### *Respective responsibilities of Executive Committee and Auditors*

As described in the statement of the Executive Committee's responsibilities, the Executive Committee is responsible for the preparation of the financial statements in accordance with applicable law and accounting standards.

Our responsibility is to audit the financial statements in accordance with relevant legal and regulatory requirements and United Kingdom auditing standards.

We report to you our opinion as to whether the financial statements give a true and fair view.

### *Basis of audit opinion*

We conducted our audit in accordance with United Kingdom 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 2002 and of the result for the year then ended.

Deloitte & Touche  
Chartered Accountants and Registered Auditors  
24 June 2003

## 17. Notes to the Accounts

The Income and Expenditure Account, the Balance sheet and the Cash Flow statement for the year ended 31 December 2002 are given in Tables 3, 4 and 5.

### 17.1. 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.

Transactions denominated in foreign currencies are translated into Swiss Francs at the rates ruling at the dates of the transactions. Monetary assets and liabilities denominated in foreign currencies at the balance sheet date are retranslated at the rates ruling at that date.

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. Profits 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 the lower of cost and net realizable value. Stocks of all other publications, including back issues of journals, are not valued for accounts purposes as sales are uncertain.

#### (e) Expenditure on premises

Expenditure on maintenance of 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 basis at a rate of 33 $\frac{1}{3}$ % per annum.

(iii) Leasehold property improvements 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 over the term of the lease. Where reduced rents are payable on property in the earlier years of the lease, the total cost for the period to the first rent review date is

spread on a straight line basis, and the appropriate creditor balance is maintained.

#### (j) Pension costs

The Union operates a defined contribution pension scheme for its employees. The assets of the scheme are held separately from those of the Union. The amount charged to income and expenditure in the year in respect of pensions represents employer's contributions payable in the year. No amounts were due to or from the pension scheme at 31 December 2002 (the same was true in 2001).

### 17.2. 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:

	2002	2001
Netherland Guilders (NLG)	–	1.4970
Euros (EUR)	0.6772	–
Danish Crowns (DKK)	5.0336	5.0606
Pounds Sterling (GBP)	0.4295	0.4242
US Dollars (USD)	0.6711	0.6061

The net assets of the Union at 1 January 2002 (CHF 5,553,575) would have had the value of USD 3,366,022 or GBP 2,355,826 if expressed in those currencies.

At 31 December 2002, the net assets (CHF 4,483,185) would have had the value of USD 3,008,665 or GBP 1,925,528, respectively, being a decrease of USD 357,357 or a decrease of GBP 430,298 from the previous year.

### 17.3. 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.

### 17.4. Tangible fixed assets

Table 6 lists the tangible fixed assets.

### 17.5. Investments

Table 7 lists the investments of the IUCr, their disposals and additions and the holding at 31 December 2002.

### 17.6. Creditors

Table 8 lists the creditors, with the amounts falling due within one year for 2001 and 2002.

### 17.7. Investment income

Table 9 lists the income from investments for 2001 and 2002.

**Table 3**  
Income and Expenditure Account for the year ended 31 December 2002.

	Note	2002	Swiss Francs	2001
<b>Income</b>				
Membership subscriptions		148,000		164,998
Sales				
Journals, back numbers and single issues		3,582,289	3,437,403	
Books		526,067	256,969	3,694,372
Investment income				
Income from investments	17.7	127,878	212,929	
Bank interest	17.8	15,534	28,029	
(Loss)/profit on sale of investments	17.9	(48,948)	(215,339)	25,619
Other income				
Grants		–	38,213	
Royalties and copyright fees		8,437	6,112	
Advertising income		146,812	198,038	242,363
<b>TOTAL INCOME</b>		<b>4,506,069</b>		<b>4,127,352</b>
<b>Expenditure</b>				
Journals				
Publication costs		838,308	929,800	
Editorial expenses		184,384	187,717	
Technical editing		1,361,346	1,309,644	
Subscription administration		33,638	44,956	2,472,117
Books				
Publication costs		57,374	95,756	
Editorial expenses		127,861	66,417	
Technical editing		176,963	192,874	355,047
Newsletter				
Publication costs		123,873	152,277	
Editorial expenses		85,851	73,175	225,452
President's Fund Grants and Young Scientists' support				
		131,874		132,288
General Assembly costs		57,155		41,397
Ewald Prize		49,005		–
Committee meetings and expenses		104,458		67,746
Publications and journals development				
General		467,958	460,387	
Electronic Publishing Committee/Section Editors meeting expenses		1,458	10,676	
STAR/CIF		621	556	
Promotions Officer		152,174	126,560	598,179
Subscriptions paid		9,971		10,568
Visiting Professorship Programme		8,570		6,937
Administration expenses:				
General Secretary and Treasurer:				
Honorarium to Treasurer		12,192	12,090	
Audit and accountancy charges		69,828	48,794	
Legal and professional fees		16,586	20,259	
Travelling expenses		6,290	8,423	
Bank charges		2,772	2,744	92,310
Executive Secretary's office:				
Salaries and expenses		351,559	290,346	
Travel expenses of IUCr Representatives on other bodies		3,379	3,840	
Commission expenses		–	10,315	
Sponsorship of meetings		46,764	1,824	
President's secretary		4,135	10,000	
IUCr/FIZ agreement		(14,874)	(8,353)	
Bad debts – subscriptions		–	8,000	315,972
Depreciation		75,127		76,013
<b>TOTAL EXPENDITURE</b>		<b>4,546,600</b>		<b>4,394,026</b>

# international union of crystallography

**Table 3 (continued)**

	Note	2002	Swiss Francs	2001
Deficit of income over expenditure			(40,531)	(266,674)
Movement in market value of investments in year	17.5		(751,472)	(563,263)
Fluctuation in rates of exchange			(792,003)	(829,937)
Trading activities	17.2	(31,058)		15,489
Investment activities	17.2	(247,329)	(278,387)	(380,429)
Total recognized gains and losses relating to the year			(1,070,390)	(1,210,366)
Opening fund accounts at 1 January			5,553,575	6,763,941
Closing fund accounts at 31 December			4,483,185	5,553,575

All the income and expenditure related to continuing activities. Historic cost results would only differ from above by the loss on sale of investments – see Note 17.9. Separate Statements of Total Recognized Gains and Losses and Reconciliation of Movements in Fund Account are not given, as the information is incorporated in the above.

**Table 4**

Balance sheet as at 31 December 2002.

	Note	2002	Swiss Francs	2001
<b>FIXED ASSETS</b>				
Tangible fixed assets	17.4		89,802	97,216
<b>CURRENT ASSETS</b>				
Stock			104,562	77,359
Cash at bank and in hand				
Current accounts		62,186		62,708
Deposit and savings accounts		414,952		244,167
Cash with Union officials		23,042	500,180	29,466
Investments at market value	17.5		3,739,292	4,772,261
Debtors, accrued income and payments in advance			280,266	450,736
Subscriptions due from Adhering Bodies			44,374	23,874
<b>TOTAL CURRENT ASSETS</b>			4,668,674	5,660,571
<i>Creditors</i> : amounts falling due within one year	17.6		(275,291)	(204,212)
<b>NET CURRENT ASSETS</b>			4,393,383	5,456,359
<b>TOTAL FUNDS</b>			4,483,185	5,553,575

## 17.8. Bank interest

Table 10 lists the bank interest for 2001 and 2002.

## 17.9. Loss/profit on disposal/redemption of investments

Table 11 lists the loss or profit on disposal/redemption of investments for 2001 and 2002.

## 17.10. Information regarding employees

Staff costs during the years 2001 and 2002 are given in Table 12.

## 17.11. Operating lease commitments

At 31 December 2002, the Union was committed to making the payments listed in Table 13 during the next year in respect of operating leases.

## 17.12. Sponsorship commitments

At 31 December 2002, the Union had authorized, but not contracted for, sponsorship grants of CHF 81,950 (2001: CHF 88,275).

**Table 5**  
Cash Flow statement for the year ended 31 December 2002.

	Note	2002	Swiss Francs	2001
Net cash inflow/(outflow) from operating activities (see below)			162,008	(409,322)
Returns on investments				
Interest received		15,534		28,029
Investment income (net of notional dividends)		38,994		78,209
Net cash inflow from returns on investments			54,528	106,238
Investing activities				
Purchase of fixed assets	17.4	(67,713)		(95,061)
Purchase of investments	17.5	(421,807)		(1,374,937)
Disposal of investments	17.9	495,910		1,912,839
Net cash inflow from investing activities			6,390	442,841
Increases in cash	17.14		222,926	139,757
<i>Reconciliation of Deficit of Income over Expenditure to Net Cash Inflow/(Outflow) from Operating Activities</i>				
Deficit of income over expenditure			(40,531)	(266,674)
Exchange rate fluctuations attributable to operating activities	17.13		28,029	12,931
Interest received	17.8		(15,534)	(28,029)
Investment income	17.7		(127,878)	(212,929)
Loss on disposal of investments	17.9		48,948	215,339
Depreciation charges			75,127	76,013
Increase in stock			(27,203)	(58,140)
Decrease/(increase) in debtors			149,970	(146,505)
Increase/(decrease) in creditors			71,080	(1,328)
Net cash inflow/(outflow) from operating activities (see above)			162,008	(409,322)

**Table 6**  
Tangible fixed assets.

	Leasehold property improvements CHF	Office equipment CHF	Computer equipment CHF	Total CHF
<b>Cost</b>				
As at				
1 January 2002	102,987	86,537	290,039	479,563
Additions	–	5,356	62,357	67,713
As at				
31 December 2002	102,987	91,893	352,396	547,276
<b>Accumulated depreciation</b>				
As at				
1 January 2002	64,132	73,099	245,116	382,347
Charge for the year	10,299	5,838	58,990	75,127
As at				
31 December 2002	74,431	78,937	304,106	457,474
<b>Net book value</b>				
31 December 2002	28,556	12,956	48,290	89,802
31 December 2001	38,855	13,438	44,923	97,216

**17.13. Exchange rate fluctuations**

Table 14 lists exchange rate fluctuations attributable to operating activities for 2001 and 2002.

**17.14. Analysis of changes in cash during the year**

Table 15 is an analysis of cash changes during 2001 and 2002.

**17.15. Analysis of balances of cash as shown in the balance sheet**

Table 16 is an analysis of cash balances as shown in the balance sheet.

Tables 17–28 give the accounts for the year ended 31 December 2002 for the various fund accounts.

# international union of crystallography

**Table 7**  
Investments.

	Holding at market value 1 January 2002	Additions during the year	Notional dividends	Disposals/ redemptions during the year	Swiss Francs Fluctuations in rates of exchange	Increase/ (decrease) in market value	Holding at market value 31 December 2002	Holding at revalued cost 31 December 2002	Holding at revalued cost 31 December 2001
Held by Merrill Lynch									
GNM P169332-2016 (USD) 2,522 Units	7,148	–	–	(2,484)	(563)	77	4,178	3,629	6,325
Hausmann Holdings (USD) 102 Units	195,972	45,012	–	–	(19,303)	(10,012)	211,669	104,759	66,495
Global Allocation Portfolio Class O (USD) 2,700 Units	96,229	–	–	–	(9,331)	(7,573)	79,325	42,443	47,000
MLBS SP PF EU EQ (US) B 3,292 Units	147,418	–	–	–	(14,295)	(17,413)	115,710	149,833	165,922
Sector SPDR Energy 2075 Units	91,414	–	–	–	(8,864)	(13,512)	69,038	72,037	79,773
ML Asian Dragon 2,600 Units	–	48,591	–	–	(2,180)	(10,886)	35,525	46,411	–
Mercury Selected Trust USD Global Bond Fund B 6,790 Units	179,479	–	–	–	(17,404)	6,980	169,055	149,258	165,285
Janus Global Life Sciences Fund 4,700 Units	71,036	–	–	–	(6,888)	(20,799)	43,349	70,620	78,203
Janus US Venture Fund 4,800 Units	51,162	–	–	–	(4,961)	(13,230)	32,971	74,125	82,084
Seligman US Comm + Info Fund 1,750 Units	49,463	–	–	–	(4,796)	(17,576)	27,091	73,953	81,894
Seligman Horizon Global Tech Fund 1,500 Units	42,125	–	–	–	(4,085)	(12,807)	25,233	73,494	81,386
Cisco Systems Inc. 1,700 Units	50,799	–	–	–	(4,926)	(12,691)	33,182	83,108	92,032
Pharmaceutical 200 Units	32,507	–	–	(31,914)	(593)	–	–	–	33,229
Global SR (DE) 600 Units	31,203	–	–	(30,636)	(567)	–	–	–	99,518
Consults Portfolios									
850-07U78	213,245	123,786	–	(138,067)	(19,565)	(17,126)	162,273	173,135	206,021
850-07A96	137,694	53,168	–	(183,512)	(10,910)	3,560	–	–	141,635
850-07U80	123,008	131,203	–	(18,104)	(12,657)	(44,644)	178,806	232,223	132,723
850-07U81	135,140	20,047	–	(140,141)	(10,858)	(4,188)	–	–	130,504
Held by Foreign & Colonial									
Reserve Asset Fund Class L (GBP) 25,538 Units	1,480,640	–	44,628	–	(18,822)	(394,449)	1,111,997	1,234,528	1,205,221
Reserve Asset Fund Class X (GBP) 2,566 Units	123,615	–	5,321	–	(1,571)	(1,331)	126,034	133,963	130,299
Reserve Asset Fund Class M (USD) 9,692 Units	708,019	–	9,381	–	(69,084)	(169,199)	479,117	479,265	520,815
Reserve Asset Fund Class E (GBP) 6,040 Units	401,727	–	29,554	–	(5,107)	2,171	428,345	432,814	408,451
	4,369,043	421,807	88,884	(544,858)	(247,330)	(754,648)	3,332,898	3,629,598	3,954,815
Treasury Stock									
7.75% UK Treasury Stock 2006 150,000 Units	403,218	–	–	–	–	3,176	406,394	370,225	374,992
	4,772,261	421,807	88,884	(544,858)	(247,330)	(751,472)	3,739,292	3,999,823	4,329,807

**Table 8**

Creditors: amounts falling due within one year.

	Swiss Francs	
	2002	2001
Creditors and accruals	227,808	161,708
Payroll creditor including tax and social security	47,483	42,504
	<u>275,291</u>	<u>204,212</u>

**Table 9**

Investment income.

	Swiss Francs	
	2002	2001
GNM P169332 - 2016	501	767
Haussmann Holdings	304	274
Foreign and Colonial – Reserve Asset Fund Class L	44,628	74,132
Foreign and Colonial – Reserve Asset Fund Class X	5,321	6,177
Foreign and Colonial – Reserve Asset Fund Class M	9,381	25,617
Foreign and Colonial – Reserve Asset Fund Class E	29,553	28,794
UK Treasury 7.75% 22.9.2006	27,493	56,381
Banco Bilbao	–	6,993
ML Debt Strategy	–	48
Sector SPDR Strategy	1,142	1,432
Pharmaceutical	143	266
Telecom	–	30
Internet Architecture	–	2
Broadband	–	1
Consults Portfolios		
850-07U78	3,817	3,508
850-07A96	1,125	3,092
850-07U80	3,651	3,341
850-07U81	819	2,074
	<u>127,878</u>	<u>212,929</u>
Allocated to:		
President's Fund	2,215	3,207
Publication and Journals Development Fund	28,869	20,714
Research and Education Fund	50,361	48,532
Ewald Fund	26,096	27,322
Balance left in General Fund	20,337	113,154
	<u>127,878</u>	<u>212,929</u>

**Table 10**

Bank interest.

	Swiss Francs			
	2002		2001	
National Westminster Bank Plc				
Manchester Business				
Reserve Account	3,055		5,544	
Manchester Capital				
Reserve Account	11,519	14,574	4,160	9,704
Merrill Lynch				
CMA Account		659		2,557
Foreign & Colonial				
Cash balance		301		325
Interest from Munksgaard		–		15,443
Allocated to General Fund		<u>15,534</u>		<u>28,029</u>

**Table 11**

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

	Swiss Francs	
	2002	2001
Proceeds	495,910	1,912,839
Book value	544,858	2,128,178
Loss allocated to General Fund	<u>(48,948)</u>	<u>(215,339)</u>

Book value represents market value at 1 January 2002 or cost if acquired after that date. The loss on disposal based on historic cost was CHF 116,449 (2001: loss of CHF 244,220). Therefore historic cost results would be as follows:

	Swiss Francs	
	2002	2001
Deficit of income over expenditure	<u>(108,032)</u>	<u>(295,555)</u>

**Table 12**

Information regarding employees.

	2002	2001
Average number of persons employed during the year	23	22

	Pounds Sterling	
	2002	2001
Staff costs incurred during the year in respect of these employees:		
Salaries	677,327	629,846
Social security	56,677	62,809
Pension	118,177	113,497
Total staff costs	<u>852,181</u>	<u>806,152</u>

	Swiss Francs	
	2002	2001
Total staff costs	<u>1,998,191</u>	<u>1,958,439</u>

# international union of crystallography

**Table 13**  
Operating lease commitments.

	Land and Buildings 2002	Other 2002	Swiss Francs	Land and Buildings 2001	Other 2001
Leases which expire:					
within one year	–	41,427		–	41,961
within two to five years	60,580	6,431		61,360	–
after five years	26,795	–		27,140	–
	<u>87,375</u>	<u>47,858</u>		<u>88,500</u>	<u>41,961</u>

**Table 14**  
Exchange rate fluctuations attributable to operating activities.

	2002	Swiss Francs 2001
Total fluctuations in exchange rates dealt with in fund accounts	(278,387)	(380,429)
Adjustments for exchange differences attributable to:		
Investments (Note 17.5)	247,329	395,918
Cash and bank balances	59,087	(2,558)
	<u>28,029</u>	<u>12,931</u>

**Table 15**  
Analysis of changes in cash during the year.

	2002	Swiss Francs 2001
Balance at 1 January 2002		336,341
Net cash inflow	222,926	139,757
Fluctuations in rates of exchange on cash and bank balances	(59,087)	163,839
Balance at 31 December 2002		500,180
		<u>336,341</u>

**Table 16**  
Analysis of cash balances as shown in the Balance sheet.

	2002	Swiss Francs 2001	Change 2002	Change 2001
Cash at bank and in hand	500,180	336,341	163,839	142,315

**Table 17**  
Fund Accounts as at 31 December 2002.

	As at 1 January 2002	Transfers between funds	(Deficit)/ excess of income over expenditure for the year	Swiss Francs		Balance at 31 December 2002	
				Loss on market value of investments	Fluctuations in exchange rates (Note 17.2)		
				Trading	Investments		
<b>FUND ACCOUNTS</b>							
General Fund	2,253,503	–	(401,439)	(751,472)	(7,178)	(247,329)	846,085
President's Fund	56,803	30,000	(17,676)	–	(451)	–	68,676
<i>Acta Crystallographica</i>	810,560	(625,000)	577,436	–	(4,977)	–	758,019
<i>Journal of Applied Crystallography</i>	202,815	(25,000)	152,190	–	(2,153)	–	327,852
<i>International Tables</i>	(2,025)	–	(22,445)	–	160	–	(24,310)
Book Fund	(31,489)	120,000	(63,071)	–	(166)	–	25,274
Publications and Journals							
Development Fund	567,419	270,000	(57,395)	–	(5,088)	–	774,936
Research and Education Fund	959,904	130,000	(70,192)	–	(6,651)	–	1,013,061
Ewald Fund	483,945	–	(22,909)	–	(3,007)	–	458,029
Newsletter Fund	148,263	50,000	(87,795)	–	(721)	–	109,747
<i>Journal of Synchrotron Radiation</i>	103,877	50,000	(27,235)	–	(826)	–	125,816
	<u>5,553,575</u>	<u>–</u>	<u>(40,531)</u>	<u>(751,472)</u>	<u>(31,058)</u>	<u>(247,329)</u>	<u>4,483,185</u>

**Table 18**

General Fund Account for the year ended 31 December 2002.

	Note	2002	Swiss Francs	2001
<b>Income</b>				
Grant received from UNESCO subvention to ICSU			–	8,656
Subscriptions from Adhering Bodies			148,000	164,998
Income from investments	17.7		20,337	113,154
Interest on bank accounts	17.8		15,534	28,029
Loss on disposal/redemption of investments	17.9		(48,948)	(215,339)
Amounts charged to the following journals and publications:				
<i>Acta Crystallographica</i>		181,534	127,294	
<i>Journal of Applied Crystallography</i>		17,107	19,727	
<i>Journal of Synchrotron Radiation</i>		9,469	30,863	177,884
		<hr/>	<hr/>	<hr/>
TOTAL INCOME		343,033		277,382
<b>Expenditure</b>				
Subscriptions to ICSU and ICSU bodies			9,971	10,568
Administrative expenses:				
General Secretary and Treasurer:				
Honorarium to Treasurer		12,192	12,090	
Audit and accountancy charges		69,828	48,794	
Legal and professional fees		16,586	20,259	
Travelling expenses		6,290	8,423	
Bank charges		2,772	2,744	
Executive Secretary's office:				
Salaries and expenses		351,559	290,346	
Depreciation of office equipment		3,238	12,642	
Depreciation of leasehold improvements		10,299	10,299	405,597
		<hr/>	<hr/>	<hr/>
Nineteenth General Assembly and Congress				
Expenses		57,155	6,620	
Programme Committee		–	34,777	
Meeting of the Executive Committee		92,439	54,892	
Finance Committee expenses		12,019	12,854	
Programming and development costs		43,828	42,361	
Promotion		16,892	14,048	
Travel expenses of IUCr Representatives on other bodies		3,379	3,840	
Commission expenses		–	10,315	
Sponsorship of meetings		46,764	1,824	
President's secretary		4,135	10,000	
IUCr/FIZ agreement		(14,874)	(8,353)	
Bad debts – subscriptions		–	8,000	191,178
		<hr/>	<hr/>	<hr/>
TOTAL EXPENDITURE			744,472	607,343
<i>Deficit of income over expenditure</i>			(401,439)	(329,961)
<b>Reconciliation of movements</b>				
Balance at 1 January			2,253,503	3,560,747
Transfers to other funds				
<i>Newsletter Fund</i>			–	(25,000)
Deficit of income over expenditure		(401,439)		(329,961)
Movement in market value of investments in the year	17.5	(751,472)	(1,152,911)	(563,263)
		<hr/>	<hr/>	<hr/>
Fluctuations in rates of exchange			(254,507)	(389,020)
Balance at 31 December			846,085	2,253,503

# international union of crystallography

**Table 19**

*Acta Crystallographica* Account for the year ended 31 December 2002.

	Note	2002	Swiss Francs	2001
<b>Income</b>				
Subscriptions to Volume 58 (2001 Volume 57) and sale of back numbers and single copies		2,831,674	2,598,837	
Distribution costs charged to subscribers		100,147	105,510	
Royalties and copyright fees		22,510	11,164	
Special Issue income		45,771	30,316	
Pay per view and secondary services (net)		10,364	4,803	
		<u>3,010,466</u>	<u>2,750,630</u>	
Less Publisher's commission on sales		205,091	185,612	2,565,018
Income from advertisements (net)			8,134	3,214
Recharge for Special Issue			(1,615)	(11,943)
<b>TOTAL INCOME</b>		<u>2,811,894</u>	<u>2,556,289</u>	
<b>Expenditure</b>				
Publication expenses:				
Production Volume 58 (2001 Volume 57)		431,187	507,782	
Distribution costs		86,030	86,147	
		<u>517,217</u>	<u>593,929</u>	
Net profit on reprints		(24,862)	(28,732)	
Special Issue costs		44,156	18,373	583,570
Editorial expenses:				
Editorial honoraria		120,495	116,035	
Secretarial assistance		8,046	8,019	
Postage, travel and sundries		21,727	24,796	
Technical editing:				
Salaries and expenses		981,341	946,969	
Computer expenses		98,051	55,591	
Subscription administration		25,228	36,255	
Promotion		68,022	56,574	
Depreciation of office equipment		13,370	11,091	1,255,330
Programming and development costs			180,133	169,449
Administration expenses recharged from General Fund			181,534	127,294
<b>TOTAL EXPENDITURE</b>		<u>2,234,458</u>	<u>2,135,643</u>	
<i>Surplus of income over expenditure</i>		<u>577,436</u>	<u>420,646</u>	
<b>Reconciliation of movements</b>				
Balance at 1 January		810,560		962,804
Transfers to other funds				
<i>International Tables</i>		–	200,000	
Book Fund		120,000	–	
Publications and Journals Development Fund		270,000	200,000	
Research and Education Fund		130,000	100,000	
<i>Newsletter</i> Fund		25,000	–	
<i>Journal of Synchrotron Radiation</i>		50,000	75,000	
President's Fund		30,000	–	(575,000)
Surplus of income over expenditure		577,436		420,646
Fluctuations in rates of exchange		(4,977)		2,110
<b>Balance at 31 December</b>		<u>758,019</u>	<u>810,560</u>	

**Table 20**
*Journal of Applied Crystallography* Account for the year ended 31 December 2002.

	Note	2002	Swiss Francs	2001
<b>Income</b>				
Subscriptions to Volume 35 (2001 Volume 34) and sale of back numbers and single copies		436,036	389,550	
Distribution costs charged to subscribers		14,623	28,889	
Royalties and copyright fees		3,575	2,120	
Advertising income		11,245	702	
Pay per view and secondary services (net)		2,960	–	
		<u>468,439</u>	<u>421,261</u>	
Less Publisher's commission on sales		<u>31,375</u>	<u>27,703</u>	
<b>TOTAL INCOME</b>		<u>437,064</u>		<u>393,558</u>
<b>Expenditure</b>				
Publication expenses:				
Production Volume 35 (2001 Volume 34)		43,874	68,595	
Distribution costs		12,080	11,726	
		<u>55,954</u>	<u>80,321</u>	
Net profit on reprints		<u>(3,376)</u>	<u>52,578</u>	<u>(4,563)</u>
				75,758
Editorial expenses:				
Editorial honoraria		8,912	4,006	
Secretarial assistance		8,717	8,785	
Postage, travel and sundries		1,211	1,074	
Technical editing:				
Salaries and expenses		136,013	134,867	
Computer expenses		9,240	8,615	
Subscription administration		5,046	7,251	
Promotion		16,739	13,921	
Depreciation of office equipment		<u>1,261</u>	<u>1,718</u>	<u>180,237</u>
Programming and development costs			28,050	26,688
Administration expenses recharged from General Fund			17,107	19,727
<b>TOTAL EXPENDITURE</b>			<u>284,874</u>	<u>302,410</u>
<i>Surplus of income over expenditure</i>			<u>152,190</u>	<u>91,148</u>
<b>Reconciliation of movements</b>				
Balance at 1 January			202,815	136,139
Transfers to other funds				
<i>Newsletter</i> Fund			(25,000)	(25,000)
Surplus of income over expenditure			152,190	91,148
Fluctuations in rates of exchange			(2,153)	528
Balance at 31 December			<u>327,852</u>	<u>202,815</u>

# international union of crystallography

**Table 21**

*Journal of Synchrotron Radiation* Account for the year ended 31 December 2002.

	Note	2002	Swiss Francs	2001
<b>Income</b>				
Subscriptions to Volume 9 (2001 Volume 8) and sales of back numbers and single issues		159,325	168,056	
Distribution costs charged to subscribers		2,441	5,143	
Special Issue income		659	125,058	
Pay per view and secondary services (net)		1,480	—	
		163,905	298,257	
<i>Less</i> Publisher's commission on sales		11,230	12,528	285,729
Income from advertisements			5,504	5,099
Income from copyright fees			1,209	1,397
Recharge for Special Issue			(659)	(5,389)
<b>TOTAL INCOME</b>		158,729		286,836
<b>Expenditure</b>				
Publication expenses:				
Special Issue costs		—	119,669	
Production Volume 9 (2001 Volume 8)		27,682	44,276	
Distribution costs		4,444	4,560	
		32,126	168,505	
Net profit on reprints		(3,562)	(8,771)	159,734
Editorial expenses:				
Editorial honoraria		8,266	9,348	
Secretarial assistance		2,777	4,770	
Postage, travel and sundries		857	408	
Technical editing:				
Salaries and expenses		100,913	30,455	
Computer expenses		5,114	13,478	
Subscription administration		3,364	1,449	
Promotion		16,739	13,921	
Depreciation of office equipment		697	2,690	76,519
Programming and development costs			9,204	9,743
Administration expenses recharged from General Fund			9,469	30,863
<b>TOTAL EXPENDITURE</b>		185,964		276,859
<i>(Deficit)/surplus of income over expenditure</i>			(27,235)	9,977
<b>Reconciliation of movements</b>				
Balance at 1 January		103,877		18,630
Transfers from other funds				
<i>Acta Crystallographica</i>		50,000		75,000
<i>(Deficit)/surplus of income over expenditure</i>			(27,235)	9,977
Fluctuations in rates of exchange			(826)	270
<b>Balance at 31 December</b>		125,816		103,877

**Table 22**

President's Fund Account for the year ended 31 December 2002.

	Note	Swiss Francs	
		2002	2001
<b>Income</b>			
Investment income	17.7	2,215	3,207
<b>Expenditure</b>			
Grants		19,891	5,196
<i>Deficit of income over expenditure</i>		(17,676)	(1,989)
<b>Reconciliation of movements</b>			
Balance at 1 January		56,803	58,644
Transfers from other funds			
<i>Acta Crystallographica</i>		30,000	–
Deficit of income over expenditure		(17,676)	(1,989)
Fluctuations in rates of exchange		(451)	148
Balance at 31 December		68,676	56,803

**Table 24**

Book Fund Account for the year ended 31 December 2002.

	Note	Swiss Francs	
		2002	2001
<b>Income</b>			
Sales of copies, net of Publisher's commission on sales			
<i>Historical Atlas of Crystallography</i>		86	140
<i>World Directory of Crystallographers</i>		1	900
<i>Escher Kaleidozyklen</i>		45	127
<i>Structure Reports</i>		70	393
Royalties			
IUCr/OUP Book Series		3,653	2,595
TOTAL INCOME		3,855	4,155
<b>Expenditure</b>			
Publication expenses			
<i>World Directory of Crystallographers</i>		1,824	1,980
Programming and development		48,211	61,002
Promotion		16,891	14,048
TOTAL EXPENDITURE		66,926	77,030
<i>Deficit of income over expenditure</i>		(63,071)	(72,875)
<b>Reconciliation of movements</b>			
Balance at 1 January		(31,489)	41,468
Transfers from other funds			
<i>Acta Crystallographica</i>		120,000	–
Deficit of income over expenditure		(63,071)	(72,875)
Fluctuations in rates of exchange		(166)	(82)
Balance at 31 December		25,274	(31,489)

**Table 23**

International Tables Account for the year ended 31 December 2002.

	Note	Swiss Francs		
		2002	2001	2000
<b>Income</b>				
Sales of copies				
Volume A		259,939	811	
Teaching Edition of Volume A		16,079	116	
Volume B		43,539	67,989	
Volume C		39,735	45,091	
Volume E		6,561	–	
Volume F		114,311	112,122	
		480,164	226,129	
Less Publisher's commission on sales		124,449	58,423	
TOTAL INCOME			355,715	167,706
<b>Expenditure</b>				
Publication expenses:				
Production Volume A		26,836	–	
Production Volume B		5,096	30,036	
Production Volume C		4,948	5,569	
Production Volume D		–	1,507	
Production Volume E		5,645	–	
Production Volume F		13,209	57,307	
Production Teaching Edition of Volume A		266	–	
		55,550	94,419	
Editorial expenses:				
Editorial honoraria		7,009	15,039	
Secretarial assistance, postage and office equipment		3,412	7,994	
Technical editing		176,963	187,384	215,907
Programming and development			118,335	114,378
Promotion			16,891	14,048
TOTAL EXPENDITURE			378,160	438,752
<i>Deficit of income over expenditure</i>			(22,445)	(271,046)
<b>Reconciliation of movements</b>				
Balance at 1 January			(2,025)	69,026
Transfers from other funds				
<i>Acta Crystallographica</i>			–	200,000
Deficit of income over expenditure			(22,445)	(271,046)
Fluctuations in rates of exchange			160	(5)
Balance at 31 December			(24,310)	(2,025)

**Table 25**

Publications and Journals Development Fund Account for the year ended 31 December 2002.

	Note	Swiss Francs	
		2002	2001
<b>Income</b>			
Investment income	17.7	28,869	20,714
<b>Expenses</b>			
Computer expenses:			
Purchase of computer equipment and software		–	9,207
Programming and development	438,279	414,414	
Recharged to other funds	(438,279)	–	(423,621)
Electronic Publishing Committee/ Section Editors' Meeting		1,458	10,676
Special Issue surplus			
recredited from other funds		(2,274)	(17,331)
NeXus		2,141	2,244
STAR/CIF		621	556
Promotion		152,174	126,560
Promotion recharged to other funds		(152,174)	(126,560)
Web input		2,981	626
Journal subscription subsidies		19,088	968
Digitisation project		15,987	32,928
Depreciation of computer equipment		46,262	37,573
<b>TOTAL EXPENDITURE</b>		<b>86,264</b>	<b>68,240</b>
<i>Deficit of income over expenditure</i>		<i>(57,395)</i>	<i>(47,526)</i>
<b>Reconciliation of movements</b>			
Balance at 1 January		567,419	413,468
Transfers from other funds			
<i>Acta Crystallographica</i>		270,000	200,000
Deficit of income over expenditure		(57,395)	(47,526)
Fluctuations in rates of exchange		(5,088)	1,477
<b>Balance at 31 December</b>		<b>774,936</b>	<b>567,419</b>

**Table 26**

Research and Education Fund Account for the year ended 2002.

	Note	Swiss Francs	
		2002	2001
<b>Income</b>			
Investment income	17.7	50,361	48,532
Refund of Congress income		–	29,556
<b>TOTAL INCOME</b>		<b>50,361</b>	<b>78,088</b>
<b>Expenditure</b>			
Young Scientists' Support	111,983	127,92	
Visiting Professorship Programme	8,570	6,937	
<b>TOTAL EXPENDITURE</b>		<b>120,553</b>	<b>134,029</b>
<i>Deficit of income over expenditure</i>		<i>(70,192)</i>	<i>(55,941)</i>
<b>Reconciliation of movements</b>			
Balance at 1 January		959,904	913,346
Transfers from other funds			
<i>Acta Crystallographica</i>		130,000	100,000
Deficit of income over expenditure		(70,192)	(55,941)
Fluctuations in rates of exchange		(6,651)	2,499
<b>Balance at 31 December</b>		<b>1,013,061</b>	<b>959,904</b>

**Table 27**

Ewald Fund Account for the year ended 31 December 2002.

	Note	Swiss Francs	
		2002	2001
<b>Income</b>			
Investment income	17.7	26,096	27,322
<b>Expenditure</b>			
Prize/Selection Committee and expenses		49,005	–
<i>(Deficit)/surplus of income over expenditure</i>		<i>(22,909)</i>	<i>27,322</i>
<b>Reconciliation of movements</b>			
Balance at 1 January		483,945	455,363
(Deficit)/surplus of income over expenditure		(22,909)	27,322
Fluctuations in rates of exchange		(3,007)	1,260
<b>Balance at 31 December</b>		<b>458,029</b>	<b>483,945</b>

**Table 28**

Newsletter Fund Account for the year ended 2002.

	Note	Swiss Francs	
		2002	2001
<b>Income</b>			
Income from advertisements		122,668	174,692
Reimbursement of 19GAC circular		(739)	14,331
<b>TOTAL INCOME</b>		<b>121,929</b>	<b>189,023</b>
<b>Expenditure</b>			
Editorial honoraria		7,284	7,260
Editorial expenses		78,567	65,915
Newsletter printing and distribution		93,207	108,604
Advertising costs		30,666	43,673
<b>TOTAL EXPENDITURE</b>		<b>209,724</b>	<b>225,452</b>
<i>Deficit of income over expenditure</i>		<i>(87,795)</i>	<i>(36,429)</i>
<b>Reconciliation of movements</b>			
Balance at 1 January		148,263	134,306
Transfers from other funds			
General Fund		–	25,000
<i>Acta Crystallographica</i>	25,000	–	–
<i>Journal of Applied Crystallography</i>	25,000	50,000	25,000
Deficit of income over expenditure			
Current year	(75,458)	–	–
Prior year	(12,337)	(87,795)	(36,429)
Fluctuations in rates of exchange		(721)	386
<b>Balance at 31 December</b>		<b>109,747</b>	<b>148,263</b>