

## **Schedule of meetings**

**Grand Hotel Panoramic, Montecatini Terme, Italy**

### **21 August**

15:00-18:30: Opening plenary session (background information)

19:00-21:00: Dinner

### **22 August**

07:00-08:30: Breakfast

08:45-12:30: Plenary session (general matters for discussion)

10:30-10:45: Coffee break

12:30-13:30: Lunch

13:30: Group photograph

13:45-17:25: Parallel journal sessions

13:45-14:55: Acta A

13:45-14:55: Acta B/C/E

13:45-17:25: Acta D/F

14:55-16:05: Acta B

14:55-17:25: Acta C/E

14:55-16:05: JSR

16:05-16:15: Coffee break

16:15-17:25: JAC

17:30-18:30: Section and Main Editors meeting

19:00-21:00: Dinner

### **23 August**

07:00-08:45: Breakfast

09:00-12:00: Final plenary session (completion of discussions, voting)

12:30: Coach to Florence

# Participants

## Grand Hotel Panoramic, Montecatini Terme, Italy

| TITLE     | FORENAMES          | SURNAME          | ADDRESS                                     | JOURNAL | ARRIVAL DETAILS      |
|-----------|--------------------|------------------|---|---------|----------------------|
| Dr        | Andrew John        | Allen            | NIST  | J       | 21 AUGUST, MORNING   |
| Dr        | Ricardo Fortunato  | Baggio           | Argentine National Atomic Energy Commission | C       | 21 AUGUST AT NOON    |
| Professor | Edward Neill (Ted) | Baker            | University of Auckland                      | D       | 21 AUGUST AT NOON    |
| Mrs       | Susan              | Barnes           | IUCr, Chester                               | A       | 21 AUGUST AT 14:00   |
| Dr        | Lonny              | Berman           | Brookhaven National Laboratory              | S       | 21 AUGUST AT 14:00   |
| Mrs       | Jill               | Bradshaw         | IUCr, Chester                               | B       | 21 AUGUST AT 14:00   |
| Professor | Carolyn            | Brock            | University of Kentucky                      | B       | 21 AUGUST AT NOON    |
| Professor | Gervais            | Chapuis          | EPFL Lausanne                               | B       | 21 AUGUST AT NOON    |
| Dr        | Vladimir V.        | Chernyshev       | Moscow State University                     | E       | 21 AUGUST AT NOON    |
| Professor | William            | Clegg            | University of Newcastle upon Tyne           | E       | 21 AUGUST AT NOON    |
| Mr        | Sean               | Conway           | IUCr, Chester                               | C,E     | 21 AUGUST AT 14:00   |
| Professor | Philip             | Coppens          | State University of New York at Buffalo     | A       | 21 AUGUST, MORNING   |
| Dr        | Jean-Claude        | Daran            | CNRS  | C,E     | 20 AUGUST, AFTERNOON |
| Professor | Gautam R.          | Desiraju         | University of Hyderabad                     | B,C     | 20 AUGUST, EVENING   |
| Dr        | Howard             | Einspahr         | Lawrenceville, USA                          | D,F     | 20 AUGUST AT 16:00   |
| Dr        | Mark Robert James  | Elsegood         | Loughborough University                     | C       | 21 AUGUST, AFTERNOON |
| Dr        | Lars               | Eriksson         | Stockholm University                        | E       | 21 AUGUST AT NOON    |
| Professor | George             | Ferguson         | University of St. Andrews                   | C       | 21 AUGUST AT 14:00   |
| Dr        | Paula              | Fitzgerald       | Merck Research Laboratories                 | F       | 21 AUGUST AT NOON    |
| Professor | Judith             | Flippen-Anderson | RCSB Protein Data Bank                      | E       | 21 AUGUST, MORNING   |
| Dr        | Frank R.           | Fronczek         | Louisiana State University                  | C       | 21 AUGUST AT NOON    |
| Dr        | Graeme J.          | Gainsford        | Industrial Research Limited                 | C       | 21 AUGUST, EVENING   |
| Dr        | John F.            | Gallagher        | Dublin City University                      | C       | 21 AUGUST AT 14:30   |
| Professor | Carl               | Görbitz          | University of Oslo                          | B       | 21 AUGUST AT NOON    |
| Dr        | Jules Mitchell     | Guss             | University of Sydney                        | D,F     | 21 AUGUST AT NOON    |
| Dr        | Ilia               | Guzei            | University of Wisconsin-Madison             | C       | 21 AUGUST, MORNING   |
| Professor | John R.            | Helliwell        | The University of Manchester                | A,D,J,S | 20 AUGUST, EVENING   |
| Dr        | Madeleine          | Helliwell        | The University of Manchester                | C       | 20 AUGUST, EVENING   |
| Professor | Jean-Louis         | Hodeau           | CNRS  | J       | 21 AUGUST AT 19:30   |
| Dr        | Gillian            | Holmes           | IUCr, Chester                               | C,E     | 21 AUGUST AT 14:00   |
| Dr        | Owen               | Johnson          | CCDC  | E       | 21 AUGUST AT NOON    |
| Mrs       | Louise             | Jones            | IUCr, Chester                               | D,F     | 19 AUGUST, EVENING   |
| Dr        | Biserka            | Kojic-Prodic     | Rudjer Boskovic Institute                   | E       | 20 AUGUST AT 19:02   |

|           |                 |               |                                    |         |                         |
|-----------|-----------------|---------------|------------------------------------|---------|-------------------------|
| Professor | Gernot          | Kostorz       | ETH Zurich                         | J,S     | 20 AUGUST, EVENING      |
| Professor | Åke             | Kvick         | ESRF                               | S       | 21 AUGUST AT NOON       |
| Professor | Claude E. P.    | Lecomte       | Université Henri Poincaré          | A,B     | 20 AUGUST, AFTERNOON    |
| Dr        | Anthony         | Linden        | University of Zurich               | C       | 20 AUGUST, AFTERNOON    |
| Dr        | Alan            | Lough         | University of Toronto              | E       | 21 AUGUST AT NOON       |
| Dr        | Dennis          | Mills         | Argonne National Laboratory        | S       | 21 AUGUST AT NOON       |
| Professor | Keiichiro       | Ogawa         | The University of Tokyo, Komaba    | B       | 21 AUGUST AT 14:00      |
| Professor | Glaucius        | Oliva         | University of Sao Paulo - Brazil   | D,S     | 21 AUGUST AT 14:00      |
| Professor | Dhananjai       | Pandey        | Banaras Hindu University, Varanasi | A,J     | 21 AUGUST AT 23:00      |
| Professor | J. Manuel       | Perez-Mato    | Univ. Pais Vasco (Bilbao)          | A       | 21 AUGUST AT NOON       |
| Professor | Dieter          | Schwarzenbach | EPFL                               | A       | 21 AUGUST AT 17:30      |
| Professor | Jim             | Simpson       | University of Otago                | E       | 21 AUGUST AT NOON       |
| Professor | William C.      | Stallings     | Pfizer PGRD                        | B,C,D,F | 20 AUGUST, AFTERNOON    |
| Professor | Helen           | Stoekli-Evans | Université de Neuchâtel            | E       | 20 AUGUST, AFTERNOON    |
| Mr        | Peter           | Strickland    | IUCr, Chester                      | J       | 19 AUGUST, EVENING      |
| Professor | Kiyoaki         | Tanaka        | Nagoya Institute of Technology     | A       | 21 AUGUST AT NOON       |
| Professor | Karl Wilhelm    | Törnroos      | University of Bergen               | C       | 20 AUGUST, AFTERNOON    |
| Dr        | David G.        | Watson        | CCDC                               | E       | 21 AUGUST AT NOON       |
| Dr        | Edgar           | Weckert       | HASYLAB at DESY                    | A       | 21 AUGUST AT 14:00      |
| Dr        | Tony            | Weight        | IUCr, Chester                      | S       | 21 AUGUST AT 14:00      |
| Professor | Thomas Richard  | Welberry      | Australian National University     | J       | 20 AUGUST, EVENING      |
| Dr        | Manfred S.      | Weiss         | EMBL Hamburg Outstation            | D       | 20 AUGUST, EVENING      |
| Professor | Stephen William | Wilkins       | CSIRO, Australia                   | S       | 21 AUGUST AT NOON       |
| Professor | Chick           | Wilson        | University of Glasgow              | B       | 21 AUGUST AT 13:00      |
| Professor | Wing-Tak        | Wong          | The University of Hong Kong        | E       | 21 AUGUST AT NOON       |
| Professor | Adriana         | Zagari        | University of Naples               | D,F     | 21 AUGUST, LATE MORNING |

# Plenary agenda

## Grand Hotel Panoramic, Montecatini Terme, Italy

21 August, 15:00-18:30; 22 August 8:45-12:30, 23 August 9:00-12:00

### CHAIR: John Helliwell

Attendees: all Editors and Co-editors

IUCr staff attending: Peter Strickland, Tony Weight, Sean Conway, Gillian Holmes, Louise Jones, Jill Bradshaw, Sue Barnes

### Agenda

1. INTRODUCTION AND WELCOME (John Helliwell)
2. BACKGROUND INFORMATION
  - 2.1. CHESTER REPORT (Peter Strickland)
    - 2.1.1. JOURNAL PRINTING AND DISTRIBUTION
    - 2.1.2. JOURNAL FINANCES AND SUBSCRIPTIONS
    - 2.1.3. STATISTICAL REPORT
    - 2.1.4. ONLINE JOURNALS
    - 2.1.5. RESEARCH AND DEVELOPMENT
    - 2.1.6. SPECIAL ISSUES
  - 2.2. REPORTS FROM THE EDITOR-IN-CHIEF, SECTION AND MAIN EDITORS
  - 2.3. JOURNALS PROMOTION REPORT (Peter Strickland)
    - 2.3.1. GENERAL PROMOTION
    - 2.3.2. ADVERTISING AND SPONSORSHIP
3. GENERAL MATTERS FOR DISCUSSION
  - 3.1. INTRODUCTION
  - 3.2. FEEDBACK FROM RECENT FC AND EC MEETINGS
  - 3.3. USE OF COLOUR
  - 3.4. ELECTRONIC SUBMISSION AND REVIEW
    - 3.4.1. GENERAL
    - 3.4.2. SECTIONS C AND E
    - 3.4.3. REVIEW BOARD
    - 3.4.4. HARD-COPY SUBMISSION
    - 3.4.5. NOTES FOR REFEREES
    - 3.4.6. REFEREE FORMS
    - 3.4.7. E-ANNOTATION OF REVIEW PDFs
    - 3.4.8. REVIEW STANDARDS
  - 3.5. NEW PUBLISHING CHALLENGES
    - 3.5.1. OPEN ACCESS
    - 3.5.2. NIH AND RCUK POLICIES
    - 3.5.3. COPYRIGHT AND LICENCING
  - 3.6. ETHICAL GUIDELINES FOR PUBLICATION
  - 3.7. TRANSFER OF PAPERS BETWEEN JOURNALS
  - 3.8. APPEALS
  - 3.9. ARTICLE CORRECTION AND RETRACTION POLICY
  - 3.10. POORLY WRITTEN ARTICLES
  - 3.11. MAXIMUM NUMBER OF REVISIONS
  - 3.12. LANGUAGE OF PUBLICATION
  - 3.13. SPELLING AND GRAMMAR
  - 3.14. REFERENCE CITATIONS AND REFERENCES
  - 3.15. COVERAGE OF EDUCATION
  - 3.16. VIRTUAL JOURNALS
  - 3.17. LEAD ARTICLES AND TOPICAL REVIEWS
  - 3.18. MATTERS ARISING FROM INDIVIDUAL JOURNAL MEETINGS
  - 3.19. ISSUES RAISED BY EDITORS AND CO-EDITORS
4. MATTERS FOR THE OPEN COMMISSION MEETINGS
5. JOURNALS' DEVELOPMENT PLANS
6. ANY OTHER BUSINESS
7. DATE AND PLACE OF NEXT MEETING

## 1. INTRODUCTION AND WELCOME (John Helliwell)

John Helliwell will give a short introduction to the meeting and welcome attendees.

As a number of attendees will be arriving during the opening session on 21 August, this session will start by considering general background reports. Main matters for discussion will be handled on 22 August under item 3 of the agenda.

## 2. BACKGROUND INFORMATION

### 2.1. CHESTER REPORT (Peter Strickland)

#### 2.1.1. JOURNAL PRINTING AND DISTRIBUTION

The Editorial Office works with 1 typesetter in the UK and 2 printers in the UK/Denmark to produce the journals. All typesetting (except Section C) is carried out by the Editorial Office using SGML created from word-processing files or from CIFs. All figures are also processed electronically by the office.

Printing of the journals is by direct-to-plate methods - a single PDF of the text of a whole issue is supplied to the printers, together with PDFs of inside and outside covers.

Our printers have access to digital presses and digital printing is used for reprints ordered after a journal has been printed or for printed reprints for electronic only journals. Litho printing is used for producing standard journal issues.

Distribution of the journals is carried out by Blackwell Publishing using Marston Book Services in Oxford, UK.

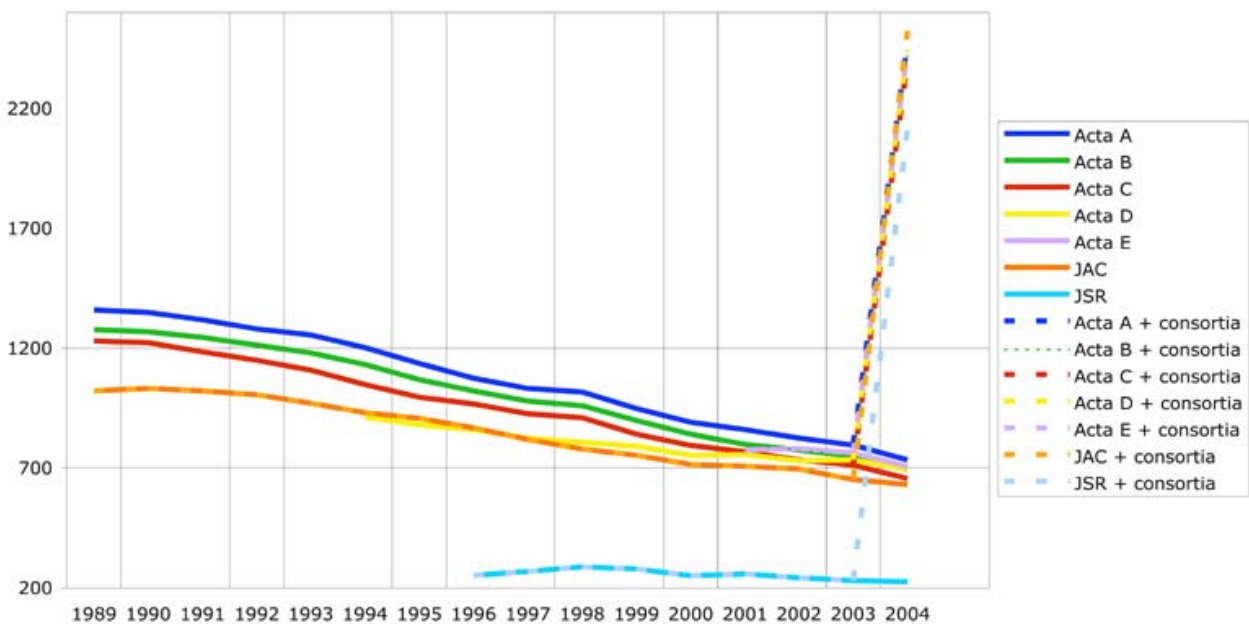
Distribution should take less than 2 weeks; Co-editors who are aware of long distribution times are invited to report this to the meeting.

Printing is currently tied into long-term contracts which will end at the start of 2007. Because of the high cost of colour printing (see point 3.3 of the agenda), investigations are being made to see whether relocation of printing to Singapore or China would be feasible and would reduce costs. Printing quality, ease of communication and distribution costs will need to be taken into account in any change of printers.

#### 2.1.2. JOURNAL FINANCES AND SUBSCRIPTIONS

A graph of the number of subscribers to the journals is shown below. The number of subscribers has decreased by 3-5 percent per annum over the last 15 years. From 2004, when the IUCr started to take part in Blackwell Synergy, the number of libraries that can access the journals has increased by approximately 1800, as libraries that have taken out a Blackwell consortial deal can now access the journals.

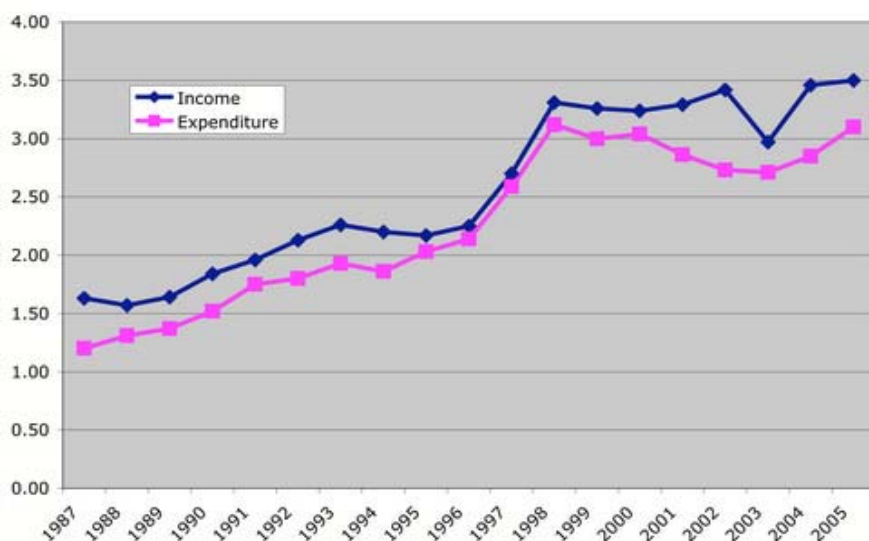
#### Number of subscribers



The revenue derived from each consortial subscriber is small compared to subscription incomes, but member libraries that previously held subscriptions to the journals are required to maintain these as part of the access conditions for the consortium.

The policy of the IUCr Finance Committee has been to try to ensure that the journals make a small surplus (10%) for use by the Union for good causes. The graph below shows that this has largely been achieved in the last two triennia.

**Income/expenditure 1987-2005(projected)  
All Journals**



For 2006, the general journal price increase will be 8.5%; the average price increase applied by Blackwell to their other journals is 9%.

There are two mechanisms that aim to allow for readers in developing countries to access the journals. The Journal Grants Fund, which is administered by the Chester Office, provides low-cost subscriptions to libraries. In addition, Blackwell Synergy provide low-cost access to consortia in developing countries. Details of the libraries with this type of access can be requested from the Editorial Office.

### 2.1.3. STATISTICAL REPORT

Full statistical reports for the years 2002, 2003 and 2004 are available for viewing at your status home page at <http://wdc.iucr.org>, by following the link "Annual reports". A summary of the statistics for 2004 is given in APPENDIX A.

The total number of pages published in 2004 was 11728, which compares with 10715 in 2003 and 9078 in 2002. Of this total, 4676 pages were published in electronic only format.

The number of manuscripts submitted to the journals was 4712 (compared with 3569 in 2003 and 2917 in 2002). The total number of accepted papers was 3346 (compared with 2899 in 2003 and 2314 in 2002).

The impact factors for 2004 have recently been released and are also reported in APPENDIX A.

### 2.1.4. ONLINE JOURNALS

The Crystallography Journals Online system now contains approximately 66000 articles and 270000 pages. The main policy aim in the last triennium has been to make the journal content as visible and accessible as possible. The two main methods for achieving this aim have been to increase the number of organisations indexing Crystallography Journals Online and the inclusion of journal articles on other online journal platforms (e.g. Blackwell Synergy).

The IUCr took part in the CrossRef search project during 2004. This led to indexing of our content by Google and Scirus, and resulted in large increases in the number of visitors to our site. We have also taken part in a number of other indexing projects, and have also started to make information about our content available by means of RSS feeds (these are a type of newsfeed).

As mentioned above, IUCr Journals are now also available via Blackwell Synergy. This service contains PDFs and links to the IUCr site for the provision of HTML content. The service currently only includes content back to 2000, but it is hoped to provide complete back content in due course. Supplementary data are not available via the Blackwell Synergy service. The Blackwell service provides access to a large number of consortia worldwide, including some in developing countries.

Linking to data from the Cambridge Structural Database has been available for some time and work has now been

carried out to link to information in the online version of Inorganic Crystal Structure Database. Linking to data in the PDB, and to other publishers' articles (e.g. via MEDLINE, CHEMPORT and CrossRef ) is also well established.

All Co-editors are entitled to free personal access to Crystallography Journals Online. If you have not already registered, send an email to [support@iucr.org](mailto:support@iucr.org) for details. Please encourage your organisation to subscribe if it does not already do so.

Editors' suggestions on how the service might be improved will be most welcome.

### 2.1.5. RESEARCH AND DEVELOPMENT

A report of research and development projects in Chester will be given. Projects that have been undertaken in the last year include:

- Searching
  - CrossRef search (with Google)
  - Scirus search
  - Distributed searching
  - IUCr search page
- Other online journals projects
  - ICSD linking
  - Openurl linking
  - RSS feeds
  - Improved metadata (article components and forward linking)
- Submission and review
  - Submission system extension to Sections C and E
  - Status system developed and integrated with the submission and review system
  - Reject and withdraw facility
- Other projects
  - CIF handling (in-house and author tool for viewing and formatting CIFs; publCIF)
  - Section F procedures and data requirements (with Howard Einspahr and the PDB)
  - Reference processing
  - Automation of figure processing
  - Increased hardware/software redundancy
  - Archiving and recovery planning
  - Usage statistics
  - CML/InChI generation

### 2.1.6. SPECIAL ISSUES

Special issues published in the last year include the following: Third European Charge-Density Meeting (Acta A, September 2004); Abstracts of ECM22 meeting 2004 (Acta A, September 2004); CCP4 - Model Building and Refinement (Acta D, December 2004); Phase Transitions (Acta A, January 2005); BioXAS and Metallogenomics (JSR, January 2005); Applications of Synchrotron Radiation to Materials Research (JSR, March 2005); Crystallization of Biological Macromolecules (ICCBM10) (Acta D, June 2005); Radiation Damage in Macromolecules (JSR, May 2005); and Softer Synchrotron Radiation X-rays in Structural Studies (JSR, July 2005)

Issues in preparation include: Structure Determination by Single Crystal X-ray Diffraction at Megabar Pressures (JSR, September 2005); CCP4 - Data Collection and Analysis (Acta D, autumn 2005); International School on Mathematical and Theoretical Crystallography (MaThCryst) (Acta A, January 2006); Abstracts of Florence Congress 2005 (Acta A, autumn 2005); Special SPINE (Structural Proteomics in Europe) issue (Acta D, spring 2006); Beijing Workshop on Recent Advances in Phasing Methods for High-throughput Protein Structure Determination (Acta D, spring 2006); and SAS2006 Small-Angle Scattering Meeting (JAC, spring 2007).

Editors will be requested to make suggestions for special issues at the individual journals meetings.

It has been proposed by the Chester Office that for future Conference special issues (large special issues for which the organisers pay a contribution towards publication) free open access will be included as part of the base price quote. This proposal will not significantly affect the cost to the organizers. The proposal mirrors the policy of the IOP for its journal "Journal of Physics: Conference Series". This approach (of open access increasing access) could reduce the risk that such issues could potentially lower the impact factor of the journal.

### 2.2. REPORTS FROM THE EDITOR-IN-CHIEF, SECTION AND MAIN EDITORS

The Editor-in-chief, Section and Main Editors will provide short reports. These will cover issues such as the progress of

their journals and new appointments to their Editorial Boards. The Editors' triennial reports to the Executive Committee for 2002-2004 are attached as APPENDIX B.

Proposed changes to the Editorial Boards of the journals are summarised below.

### Editorial Board changes

|                 | Due to retire                                 | New appointments  |
|-----------------|---|---|
| Editor-in-Chief | John Helliwell                                | Gernot Kostorz  |
| Acta A          | Giacovazzo, Helliwell, Moore                  | Dmitrienko, Fewster, Krebs-Larsen                           |
| Acta B          | Jones, Nassimbeni, Taylor                     | Kaduk, Krebs-Larsen, McCusker, Rychlewska, Spackman         |
| Acta C          | Daniels, Fronczek, Stallings                  | No changes immediately as new Co-editors recently appointed |
| Acta D          | Helliwell, Tsukihara                          | Miki, Murthy  |
| Acta E          |   | No changes immediately as new Co-editors recently appointed |
| Acta F          |   | No changes immediately as new Co-editors recently appointed |
| JAC             | Hasnain, Moore, Oskarsson, Pandey, Zimmermann | Ciccariello, David, Fewster, Kantardjieff                   |
| JSR             | Helliwell, Kirz, Penner-Hahn                  | McSweeney, Wakatsuki  |

### 2.3. JOURNALS PROMOTION REPORT (Peter Strickland)

A summary of the journals promotion work carried out in the last year by Andrea Sharpe and the Journals Working Group will be provided and plans for the Congress and 2006 outlined.

The Journals Working Group are interested to hear the views of the Commission on ideas that would help in the promotion of the journals. The main roles of the Journals Working Group are: (a) the preparation and updating of leaflets including where they should be distributed, and (b) journals' development ideas in general.

#### 2.3.1. GENERAL PROMOTION

An IUCr folder and a full-colour IUCr Journals brochure are now a regular feature of the promotional campaign. Journal-specific leaflets have now been produced for Acta A and F, Journal of Applied Crystallography and Journal of Synchrotron Radiation. There is also an Acta B/C/E leaflet and an Acta D leaflet is in preparation for the Congress. Japanese versions of some of the leaflets are also being produced. The current leaflets will be circulated at the meeting and suggestions for improvements to the leaflets and new leaflet features will be sought.

Journal article press releases have a regular slot in the IUCr Newsletter, which also features occasional articles to promote specific matters. Promotional articles are also sometimes contributed to other crystallographic newsletters.

The journals continue to be promoted at the major crystallographic meetings and at other meetings outside the community. Details of meetings attended in 2005 and meetings planned for 2006 are given below. Recommendations for additional meetings for 2006-2008 are welcome.

#### Promotion at meetings

|      |   |
|------|---|
| 2005 | DGK, Germany (February/March)   |
|      | West Coast Protein Crystallography Workshop, USA (March) (Howard Einspahr)        |
|      | Recent Advances in Macromolecular Crystallization, France (May) (Howard Einspahr) |
|      | ACA, USA (May/June) (Howard Einspahr)   |
|      | IUCrXX, Italy (August)  |
|      |   |
| 2006 | ACA, USA (July)   |
|      | ECM, Belgium (August)   |

Promotional materials (posters and leaflets) are available via the link "Promotional materials" in the online status home pages for editors. Editors are welcome to print out these materials and take them to meetings that they attend.

#### 2.3.2. ADVERTISING AND SPONSORSHIP

The journals have been more successful over the last triennium in attracting advertising than in previous triennia. Advertising revenue was USD 16204 in 2002, USD 28294 in 2003 and USD 74266 in 2004. The 2004 figure includes

income from the Facility Information pages in Journal of Synchrotron Radiation.

Sponsorship of the online journals has been developing over the last triennium and now provides a small revenue stream. Areas that have been considered for sponsorship include:

- Online journal home pages, e.g. <http://journals.iucr.org/f/>
- E-mail alerting services
- Home pages for special issues
- checkCIF service

Other potential ideas for sponsorship include:

- Company sponsorship of open-access articles
- Linking to products mentioned in journal articles

Editors are encouraged to suggest new advertising ideas, and will also be asked for their views on where advertising should be allowed in the online version of the journals.

### **3. GENERAL MATTERS FOR DISCUSSION**

#### **3.1. INTRODUCTION**

John Helliwell will give an introduction to the main policy issues to be considered at the meeting. Attendees will be asked to say a few words to introduce themselves to others at the meeting, and will also be asked if there are any general policy issues not already on the agenda that they would like to see discussed.

#### **3.2. FEEDBACK FROM RECENT FC AND EC MEETINGS**

John Helliwell and Gernot Kostorz will meet with the IUCr Finance and Executive Committees on 18 and 19 August 2005, respectively. Feedback from these meetings will be reported, as will any matters that need to be prepared for the next Executive Committee meeting and the IUCr General Assembly.

#### **3.3. USE OF COLOUR**

In the last 1-2 years there have been significant increases in the cost of printing the journals. These cost increases can be linked to the use of extra colour by authors.

This matter needs to be discussed on a journal by journal basis, but the overall views of the meeting would be useful ahead of the individual journal meetings. For most journals the Notes for Authors currently state:

"Figures in colour are accepted at no cost to the author provided that the editor agrees that they improve the understanding of the paper. At the editor's discretion, figures printed in black and white may appear in colour in Crystallography Journals Online."

Options for controlling costs include:

- Make Notes for Authors stricter - perhaps by adding "significantly" at the end of the first sentence above
- Emphasize restrictions to reviewers - in Notes for Reviewers
- Ask Main and Section Editors to review all colour at the proof stage
- Only allow colour online - currently the case for Section C
- Relax rules on the running order of articles in an issue
- Charge for colour
- Find cheaper colour printers

The meeting will be asked if any of the above options should be ruled out for consideration by individual journal meetings.

The Chester Office would also like the views of the meeting on handling captions for figures that are made black and white in print, but colour online. In such cases, where possible we remove reference to colour in the figure caption; where this is not possible we leave the colour reference in the caption, but add the sentence

"This figure is in colour in the electronic version of this paper."

Is this approach satisfactory?

Another option is to convert a journal to online-only publication. This may become necessary for individual IUCr Journals at some stage if the number of print subscriptions falls below a level at which it is economic to continue printing. The views of the meeting on this subject are invited.

### **3.4. ELECTRONIC SUBMISSION AND REVIEW**

#### **3.4.1. GENERAL**

The submission system has been running for over two years. Comments on the system (e.g. on the wording of template messages, system functionality etc.) will be welcome at the meeting.

The Chester Office is currently developing tools for Co-editors that will allow functions such as (1) inviting a reviewer, (2) sending out review comments, (3) paper acceptance, (4) paper rejection etc. to be carried out online. The tools will be demonstrated in the context of the new submission system for Sections C and E (see below).

It is expected that an option for password-controlled submission via the status system will be introduced in the next 1-2 years. Co-editors wishing to volunteer to try out this system, should let Chester staff know this during the meeting.

#### **3.4.2. SECTIONS C AND E**

A new submission system is being set up for Sections C and E. The Chester Office will give a very brief demonstration of this and answer questions. More details will be given in the C/E meeting. The system should be operational by the time of the meeting; it allows all source files to be uploaded during the initial submission process.

#### **3.4.3. REVIEW BOARD**

The idea of a review board (i.e. a set of reviewers who agree to handle a defined number of papers per year for a journal) has been suggested for Section F. The views of the meeting on this idea are welcomed. Any work in this area would most likely be a pilot project involving one or two Section F Editors, with the results reported back to JComm.

Mitchell Guss will give a brief presentation on the merits of a fully integrated web-based management system for handling papers.

#### **3.4.4. HARD-COPY SUBMISSION**

Sections C, D, E and F, and JSR no longer allow hard-copy submissions. Editors of Sections A and B and JAC will be asked in the individual journal meetings to decide whether hard-copy submission should also be phased out for their journals.

#### **3.4.5. NOTES FOR REFEREES**

Reviewers are alerted to Notes for Reviewers in the template referee invite email. For example, the notes for Journal of Applied Crystallography are available from <http://journals.iucr.org/j/services/referees/notes.html>

The Notes are also reproduced in Appendix C. Suggestions for changes to the Notes should be discussed at individual journal meetings and requests for changes reported back to the general meeting as appropriate.

#### **3.4.6. REFEREE FORMS**

Reviewers are currently asked to reply to a number of questions (see Appendix C). Suggestions for changes to the forms should be discussed at individual journal meetings and requests for changes reported back to the general meeting as appropriate.

It is expected that an online version of the forms will be implemented shortly.

#### **3.4.7. E-ANNOTATION OF REVIEW PDFs**

A new development in Acrobat 7 may be used in future to give reviewers and Co-editors an extra option in the review process. A REVIEW PDF is made available in the normal way via the web site but the PDF is created in Acrobat 7 in a way that allows it to be annotated electronically. The reviewer and Co-editor can then use a free Acrobat Reader 7 as an electronic annotation tool for the communication and the exchange of corrections. The view of the meeting on this possible development is welcomed.

#### **3.4.8. REVIEW STANDARDS**

This is an opportunity for a general discussion of ideas on how we can ensure that consistent standards are applied to the review process. The risk of variation is at present mitigated against mainly by Section Editors seeing proofs. Notes for Co-editors and Notes for Authors also aim to ensure a uniformity of the procedures and, partly, science. Journal specific

ideas should be discussed at individual journal meetings.

### **3.5. NEW PUBLISHING CHALLENGES**

#### **3.5.1. OPEN ACCESS**

Open access became available on Crystallography Journals Online from January 2004. After acceptance, authors are given the opportunity, by payment of a fee (USD 900), to make their papers available as open-access articles in the electronic version of the journal. The fees will be used to keep down the costs of subscriptions. More details of the policy are available at <http://journals.iucr.org/services/openaccess.html>. The IUCr made an agreement with the UK Joint Information Systems Committee (JISC) which means that open-access charges have been waived for 2004 and 2005 for UK further education staff publishing in IUCr journals (for more details see <http://journals.iucr.org/services/openaccessuk.html>).

The open-access policy has been successful with approximately 25 articles being made open access by direct author payment, and over 450 articles being made open access as a result of the JISC funding.

In addition to the above policy, the IUCr allows authors to load preprints of their articles on a preprint server, and authors may also make their electronic reprints available on the web.

Editors will be encouraged to give their views on the above policies at the meeting, together with any suggestions for improvements.

#### **3.5.2. NIH AND RCUK POLICIES**

NIH and RCUK have recently announced policies that aim to ensure that research papers that they have funded are available in the *public domain*, either immediately after publication or within 12 months of publication. They are asking that authors deposit their papers either in PubMed Central or an equivalent public institutional or subject repository.

A number of publishers have started to look at whether they can offer such deposition as part of their services to authors. The American Chemical Society (ACS) plans to submit published papers to PubMed Central, with the papers being viewable electronically a year after original publication. This gives the publisher some degree of control over what is deposited and specification of any linking back to the paid service.

Editors' views on this matter are requested. For example, should the IUCr start a dialogue with PubMed Central on deposition of papers from IUCr Journals? If so, should this be for a limited set of papers (paid open access papers, NIH-funded papers, RCUK-funded papers)?

#### **3.5.3. COPYRIGHT AND LICENCING**

It is proposed that the transfer of copyright form be modified to specifically allow authors the right to deposit their electronic reprints in PubMed Central or other appropriate repository as required by their funding agency.

The IUCr reviews the situation on copyright on a regular basis with Blackwell Publishing; this may lead to a move towards an exclusive licence rather than transfer of copyright in the future.

The main reasons quoted by Blackwell for copyright transfer are:

- (a) ownership of copyright by one central organisation facilitates international protection against infringement, libel or plagiarism;
- (b) it enables the most efficient processing of permissions and licensing in order that the Article can be made available to the fullest extent both directly and through intermediaries, and in both print and electronic form;
- (c) it enables the copyright holder to maintain the integrity of an article once refereed and accepted for publication, by facilitating centralised management of all media forms including linking, reference validation and distribution.

The IUCr copyright form also covers the transfer of data associated with a publication. It is intended that in the next year the IUCr will review the conditions under which it makes associated data available. Use of the data will remain free except in the case of use for commercial purposes.

### **3.6. ETHICAL GUIDELINES FOR PUBLICATION**

In some cases it is difficult to determine who should be included as an author of a paper. It is proposed that a more formal statement concerning authorship be added as a second paragraph to the "Author's warranty" section in the Notes for Authors. Suggested wording for the paragraph is as follows:

"The co-authors of a paper should be all those persons who have made significant scientific contributions to the work

reported, including the ideas and their execution, and who share responsibility and accountability for the results. Other contributions should be indicated in an 'Acknowledgments' section. An administrative relationship to the investigation does not of itself qualify a person for co-authorship (but it may be appropriate to acknowledge major administrative assistance)."

It should be possible to query the roles of authors during the submission process if a paper has a large number of authors. Individual journal meetings will be asked to discuss this matter.

### **3.7. TRANSFER OF PAPERS BETWEEN JOURNALS**

A pilot scheme is currently being set up for the transfer of papers from Section C to Section E with the same Co-editor handling the paper through to acceptance. More details of this are given in the Section C/E agenda notes.

This arrangement raised the general question as to whether such a scheme could be applied to other journal borderlines and, if so, what would the transfer mechanism involve.

It is proposed that a general transfer mechanism be set up within the online submission and review system that would allow a Co-editor to transfer and accept a paper to a journal other than one on which they usually work. The main idea of the scheme is to avoid multiple reviewing of a paper by different Co-editors and reviewers. The proposed steps are as follows:

- (1) Carry out the review as usual unless it is immediately clear that the paper should be in another journal (in this case an early decision as to whether to continue with the paper or to ask the authors to resubmit to another journal should be made).
- (2) After the review has been completed and a transfer looks appropriate, consult with a Section or Main Editor of the new journal about whether a transfer makes sense.
- (3) Consult with the author giving reasons why a transfer would be appropriate.
- (4) If the author agrees to the transfer, use the submission and review system to transfer and accept the paper for the new journal.

Editors comments are invited on the above procedure. It is expected that Chester could implement this within 12 months if the meeting agrees that this would be helpful.

### **3.8. APPEALS**

The current Notes for authors for most journals state the following in relation to appeals:

"An author who believes that a paper has been unjustifiably treated by the Co-editor may appeal initially to the Section Editor and then to the Editor-in-chief if still aggrieved by the decision."

We would propose that this statement is extended to include a time limit (to ensure that all relevant materials are still available) and strengthened to make it clear that the appeal to the Editor-in-chief is final:

"An author who believes that a paper has been unjustifiably treated by the Co-editor may appeal initially to the Section Editor and then to the Editor-in-chief if still aggrieved by the decision. The initial appeal must be made within 12 months of rejection of the paper. The decision of the Editor-in-chief is final."

Individual journals may need to set different time limits, as it may be more difficult to ensure that all relevant materials are still available for Editors handling high number of papers. In addition it is proposed that statistics on appeals (number of appeals, number upheld) be published as part of the annual reports to the Executive Committee.

### **3.9. ARTICLE CORRECTION AND RETRACTION POLICY**

It is proposed that a web page giving our policy on article correction and retraction be made available. The proposed policy is given below for discussion. It is largely derived from the policies available on the Nature and Elsevier web sites.

#### **Article correction and retraction policy**

Corrections are published if the publication record is seriously affected, for example with regard to the scientific accuracy of published information, or the reputation of the authors, or the reputation of the journal. Corrections that do not affect the contribution in a material way or significantly impair the reader's understanding of the contribution (e.g. a spelling mistake or grammatical error) will not be published.

When an amendment is published, it is linked bi-directionally to and from the article being corrected. A PDF version of the correction is appended to the last page of the original article PDF so that the original article PDF will remain the

same as the printed page and readers downloading the PDF will receive the original article plus amendment.

Amendments are published in the article category "Addenda and Errata" and will be further classified as an "Erratum", "Corrigendum", "Addendum" or "Retraction". All such amendments should be as concise as possible, containing only material strictly relevant to the contribution being corrected. In very rare circumstances, the IUCr also reserves the right to remove articles (see Article removal).

### **Errata**

Errata concern the amendment of mistakes introduced by the journal in editing or production, including errors of omission such as failure to make factual proof corrections requested by authors within the deadline provided by the journal and within journal policy. Errata are generally not published for simple, obvious typing errors, but are published when an apparently simple error is significant (for example a greek mu for an 'm' in a unit, or a typing error in the corresponding author's email address).

If there is an error in a figure or table, the usual procedure is to publish a sentence of rectification. A significant error in the figure or table is corrected by publication of a new corrected figure or table as an erratum. The figure or table is republished only if the editor considers it necessary. If the colours of histogram bars were wrongly designated in the figure legend, for example, a sentence of correction would be published as an erratum; the entire figure would not be reproduced.

### **Corrigenda**

Corrigenda submitted by the original authors are published if the scientific accuracy or reproducibility of the original paper is compromised. IUCr journals will publish corrigenda if there is an error in the published author list, but not usually for overlooked acknowledgements.

Readers wishing to draw the journal's attention to a significant published error should submit their comments as a "Letter to the Editor". Such "Letters to the Editor" will be carefully reviewed by unrelated and neutral referees. On editorial acceptance, the paper will be sent to the authors of the original paper to provide an opportunity for their early response.

### **Addenda**

Addenda are judged on the significance of the addition to the interpretation of the original publication. Addenda do not contradict the original publication, but if the authors inadvertently omitted significant information available to them at the time, this material will be published as an addendum after peer review.

### **Retractions**

Retractions are judged according to whether the main conclusion of the paper is seriously undermined as a result, for example, of subsequent information coming to light of which the authors were not aware at the time of publication. In the case of experimental papers, this can include e.g. further experiments by the authors or by others which do not confirm the main experimental conclusion of the original publication.

Readers wishing to draw the editors' attention to published work requiring retraction should first contact the authors of the original paper and then write to the journal, including copies of the correspondence with the authors (whether or not the correspondence has been answered). The editors will seek advice from reviewers if they judge that the information is likely to draw into question the main conclusions of the published paper.

Infringements of professional ethical codes, such as multiple submission, bogus claims of authorship, plagiarism, fraudulent use of data, or the like, will also result in an article being retracted.

All coauthors will be asked to agree to a retraction. In cases where some coauthors decline to sign a retraction, the editors reserve the right to publish the retraction with the dissenting author(s) identified.

### **Article removal**

In very rare circumstances it may be necessary to remove an article from the online journal. This will only occur where the article is clearly defamatory, or infringes others' legal rights, or where the article is, or there is good reason to expect it will be, the subject of a court order, or where the article, if acted upon, might pose a serious health risk.

In these circumstances, while the bibliographic information (title and authors) will be retained online, the text will be replaced with a page indicating that the article has been removed for legal reasons.

### 3.10. POORLY WRITTEN ARTICLES

The Section C Notes for Authors were modified in 2005 to put more emphasis on the authors being responsible for correcting poorly written articles. It is proposed that the Notes for Authors for other journals also include similar wording:

#### Quality of writing

Papers should be clearly written and grammatically correct. Authors who do not have good language skills in the language of submission are expected to seek local assistance before submission of their paper.

In addition, special measures for Section E are noted in the agenda notes for the Section C/E meeting. There will be a brief demonstration of the new pubCIF tool.

Another proposal that has been suggested to resolve such problems is that for-profit services be investigated to offer language and scientific consultations to authors who need this help. Editors' views on such services are welcome.

### 3.11. MAXIMUM NUMBER OF REVISIONS

It is proposed that the Notes for Authors be modified to indicate a maximum number of revisions for a paper. It would then be at the discretion of the Co-editor as to how they wish to apply this limit.

The current wording:

"If changes to a manuscript requested by the Section Editor, a Co-editor or the editorial staff are not received within two months of transmittal to the author, the submission will automatically be withdrawn. Should the manuscript require further revision, this would normally be expected to be completed within one month of the revision having been requested. Any subsequent communication of the material will be treated as a new submission in the editorial process."

would be changed to:

"If changes to a manuscript requested by the Section Editor, a Co-editor or the editorial staff are not received within two months of transmittal to the author, the submission will automatically be withdrawn. Should the manuscript require further revision, this would normally be expected to be completed within one month of the revision having been requested. If a manuscript is not acceptable after two revisions it will not be considered further. Any subsequent communication of the material will be treated as a new submission in the editorial process."

NB Some journals have a "one month" rather than a "two month" time limit in the first sentence of the above paragraph.

### 3.12. LANGUAGE OF PUBLICATION

The number of papers in languages other than English has decreased in recent years. In 2004, out of over 3500 papers only 4 were in French and none were in German or Russian. The figures for 2000-2005 were as follows:

#### Language of publication (2000-2005)

| Journal | Language | No. of articles |
|---------|----------|-----------------|
| Acta A  | English  | 3416            |
|         | French   | 1               |
| Acta B  | English  | 617             |
|         | German   | 1               |
| Acta C  | English  | 3353            |
|         | French   | 16              |
|         | German   | 8               |
| Acta D  | English  | 2343            |
| Acta E  | English  | 6506            |
|         | French   | 33              |
| Acta F  | English  | 213             |
|         | French   | 2               |
| JAC     | English  | 1100            |
|         | French   | 2               |
| JSR     | English  | 849             |

It is proposed that from 2006, the IUCr should only support publication in English. Any recommendation to make a change to the languages of publication would be referred to the IUCr Executive Committee for approval.

### 3.13. SPELLING AND GRAMMAR

Papers are currently edited in Chester to have British or American English spelling depending on the predominant spelling in the accepted paper. However, grammar has always been edited to British English standards as the Chester staff are not expert in American English grammar.

Is this situation acceptable? If not, the Chester staff suggest that all papers are edited to have British English spelling and grammar.

### 3.14. REFERENCE CITATIONS AND REFERENCES

In the text, all citations with three or more authors are currently shortened to "First author et al." The exception to this rule is where such a treatment would leave an ambiguous citation. For example, consider the following references:

Smith, A., Jones, B., Bloggs, C. & Another, D. (2004). *J. Appl. Cryst.* 37, 325-327.

Smith, A., Jones, B., Bloggs, C., Another, D. & Yetanother, E. (2004). *J. Appl. Cryst.* 37, 328-329.

These would need to be cited in full to avoid ambiguity (i.e. Smith, Jones, Bloggs & Another, 2004; Smith, Jones, Bloggs, Another & Yetanother, 2004), as we currently only assign a label "a", "b" etc. to references where the list of authors is identical.

It is proposed that a label "a", "b" etc. should be assigned for all "et al." references that require such a label to avoid ambiguity. For example, the above references would become:

Smith, A., Jones, B., Bloggs, C. & Another, D. (2004a). *J. Appl. Cryst.* 37, 325-327.

Smith, A., Jones, B., Bloggs, C., Another, D. & Yetanother, E. (2004b). *J. Appl. Cryst.* 37, 328-329.

and then could be cited in shorter form in the text (i.e. Smith et al., 2004a,b).

### 3.15. COVERAGE OF EDUCATION

The IUCr has received input from various sources indicating that the handling of education papers in IUCr journals should be reviewed. "Teaching and Education" papers are presently 'open access' and may theoretically appear in any IUCr journal: it would therefore be possible to create a 'virtual' online journal bringing all these papers together, and perhaps link to education papers appearing in journals from other publishers. Also, papers not formally classified as "Teaching and Education" papers, but of educational interest, might be included. Following the recommendation of the Journals Working Group, the Chair of the Commission on Crystallographic Teaching (P. Spadon) was consulted and a circular also sent to the Chairs of the three Regional Associates asking for their views. The responses were uniformly in favour of some form of virtual journal.

Editors' views on the breadth of coverage of education are welcomed.

### 3.16. VIRTUAL JOURNALS

The meeting will be asked for ideas on virtual journals. The following ideas are based on other publishers' virtual journals:

- (1) The journal would have an Editor and small Editorial Board, who would each be Co-editors of particular IUCr journals. These editors would be responsible for selecting articles for inclusion in the journal and perhaps providing the necessary bibliographic information via a web form. They would also work to commission articles that would go into the source journals.
- (2) An article would appear in the virtual journal if it falls within the scope of the virtual journal and is published in one of the participating source journals.
- (3) Agreements would need to be made with publishers of source journals to allow their bibliographic information to be given and linking to be set up.
- (4) When citing an article that is in the virtual journal, the source journal article would be cited - the virtual journal itself would not be cited.
- (5) The journal contents page would include links to the articles on the source publishers site. Access to the articles would be dependent on the reader having access rights to the article in the source journal.
- (6) The journal might include links to relevant non-journal material (e.g. tutorials, workshop notes etc.) providing this had been reviewed for quality.

### **3.17. LEAD ARTICLES AND TOPICAL REVIEWS**

The description of Lead Articles and Topical Reviews in the Notes for Authors are as follows:

Lead Articles are authoritative, comprehensive and forward-looking reviews of major areas of research interest. They are always commissioned by the Section Editor, on the advice of the Editorial Board. Suggestions for suitable topics and of potential author(s) are welcomed by the Section Editor for discussion with the Board. The Editor will discuss the treatment of the topic, the length of the Article and the delivery date of the manuscript with invited author(s). Lead Articles will be refereed in the normal manner.

A Topical Review is a short, highly focused survey covering a relatively narrow area of current research interest. It should not aim to be comprehensive, but a brief introduction should provide historical perspective and a brief conclusion should indicate likely future directions. Topical Reviews will be limited to about ten journal pages (10 000 words) except in special agreed circumstances. Shorter reviews on rapidly evolving areas are also actively encouraged. They will be commissioned by the Section Editor either personally, or following a formal proposal by prospective author(s). Topical Reviews will be refereed in the normal way.

Are these descriptions still appropriate, or do they require modification?

### **3.18. MATTERS ARISING FROM INDIVIDUAL JOURNAL MEETINGS**

Reports back from the individual journal meetings on items discussed, including:

- a. Journal development
  - How can we encourage good authors to submit?
  - How can we attract papers that will be highly cited?
  - How can we improve the impact factor?
  - Are there particular special issues that would help the impact factor?
  - How can we improve services to authors?
- b. Submission and review system
  - What new features would be useful for Co-editors?
  - How can the Notes for referees be improved?
  - How can the review form be improved?
  - Are there any measures that would improve the consistency of the review process?
  - Should hard-copy submission continue?
- c. Journals promotion and sponsorship
  - How can promotion of the journals be improved?
  - How can advertising revenues be increased?
- d. Journal design
  - How can the print journals be improved?
  - How can online services be improved?
  - Are there any items that can be removed from the print journal?
- e. Notes for authors
- f. Use of colour
  - Should the policy of the journal regarding colour be changed?
- h. Other general matters arising

### **3.19. ISSUES RAISED BY EDITORS AND CO-EDITORS**

Issues raised by Editors and Co-editors in response to circulation of these agenda notes will be discussed here.

## **4. MATTERS FOR THE OPEN COMMISSION MEETINGS**

The Abstracts of the presentations for the Open Commission Meetings (to be held on 24 and 25 August in Florence) are attached as APPENDIX C.

A powerpoint containing information and images for use by Section Editors in the Open Commission meeting is

available by following the link "JComm2005" from the status home page at <http://wdc.iucr.org>.

## **5. JOURNALS' DEVELOPMENT SUMMARY**

A personal summary of IUCr Journals' Development Plans 1996-2005 will be given by John Helliwell, whose aims are firstly to expedite an efficient handover to the incoming Editor-in-chief and secondly to offer modern management analyses, such as risk, SWOT, sensitivity and scenario, to the Journals Commission.

## **6. ANY OTHER BUSINESS**

## **7. DATE AND PLACE OF NEXT MEETING**

The next formal meeting of the Commission on Journals will be held in conjunction with the 2008 IUCr Congress, which is to be held in Japan. It is expected that the Commission will meet informally during 2006 and 2007 to coincide with at least one of the meetings of the IUCr regional associates.

## APPENDIX A

### Statistical report

#### A.1. Manuscripts received by Co-editors

The number of manuscripts submitted to Acta in 2004 was 35% higher than in 2003. All Sections of Acta showed increases in submission levels except Section D. However, the combined number of submissions to Sections D and F did increase. The largest change was for Section E, which increased from 1595 to 2383; the total number of short structural papers submitted to Sections C and E increased from 2445 to 3460. In total, 4353 Acta manuscripts were submitted, compared with 3220 in 2003 and 2543 in 2002.

The number of manuscripts submitted to JAC was 226, compared with 216 in 2003 and 260 in 2002. It should be noted that the 2002 figure includes 68 manuscripts submitted for the SAS2002 Conference Issue.

A total of 133 manuscripts were submitted to JSR, compared with 133 for 2003 and 114 for 2002.

#### Manuscripts received by Co-editors

|            | 1998 | 1999 | 2000 | 2001 | 2002 | 2003 | 2004 |
|------------|------|------|------|------|------|------|------|
| Acta A     | 153  | 88   | 117  | 121  | 124  | 123  | 135  |
| Acta B     | 117  | 128  | 131  | 148  | 141  | 122  | 143  |
| Acta C     | 1147 | 1189 | 1233 | 733  | 738  | 850  | 1077 |
| Acta D     | 297  | 313  | 376  | 432  | 504  | 530  | 499  |
| Acta E     |      |      | 119  | 883  | 1036 | 1595 | 2383 |
| Acta F     |      |      |      |      |      |      | 116  |
| Acta total | 1714 | 1718 | 1976 | 2317 | 2543 | 3220 | 4353 |
| JAC        | 192  | 326  | 165  | 175  | 260  | 216  | 226  |
| JSR        | 326  | 86   | 420  | 98   | 114  | 133  | 133  |
| TOTAL      | 2232 | 2130 | 2561 | 2590 | 2917 | 3569 | 4712 |

#### A.2. Papers accepted

The number of Acta papers accepted by Co-editors in 2003 was 3149, a 25% increase on 2003 when 2525 were accepted. Sections A, B, C and E showed increases in the number of papers accepted of 27%, 11%, 10% and 39%, respectively; Section D showed a decrease of 9%, but the overall number of papers accepted for Sections D and F increased by 3%.

The number of papers accepted for JAC was 167, compared with 277 in 2003 and 138 in 2002. It should be noted that the high number of accepted papers in 2003 included papers for the SAS2002 Conference Issue.

A total of 86 papers were received for JSR, compared with 97 in 2003 and 99 in 2002.

#### Accepted papers received in Chester

|            | 1998 | 1999 | 2000 | 2001 | 2002 | 2003 | 2004 |
|------------|------|------|------|------|------|------|------|
| Acta A     | 133  | 71   | 92   | 85   | 84   | 75   | 95   |
| Acta B     | 104  | 119  | 122  | 106  | 118  | 82   | 91   |
| Acta C     | 944  | 962  | 915  | 510  | 471  | 512  | 561  |
| Acta D     | 271  | 304  | 349  | 395  | 467  | 486  | 446  |
| Acta E     |      |      | 77   | 794  | 937  | 1370 | 1899 |
| Acta F     |      |      |      |      |      |      | 57   |
| Acta total | 1452 | 1456 | 1555 | 1890 | 2077 | 2525 | 3149 |
|            |      |      |      |      |      |      |      |
| JAC        | 152  | 220  | 178  | 138  | 138  | 277  | 167  |
| JSR        | 243  | 155  | 327  | 82   | 99   | 97   | 86   |
|            |      |      |      |      |      |      |      |
| TOTAL      | 1847 | 1831 | 2060 | 2110 | 2314 | 2899 | 3402 |

### A.3. Papers published

Overall, 10175 Acta pages were published in 2004, compared with 8735 in 2003 and 7905 in 2002. This represents an increase of 16% on the 2003 level; the number of printed pages increased from 5316 to 5507. 644 pages were printed for Section A (628 in 2003), 763 for Section B (821 in 2003), 1694 for Section C (1482 in 2003) and 2406 for Section D (2385 in 2003). Section E published 4676 electronic only pages (3419 in 2003).

The average length of Full Articles in Sections A, B and D decreased to 7.8, 8.9 and 4.9 pages, respectively, and the average lengths of Full Articles in Sections C and E increased to 3.0 and 2.6 pages, respectively. Average publication times increased for Section A (6.2 months) and C (2.3 months) and fell for Section B (4.8 months), Section D (4.3 months) and Section E (0.8 months).

The number of Full Articles published in JAC in 2004 was 110 (down from 225 in 2003 when the number was large as a result of the publication of the SAS2002 Proceedings). The number of pages also decreased for the same reason, from 1505 to 1044. The average review time decreased to 4.4 months and the technical editing time decreased to 2.2 months; the overall publication time was 6.7 months.

The number of Full Articles published in JSR in 2004 was 85 (77 in 2003). The number of pages increased to 512 in 2004 (475 in 2003). The average review time decreased to 4.9 months and the technical editing time decreased to 1.7 months; the overall publication time decreased to 6.5 months.

#### Pages(papers) published

|            | 1999       | 2000       | 2001       | 2002       | 2003        | 2004        |
|------------|------------|------------|------------|------------|-------------|-------------|
| Acta A     | 1073(122)  | 649(82)    | 803(103)   | 630(102)   | 628(83)     | 644(96)     |
| Acta B     | 1128(126)  | 1127(137)  | 877(110)   | 1088(132)  | 821(88)     | 763(87)     |
| Acta C     | 2192(929)  | 2179(943)  | 1504(545)  | 1570(535)  | 1482(482)   | 1694(556)   |
| Acta D     | 2079(394)  | 1723(339)  | 1980(390)  | 2243(457)  | 2385(466)   | 2406(511)   |
| Acta E     |            |            | 1998(800)  | 2374(922)  | 3419(1305)  | 4676(1811)  |
| Acta total | 6472(1571) | 5678(1501) | 7162(1948) | 7905(2148) | 8735(2424)  | 10183(3061) |
|            |            |            |            |            |             |             |
| JAC        | 1208(192)  | 1468(259)  | 798(140)   | 760(128)   | 1505(282)   | 1041(170)   |
| JSR        | 1209(311)  | 419(65)    | 1255(376)  | 413(93)    | 475(108)    | 512(119)    |
|            |            |            |            |            |             |             |
| TOTAL      | 8889(2074) | 7565(1825) | 9215(2464) | 9078(2369) | 10715(2814) | 11736(3350) |

#### Average publication times for full articles

|        | Year | Review process (months) | Editing/printing (months) | Publication time (months) |
|--------|------|-------------------------|---------------------------|---------------------------|
| Acta A | 2004 | 4.2                     | 2.0                       | 6.2                       |
|        | 2003 | 2.7                     | 1.8                       | 4.5                       |
|        | 2002 | 3.1                     | 2.5                       | 5.6                       |
|        | 2001 | 3.1                     | 4.1                       | 7.2                       |
|        | 2000 | 3.1                     | 3.7                       | 6.8                       |
|        | 1999 | 4.6                     | 6.5                       | 11.1                      |
| Acta B | 1998 | 4.1                     | 5.3                       | 9.4                       |
|        | 2004 | 2.9                     | 1.9                       | 4.8                       |
|        | 2003 | 3.2                     | 2.2                       | 5.4                       |
|        | 2002 | 2.9                     | 3.3                       | 6.2                       |
|        | 2001 | 3.5                     | 3.6                       | 7.2                       |
|        | 2000 | 3.5                     | 5.1                       | 8.5                       |
| Acta C | 1999 | 5.1                     | 6.4                       | 11.6                      |
|        | 1998 | 5.3                     | 7.9                       | 13.1                      |
|        | 2004 | 1.1                     | 1.2                       | 2.3                       |
|        | 2003 | 1.1                     | 1.1                       | 2.2                       |
|        | 2002 | 1.3                     | 1.4                       | 2.7                       |

|        |      |     |     |      |
|--------|------|-----|-----|------|
|        | 2001 | 2.0 | 2.8 | 4.8  |
|        | 2000 | 2.3 | 2.9 | 5.2  |
|        | 1999 | 2.8 | 4.0 | 6.8  |
|        | 1998 | 3.2 | 5.2 | 8.4  |
| Acta D | 2004 | 2.5 | 1.8 | 4.3  |
|        | 2003 | 2.9 | 2.0 | 4.9  |
|        | 2002 | 3.2 | 2.0 | 5.2  |
|        | 2001 | 3.0 | 2.5 | 5.5  |
|        | 2000 | 3.2 | 2.4 | 5.7  |
|        | 1999 | 3.4 | 3.7 | 7.0  |
|        | 1998 | 3.5 | 7.1 | 10.6 |
| Acta E | 2004 | 0.5 | 0.2 | 0.8  |
|        | 2003 | 0.5 | 0.4 | 0.9  |
|        | 2002 | 0.6 | 0.4 | 0.9  |
|        | 2001 | 0.6 | 0.4 | 1.0  |
| JAC    | 2004 | 4.4 | 2.2 | 6.7  |
|        | 2003 | 4.7 | 2.6 | 7.3  |
|        | 2002 | 4.5 | 2.7 | 7.1  |
|        | 2001 | 4.7 | 3.3 | 8.0  |
|        | 2000 | 5.4 | 4.4 | 9.8  |
|        | 1999 | 4.9 | 5.2 | 10.1 |
|        | 1998 | 5.0 | 7.6 | 12.5 |
| JSR    | 2004 | 4.9 | 1.7 | 6.5  |
|        | 2003 | 5.5 | 2.7 | 8.2  |
|        | 2002 | 4.6 | 2.0 | 6.6  |
|        | 2001 | 3.5 | 2.6 | 6.1  |
|        | 2000 | 3.9 | 2.5 | 6.3  |
|        | 1999 | 3.6 | 2.8 | 6.4  |
|        | 1998 | 4.2 | 3.1 | 7.3  |

#### A.4. Manuscripts rejected and withdrawn

The overall rejection rate for the journals (13%) was up from 2003 (8%). The rejection rate was highest for Section C (22%) and lowest for Sections D (7%) and F (2%). Withdrawal rates were highest for Section C (27%, up from 23% for 2003); the overall withdrawal rate was 13%.

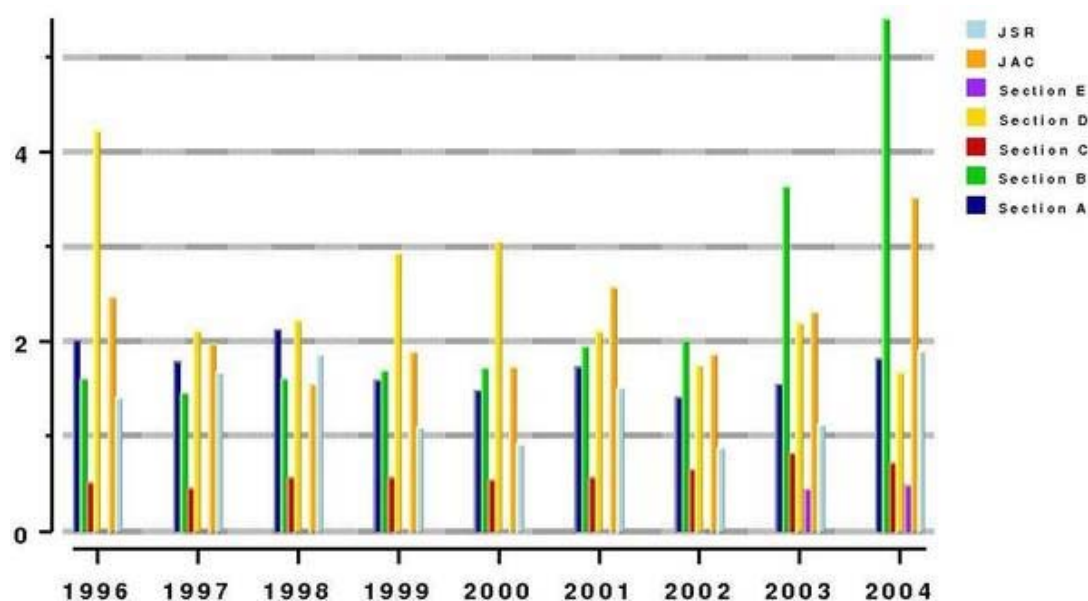
#### Manuscripts rejected and withdrawn

|        | Year | Number accepted | Number rejected | Number withdrawn | Rejection (%) | Withdrawal (%) |
|--------|------|-----------------|-----------------|------------------|---------------|----------------|
| Acta A | 2004 | 95              | 23              | 21               | 17            | 15             |
|        | 2003 | 75              | 26              | 26               | 20            | 20             |
|        | 2002 | 84              | 23              | 10               | 20            | 9              |
|        | 2001 | 85              | 14              | 10               | 10            | 5              |
|        | 2000 | 92              | 18              | 8                | 15            | 7              |
|        | 1999 | 71              | 11              | 9                | 12            | 10             |
| Acta B | 2004 | 91              | 27              | 26               | 19            | 18             |
|        | 2003 | 82              | 22              | 21               | 18            | 17             |
|        | 2002 | 118             | 20              | 8                | 14            | 5              |
|        | 2001 | 106             | 12              | 6                | 10            | 5              |
|        | 2000 | 122             | 24              | 9                | 15            | 6              |
|        | 1999 | 119             | 11              | 8                | 8             | 6              |

|         |      |      |     |     |    |    |
|---------|------|------|-----|-----|----|----|
| Acta C  | 2004 | 561  | 239 | 291 | 22 | 27 |
|         | 2003 | 512  | 121 | 191 | 15 | 23 |
|         | 2002 | 471  | 101 | 176 | 14 | 24 |
|         | 2001 | 511  | 74  | 220 | 9  | 27 |
|         | 2000 | 915  | 78  | 298 | 6  | 23 |
|         | 1999 | 766  | 76  | 224 | 7  | 21 |
| Acta D  | 2004 | 446  | 37  | 33  | 7  | 6  |
|         | 2003 | 486  | 23  | 24  | 4  | 5  |
|         | 2002 | 467  | 19  | 10  | 4  | 2  |
|         | 2001 | 396  | 9   | 11  | 2  | 3  |
|         | 2000 | 349  | 22  | 6   | 6  | 2  |
|         | 1999 | 304  | 9   | 11  | 3  | 3  |
| Acta E  | 2004 | 1899 | 253 | 203 | 11 | 9  |
|         | 2003 | 1370 | 81  | 117 | 5  | 7  |
|         | 2002 | 937  | 37  | 67  | 4  | 6  |
|         | 2001 | 794  | 24  | 53  | 3  | 6  |
|         | 2000 | 77   | 1   | 6   | 1  | 7  |
| Acta F  | 2004 | 57   | 1   | 1   | 2  | 2  |
| JAC     | 2004 | 167  | 26  | 33  | 12 | 15 |
|         | 2003 | 277  | 25  | 28  | 8  | 8  |
|         | 2002 | 138  | 26  | 18  | 14 | 10 |
|         | 2001 | 138  | 17  | 33  | 9  | 18 |
|         | 2000 | 178  | 13  | 18  | 6  | 9  |
|         | 1999 | 220  | 23  | 17  | 9  | 7  |
| JSR     | 2004 | 86   | 10  | 13  | 9  | 12 |
|         | 2003 | 97   | 9   | 10  | 8  | 9  |
|         | 2002 | 99   | 3   | 3   | 3  | 3  |
|         | 2001 | 82   | 13  | 20  | 11 | 17 |
|         | 2000 | 327  | 37  | 13  | 10 | 3  |
|         | 1999 | 155  | 8   | 7   | 5  | 4  |
| Overall | 2004 | 3402 | 616 | 621 | 13 | 13 |
|         | 2003 | 2899 | 307 | 417 | 8  | 12 |
|         | 2002 | 2314 | 229 | 292 | 8  | 10 |
|         | 2001 | 2112 | 163 | 353 | 6  | 13 |
|         | 2000 | 2060 | 193 | 358 | 7  | 14 |
|         | 1999 | 1635 | 138 | 276 | 7  | 13 |

## A.5. Citation statistics

The citation statistics for 1996-2004 are shown below.



IUCr journals continued to be highly ranked amongst crystallographic journals. Section B occupied the top ranking with an impact factor 5.418. Citation information is also reported in the Appendices to the individual journal meetings.

### Crystallography

| Abbreviated Journal Title | 2004 Total Cites | Impact Factor | Immediacy Index | 2004 Articles | Cited Half life |
|---------------------------|------------------|---------------|-----------------|---------------|-----------------|
| <b>ACTA CRYSTALLOGR B</b> | <b>9,852</b>     | <b>5.418</b>  | <b>0.452</b>    | <b>84</b>     | <b>&gt;10.0</b> |
| <b>J APPL CRYSTALLOGR</b> | <b>12,629</b>    | <b>3.534</b>  | <b>0.637</b>    | <b>146</b>    | <b>&gt;10.0</b> |
| J MOL GRAPH MODEL         | 2,579            | 3.036         | 0.362           | 58            | 8.3             |
| CRYST GROWTH DES          | 954              | 2.856         | 0.782           | 170           | 1.9             |
| CRYSTENGCOMM              | 808              | 2.596         | 0.480           | 102           | 2.5             |
| <b>ACTA CRYSTALLOGR A</b> | <b>9,186</b>     | <b>1.829</b>  | <b>0.417</b>    | <b>84</b>     | <b>&gt;10.0</b> |
| J CRYST GROWTH            | 18,949           | 1.707         | 0.301           | 1249          | 6.1             |
| <b>ACTA CRYSTALLOGR D</b> | <b>8,772</b>     | <b>1.693</b>  | <b>0.347</b>    | <b>495</b>    | <b>6.1</b>      |
| POLYHEDRON                | 8,929            | 1.586         | 0.350           | 383           | 7.2             |
| Z KRISTALLOGR             | 2,912            | 1.390         | 0.611           | 108           | >10.0           |
| LIQ CRYST                 | 3,483            | 1.056         | 0.207           | 184           | 7.2             |
| CRYST ENG                 | 239              | 0.945         | -               | 0             | 4.2             |
| STRUCT CHEM               | 424              | 0.833         | 0.211           | 71            | 6.4             |
| J INCL PHENOM MACRO       | 1,404            | 0.825         | 0.165           | 103           | 6.2             |
| CRYST RES TECHNOL         | 1,188            | 0.770         | 0.158           | 152           | 5.9             |
| CHINESE J STRUC CHEM      | 521              | 0.734         | 0.088           | 274           | 3.2             |
| <b>ACTA CRYSTALLOGR C</b> | <b>6,751</b>     | <b>0.728</b>  | <b>0.286</b>    | <b>553</b>    | <b>9.3</b>      |
| PHASE TRANSIT             | 698              | 0.581         | 0.210           | 62            | >10.0           |
| PROG CRYST GROWTH CH      | 390              | 0.531         | -               | -             | 8.9             |
| MOL CRYST LIQ CRYST       | 5,267            | 0.529         | 0.050           | 522           | 9.7             |
| J CHEM CRYSTALLOGR        | 533              | 0.512         | 0.074           | 136           | 5.5             |
| CRYSTALLOGR REP+          | 1,715            | 0.496         | 0.180           | 150           | >10.0           |
| <b>ACTA CRYSTALLOGR E</b> | <b>2,083</b>     | <b>0.491</b>  | <b>0.380</b>    | <b>1802</b>   | <b>1.5</b>      |
| Z KRISTNEW CRYST ST       | 561              | 0.330         | 0.075           | 228           | 3.8             |

## Instruments and Instrumentation

| Abbreviated Journal Title   | 2004 Total Cites | Impact Factor | Immediacy Index | 2004 Articles | Cited Half life |
|-----------------------------|------------------|---------------|-----------------|---------------|-----------------|
| APPL SPECTROSC REV          | 301              | 2.194         | 0.077           | 13            | 9               |
| SENSOR ACTUAT BCHEM         | 9058             | 2.083         | 0.211           | 436           | 5               |
| J MICROMECH MICROENG        | 2054             | 2.048         | 0.345           | 252           | 4.3             |
| <b>J SYNCHROTRON RADIAT</b> | <b>1571</b>      | <b>1.919</b>  | <b>0.494</b>    | <b>87</b>     | <b>5.3</b>      |
| CHEMOMETR INTELL LAB        | 2282             | 1.899         | 0.148           | 115           | 6.7             |
| APPL SPECTROSC              | 5680             | 1.848         | 0.297           | 219           | 7.2             |
| SMART MATER STRUCT          | 1856             | 1.522         | 0.082           | 170           | 5.4             |
| SENSOR ACTUAT APHYS         | 5051             | 1.462         | 0.123           | 464           | 5.3             |
| NUCL INSTRUM METH A         | 16582            | 1.349         | 0.288           | 1692          | 5.3             |
| METROLOGIA                  | 1244             | 1.314         | 0.481           | 79            | 7.5             |
| REV SCI INSTRUM             | 14434            | 1.226         | 0.186           | 1041          | 7.6             |
| INFRARED PHYS TECHN         | 767              | 1.128         | 0.147           | 75            | 9.1             |
| J RES NATL INST STAN        | 1469             | 1.123         | 0.088           | 34            | >10.0           |
| MEAS SCI TECHNOL            | 2983             | 1.118         | 0.217           | 345           | 5.4             |
| IEEE CIRCUITS DEVICE        | 236              | 1.115         | 0.179           | 28            | 5.4             |
| RADIO SCI                   | 2905             | 1.007         | 0.348           | 141           | 10              |
| NUCL INSTRUM METH B         | 12441            | 0.997         | 0.231           | 1095          | 6.6             |
| SENSORSBASEL                | 123              | 0.990         | 0.059           | 17            | 2.4             |
| IEEE T IND ELECTRON         | 1926             | 0.976         | 0.097           | 155           | 6.4             |
| SCANNING                    | 606              | 0.892         | 0.123           | 57            | 7.1             |
| ACCREDIT QUAL ASSUR         | 408              | 0.861         | 0.240           | 121           | 3.5             |
| J GUID CONTROL DYNAM        | 2054             | 0.852         | 0.061           | 131           | 9.3             |
| DISPLAYS                    | 275              | 0.800         | 0.000           | 31            | 5.4             |
| PRECIS ENG                  | 608              | 0.796         | 0.188           | 48            | 8.1             |
| INSTRUM SCI TECHNOL         | 166              | 0.681         | 0.121           | 58            | 3.5             |

## Optics

| Abbreviated Journal Title   | 2004 Total Cites | Impact Factor | Immediacy Index | 2004 Articles | Cited Half life |
|-----------------------------|------------------|---------------|-----------------|---------------|-----------------|
| PROG OPTICS                 | 1,046            | 7.846         | 0.400           | 5             | 9               |
| ADV ATOM MOL OPT PHY        | 871              | 7.214         | -               | -             | 8.5             |
| OPT LETT                    | 25,479           | 3.882         | 0.821           | 836           | 6.2             |
| OPT EXPRESS                 | 4,442            | 3.797         | 0.731           | 780           | 2.1             |
| J BIOMED OPT                | 1,570            | 3.455         | 0.592           | 152           | 3.6             |
| IEEE J SEL TOP QUANT        | 4,017            | 3.048         | 0.141           | 170           | 4.8             |
| PHYS REV A                  | 58,306           | 2.902         | 0.641           | 1699          | 8.4             |
| J OPT SOC AM B              | 8,632            | 2.649         | 0.562           | 265           | 7.4             |
| IEEE PHOTONIC TECH L        | 11,062           | 2.552         | 0.444           | 867           | 4.8             |
| APPL PHYS BLASERS O         | 5,415            | 2.215         | 0.439           | 337           | 4.9             |
| J LIGHTWAVE TECHNOL         | 8,703            | 2.113         | 0.428           | 318           | 6.7             |
| J OPT SOC AM A              | 9,563            | 2.012         | 0.435           | 271           | 8.9             |
| <b>J SYNCHROTRON RADIAT</b> | <b>1,571</b>     | <b>1.919</b>  | <b>0.494</b>    | <b>87</b>     | <b>5.3</b>      |
| APPL OPTICS                 | 25,477           | 1.799         | 0.451           | 781           | 9.2             |
| J PHYS BAT MOL OPT          | 11,588           | 1.761         | 0.564           | 427           | 8.5             |
| J OPT BQUANTUM S O          | 1,044            | 1.746         | 0.338           | 204           | 2.6             |
| J LUMIN                     | 4,298            | 1.684         | 0.242           | 244           | 6               |

|                   |        |       |       |     |     |
|-------------------|--------|-------|-------|-----|-----|
| OPT FIBER TECHNOL | 324    | 1.622 | 0.429 | 21  | 4.8 |
| OPT COMMUN        | 11,815 | 1.581 | 0.361 | 785 | 6.2 |

### Physics, applied

| Abbreviated Journal Title   | 2004 Total Cites | Impact Factor | Immediacy Index | 2004 Articles | Cited Half life |
|-----------------------------|------------------|---------------|-----------------|---------------|-----------------|
| MAT SCI ENG R               | 2,066            | 14.233        | 0.846           | 13            | 4.9             |
| NAT MATER                   | 2,462            | 13.531        | 2.182           | 132           | 1.6             |
| ADV FUNCT MATER             | 2,024            | 5.679         | 0.797           | 148           | 2.3             |
| APPL PHYS LETT              | 112,516          | 4.308         | 0.567           | 3731          | 5.2             |
| IEEE J QUANTUM ELECT        | 10,875           | 3.675         | 0.486           | 208           | >10.0           |
| ORG ELECTRON                | 332              | 3.636         | 0.351           | 37            | 2.9             |
| MRS BULL                    | 3,099            | 3.444         | 0.446           | 74            | 5.2             |
| NANOTECHNOLOGY              | 2,858            | 3.322         | 0.473           | 450           | 2.9             |
| IEEE T NANOTECHNOL          | 311              | 3.176         | 0.309           | 68            | 2.2             |
| CURR OPIN SOLID ST M        | 1,310            | 2.846         | 0.211           | 19            | 5.2             |
| IEEE PHOTONIC TECH L        | 11,062           | 2.552         | 0.444           | 867           | 4.8             |
| J APPL PHYS                 | 84,947           | 2.255         | 0.383           | 2684          | 7.7             |
| APPL PHYS BLASERS O         | 5,415            | 2.215         | 0.439           | 337           | 4.9             |
| PHILOS MAG A                | 4,508            | 2.136         | -               | 0             | 8.6             |
| IEEE T ELECTRON DEV         | 10,013           | 2.036         | 0.402           | 333           | 7.6             |
| <b>J SYNCHROTRON RADIAT</b> | <b>1,571</b>     | <b>1.919</b>  | <b>0.494</b>    | <b>87</b>     | <b>5.3</b>      |
| EUR PHYS J E                | 1,412            | 1.903         | 0.240           | 129           | 3.1             |
| GRANUL MATTER               | 231              | 1.897         | 0.206           | 34            | 4.1             |
| PLASMA CHEM PLASMA P        | 742              | 1.847         | 0.182           | 33            | 8.3             |
| J OPT BQUANTUM S O          | 1,044            | 1.746         | 0.338           | 204           | 2.6             |
| J VAC SCI TECHNOL B         | 10,710           | 1.664         | 0.202           | 648           | 6.3             |
| THIN SOLID FILMS            | 20,557           | 1.647         | 0.226           | 1403          | 6.2             |
| J PHYS D APPL PHYS          | 9,220            | 1.642         | 0.273           | 516           | 6.5             |
| J VAC SCI TECHNOL A         | 9,683            | 1.557         | 0.207           | 421           | 8.3             |
| SUPERCOND SCI TECH          | 2,769            | 1.556         | 0.355           | 389           | 3.7             |
| MICROELECTRON ENG           | 3,028            | 1.514         | 0.244           | 398           | 3.6             |
| J ELECTRON MATER            | 3,433            | 1.507         | 0.179           | 235           | 5.6             |

## APPENDIX B

### Commission on Journals Triennial Reports to the Executive Committee

#### Overview

Comparing the year-ends of the last three triennia, 11,736 journal pages were published in 2004, compared with 9,215 in 2001 and 7,937 in 1998. This increase in the number of pages has been accompanied by a major reduction in publication times for all sections of *Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.* Thus, for *Acta Cryst.* Sections A, B, C and D in 2004 publication times were 6.2, 4.8, 2.3 and 4.3 months versus 12 months for each in 1995; the 2004 times for *Acta Cryst.* Section E, *J. Appl. Cryst.* and *J. Synchrotron Rad.* were 0.8, 6.7 and 6.5 months, respectively. This improvement has happened owing to measures introduced to metricate individual Co-editor review times and to improved efficiency in the technical editing, all aided by e-mail and use of the web. The latest initiative aimed at efficiency, an electronic submission system for articles, introduced in 2003, has been very popular with Co-editors and authors.

Financially, the overall subscriptions situation has remained positive in a challenging climate. There is an annual attrition of subscriptions but at approximately 5% this is less than the average of 7% generally experienced by science journals. Prudent attention to setting of year-on-year subscription rates by the IUCr Finance Committee through the triennium has kept IUCr journals generating a surplus overall. Strong challenges have surfaced in 2004 as the US National Institutes of Health (NIH) and the UK Science and Technology Parliamentary Committee have both investigated science publishing and recommended that for government-funded research the results and data should be made freely available within 12 months of publication. These developments will require very careful discussion within the IUCr Finance Committee.

The citation impact of IUCr journals continued to be high, effectively occupying two or three of the top five ranking positions in crystallography.

The overall withdrawal plus rejection rate for the journals was 26% in 2004, up compared with 2003 (20%) and 2002 (18%). Looking into this there is a noticeable effect from Acta C in 2004 of 49% versus 38% in both 2002 and 2003, which in turn analyses as being heavily biased by high rejection rate by country of origin.

An open-access option for authors was introduced on a fee payment basis in 2004. In the case of authors from the UK, however, a grant from the UK Joint Information Systems Committee allowed all UK papers to be published as open access in 2004 and another award makes this possible for 2005.

Acta E is attracting ever-increasing numbers of electronic structure reports; the number of electronic pages produced in 2004 is approximately 85% of all the printed pages published for *Acta Cryst.* in 2002! This success has required an expansion of the Acta E Editorial Board. This is a major achievement to publish so many papers, all of which are of course citable and citation ranked by ISI.

Acta C has not suffered from the Acta E launch. Acta C subscribers in any case receive Acta E within the Acta C subscription. Rather, Acta C is now showing that it is increasingly the premier home of important and high-quality crystal structure communications; evidence that this is happening is in the citation impact rising from 0.571 in 2001, to 0.659 in 2002 and 0.828 in 2003.

Discussions concerning a new Section of *Acta Cryst.* catering for high-throughput crystallization communications started in about 1997. As structural genomics programmes became funded in the early 2000s the issue broadened as to how to handle high-throughput short structural biology communications. In terms of quantity, approximately half of any single issue of Acta D had become regularly devoted to crystallization communications. The structural genomics funding, in addition, was very healthy and a journal outlet might be optimized for them as well. Thus, through 2003 and 2004, the situations of crystallization and high-throughput structural biology/genomics reports were monitored carefully by IUCr journals staff and the Editor-in-Chief. In 2004 the final decision was taken to bud part of Acta D into a new Acta F. The launch of Acta F was agreed in mid-2004 with a launch date of January 2005. The name of Acta F was also finalized as Structural Biology and Crystallization Communications. New Section Editors (H.M. Einspahr and J.M. Guss) and a new Editorial Board were appointed. Extensive work has been made jointly with the Protein Data Bank by H.M. Einspahr concerning streamlined deposition-to-publication methodologies. We acknowledge the cooperation of the Protein Data Bank in this work. The first issue was published in January 2005. Acta D subscribers receive Acta F free.

This is my final triennial report. 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 Chester. I have enjoyed many science interactions with fellow IUCr journals' Editors and Co-editors (*Acta Cryst.*, *J. Appl. Cryst.* and *J. Synchrotron Rad.*) and with our submitting authors, as well as with many fellow diffraction physicists, crystallographers and structural scientists who care deeply about the IUCr, through my nine years as Editor-in-Chief of *Acta Cryst.* I acknowledge also very good collaborations with the Executive and Finance Committees and with the IUCr Newsletter Editors. I thank here also, most heartily, the many scientists who helped me as referees. Overall I wish to record here that to have had the chance to contribute to the International Union of Crystallography by serving the IUCr journals learned

society style of publishing enterprise, as well as authors, subscribers and readers, has been a deeply fulfilling experience for me.

**J.R. Helliwell**, Editor-in-Chief and Chair of Commission

### **Acta Crystallographica Section A**

Basic statistics for Section A are shown below:

| Year | Total pages | Pages for science | No. of Research Papers                       | No. of Short Communications | Average length of Research Papers | Publication time (months) | Europe (%) | Asia (%) | Americas (%) |
|------|-------------|-------------------|--|-----------------------------|-----------------------------------|---------------------------|------------|----------|--------------|
| 2002 | 630         | 551               | 65   | 14                          | 8.0                               | 5.6                       | 50         | 25       | 25           |
| 2002 | 375         | 372               | Supplement, Abstracts of the Geneva Congress |                             |                                   |                           |            |          |              |
| 2003 | 628         | 474               | 58   | 6                           | 7.9                               | 4.5                       | 54         | 10       | 36           |
| 2004 | 644         | 626               | 78   | 7                           | 7.8                               | 6.2                       | 61         | 14       | 25           |
| 2004 | 308         | 308               | Abstracts of ECM-22                          |                             |                                   |                           |            |          |              |

Pages for science comprise only Research Papers, Short Communications and Letters to the Editor; publication time applies to research papers; the origin of articles binned for Europe, Asia+Australia and the Americas comprises Research Papers and Short Communications counted as integral or half-integral numbers.

Section A published 18 issues, 6 per year. The numbers for 2002 are comparable to those for 2000, but lower than those for 2001 by 10 Research Papers. A further notable dip occurs in 2003, but the results for 2004 again reach levels comparable to those of 2001. This appears to indicate that Section A on average retains its volumetric importance. The good results for 2004 are in part due to the September Special Issue containing 21 articles in 160 pages (see below). Still, the five regular issues of 2004 comprise as many pages and articles as the six issues of 2003. The rejection plus withdrawal rates oscillate around 33%, being 29%, 40% and 32%, respectively. The geographical origins of the papers show a European preponderance. The electronic submission procedure works very well and is used by a large majority of authors.

In 2002 and 2003, no Lead Articles, Topical Reviews or Special Issues were published. In 2004, two contributions to the Microsymposium on Quantum Crystallography of the Geneva Congress in 2002 were published with an introduction by the Chair S. Manninen. In September 2004, a Special Issue was published on New Information from Modern Charge Density Methods, containing work presented at the Third European Charge Density Meeting ECDM-III at Sandbjerg Estate, Denmark. The Guest editor was the conference organizer F.K. Larsen.

Section A covers a broad interdisciplinary spectrum of the exact sciences. It has retained its comparative international rating during the past five years with impact factors oscillating between 1.42 and 1.75. It is indubitably the leading journal for work in Foundations of Crystallography. We hope to publish in the near future two Special Issues and three Lead Articles/Topical Reviews. I thank the Co-editors and the referees for their work.

**D. Schwarzenbach**, Editor

### **Acta Crystallographica Section B**

During the triennium 2002-2004 Section B published six issues per year. In the years 2002-2004 the numbers of articles were 132, 88 and 87, with the high value for 2002 a partial consequence of a very successful Special Issue (jointly with Section D) on crystallographic databases. The numbers of pages per year were 1,088, 821, and 763. Papers came from 27 different countries. All papers were written in English.

A comparison of the statistics for the years 2002-2004 shows that the distribution of articles between the inorganic, metal-organic and organic sections of the journal varies from year to year. Overall the ratio of papers that discuss inorganic and molecular compounds is about 35:65.

A comparison of numbers of articles and pages for this and the previous triennium indicates that the number of pages per year has been decreasing. It may be that work is now being reported in a more concise way. Because access to archived CIFs and to other Supplementary Material is now easy, the number of tables in the printed papers can be reduced. On the other hand, the number of papers per year is also down. It is possible that some papers that would in the past have appeared in Section B are now appearing in Section C because structures that were once considered difficult or unusual (e.g. because of twinning or a large number of molecules in the asymmetric unit) have become more routine. This factor might help explain the rise of the combined rejection/withdrawal rate for Section B from 17% in 1999-2001 to ca 35% in 2003-2004. Finally, it seems almost certain that competition from CrystEngComm (started in 1999 by the Royal Society

of Chemistry) and Cryst. Growth Design (started in 2001 by the American Chemical Society) is a factor in the decreased number of papers. Ways of enhancing the competitive position of Section B are being considered. One Topical Review was published in 2004. Another is being written and several others are in the discussion stage.

A very positive development is the continuing increase of the impact factor from 1.73 for 2000 (announced in 2001) to 3.64 for 2003 (announced in 2004). This increase has brought Section B greater visibility and very favourable publicity. The heavily cited 2002 Special Issue on databases is an important factor in the rise.

The electronic submission system first implemented in 2003 is now fully operational. The system is popular with both authors and editors. Time to publication dropped from 7.2 months in 2001 to 4.8 months in 2004. Communication between authors, Co-editors, referees and the Chester Office is now essentially instantaneous and all file processing is highly automated.

Colour figures have become so common that the journal pages look quite different than they did three years ago. The colour enhances the visual appeal, but more colour is being used than seems necessary.

It is, as always, a pleasure to thank the Chester staff for their skill in producing attractive journal pages that are easily read. Placing the many tables, figures, and footnotes in logical positions relative to the text is no easy task. The considerable work necessary to make sure the text conforms to reasonable standards is also very much appreciated.

**C.P. Brock**, Editor

### **Acta Crystallographica Section C**

Section C continues to specialize in the rapid publication of high-quality studies of novel and challenging crystal and molecular structures. Publication times continue their downward trend with the majority of technically correct and well written papers appearing online (<http://journals.iucr.org/c>) within one to two months of submission. In 2003 Section C published 478 papers (49 inorganic, 186 metal-organic and 243 organic) in a total of 1,482 pages. In 2004, Section C published 554 papers (42 inorganic, 227 metal-organic, 285 organic) in a total of 1,686 pages - a 15% increase in papers and pages over 2003. Section C is now showing that it is increasingly the premier home of important and high-quality crystal structure communications; evidence that this is happening is in the citation impact rising from 0.571 in 2001, to 0.659 in 2002 and 0.828 in 2003.

There has been a significant increase in the number of submissions to Section C in the last triennium and this has resulted in a major increase in editorial workload. Some 39% of original technically correct submissions to Section C in 2003 were subsequently withdrawn or rejected; this withdrawal/rejection rate climbed to 48% in 2004. The principal reasons for this significant increase in the withdrawal/rejection rate were either that the text in the Comment section of the CIF was deemed not to provide the "significant added value to the numerical data freely available in the CIF" as detailed in Notes for Authors, or (increasingly) that the text in the Comment section was very poorly crafted and difficult to understand.

Some changes have been made to the 2005 Notes for Authors in an attempt to improve the quality of initial submissions. It is a requirement that the text sections of the paper be written in clear and correct English (or one of the other accepted languages). Papers with text sections containing consistently poor grammar or incomprehensible statements are now being rejected promptly by the assigned Co-editor. While the editors and Chester editorial office staff are very willing to provide help with any technical CIF problems, they cannot be expected to assist with major corrections or re-drafting of inadequately prepared text. To assist Co-editors with the initial review of new submissions we are now asking that the submitting author consider providing in the `_publ_contact_letter` section of the CIF a brief statement of what is new, novel or interesting about the structure(s) in the submitted CIF that merits publication in the printed form in Section C. Given the ever increasing number of structures determined, the pressure on space in Section C is such that we must serve our chemical- and materials-structure communities by keeping Section C as a premier outlet for the best crystal structures, both technically and scientifically.

It was with deep regret that we learned of the death in 2004 of Professor Mario Nardelli, a highly respected and long-time member of the Section C Editorial Board.

It is always a pleasure to thank the many Co-editors, referees, and the Chester staff for their superb work in the preparation of Section C; their fine efforts make my job as Editor much easier and I look forward to our continuing partnership.

**G. Ferguson**, Editor

### **Acta Crystallographica Section D**

The past three years have seen major changes, both in Section D and in biological crystallography itself. First and foremost has been the retirement of our founding Editor, Jenny Glusker. Jenny approached her task of developing the new journal, from its inception in 1993, with enormous wisdom and personal commitment, and for this we owe her a

huge debt of gratitude. Perhaps significantly, it has taken the two of us, E.N. Baker and Z. Dauter, to replace her! Coinciding with Jenny's retirement as Editor, and celebrating 10 years of publication of Section D, a number of invited articles were published, from leading crystallographers.

The first 10 years of Section D coincided with a boom in biological crystallography that shows no sign of stopping. In 1993 there were less than 2,000 experimentally determined protein structures in the Protein Data Bank; in 2003 there were 22,000 and today there are more than 30,000. This growth in biological crystallography is driven by the importance of protein structures for biotechnology, medicine and functional genomics. In parallel there have been many changes in crystallographic methods, technologies and practice, including the development of crystallization robotics, the much wider use of anomalous scattering (MAD and SAD), automated map interpretation and model building, many improved protocols for structure solution and refinement, and major synchrotron developments.

The task of Section D is to capture the dynamism of this field, and provide a high quality publication venue for the biological crystallography community. The journal looks superb, and the quality of production is excellent. The electronic submission system, which was introduced in 2003, works very well for authors, reviewers and Co-editors, and has also helped reduce average publication times; these have steadily decreased from 5.2 months for full articles in 2002, to 4.9 in 2003, to 4.3 in 2004. The journal has also grown, from 2,243 pages in 2002 to 2,406 in 2004.

In terms of content, Section D remains pre-eminent in the publication of new methods in biological crystallography. This makes it a very important resource for the crystallographic community, and many of these methodological papers are highly cited. The publication of the very popular CCP4 study weekend series (see below) is similarly important. In some other respects the journal is not yet meeting its full potential, however. The number of structural papers published averages about 10 per issue, but we wish to increase this and attract more high-profile structures. Of some concern here is the impact factor, which was 1.76 in 2002 and 2.21 in 2003, lower than some competitor structural biology journals.

The place of crystallization papers has stimulated much discussion. Whereas the number of full research articles has remained steady at about 12 per monthly issue, the number of crystallization papers has increased from an average of 16.8 in 2002, to 20.6 in 2003, to 24.6 in 2004; in 2004, crystallization papers accounted for 60% of articles and 37% of pages. Crystal growth is a key part of crystallography, often requiring great skill, and full documentation of protein production and crystallization is essential for the reproducibility of a crystallographic structure determination. Paradoxically, despite the importance of these papers, they are seldom cited and thus depress the impact factor of the journal. From 2005, they will instead be published in the new all-electronic journal, Acta F, leaving Acta D to focus on crystallographic methods and structures.

Notable features of the past three years have been the Special Issues devoted to methods. These are also available as stand-alone publications. The CCP4 study weekend issue is published towards the end of each year, with Guest Editors who are responsible for the issue. In 2002, the topic was high-throughput structure determination, with guest editors R. Esnouf, D. Stuart and K. Wilson; in 2003, A. McCoy and N. McDonald were Guest Editors for an issue focusing on experimental phasing; and in 2004 the topic was model building and refinement, with Guest editors A. Perrakis and M. Noble. These are always eagerly awaited issues, and the papers give a snapshot of the leading edge of the field. We are enormously grateful both to CCP4 and to the Guest Editors for the continued publication of this series. The other Special Issue from the past three years, in October 2002, presented the Proceedings of the 9th International Conference on the Crystallization of Biological Macromolecules. Again, this contains seminal methodological papers, and we are very grateful to the Guest Editors M. Riès-Kautt and R. Hilgenfeld.

Finally we thank the many people who contribute to the success of the journal; our authors and readers; the reviewers whose efforts are critical for maintaining quality; our Co-editors who give their time and wisdom in shepherding papers through to acceptance; Louise Jones and Simon Glynn for their efforts at Chester in maintaining superb production quality; and Peter Strickland, as Managing Editor, and John Helliwell, Editor-in-Chief, for their guidance and management.

**E.N. Baker and Z. Dauter**, Editors

### **Acta Crystallographica Section E**

This is the first full triennial report for the journal; three years ago we were able to give a report for only one year, 2001, the first year of publication. A great deal has happened since then!

From its inception in 2001, Section E of Acta Crystallographica has experienced a steady and remarkable growth, as evidenced by the statistics reported below for the three years covered by this report.

|                      | 2002 | 2003 | 2004 |
|----------------------|------|------|------|
| Manuscripts received | 1036 | 1595 | 2383 |
| Manuscripts accepted | 937  | 1370 | 1899 |
| Manuscripts rejected | 37   | 81   | 253  |

|                        |      |      |      |
|------------------------|------|------|------|
| Manuscripts withdrawn  | 67   | 117  | 203  |
| Inorganic papers       | 49   | 59   | 57   |
| Metal-organic papers   | 295  | 444  | 743  |
| Organic papers         | 577  | 794  | 1003 |
| Total papers published | 922  | 1305 | 1811 |
| Pages published        | 2374 | 3419 | 4676 |

In terms of both published papers and pages, the journal in 2004 was well over twice the size of 2001. This rate of growth shows no sign of abating.

Over the same period, there has been a slight decrease in the average time taken from receipt to publication, from 1 month to 0.8 months. Authors are asked to make revisions within one month, otherwise papers are considered to be withdrawn; in some cases, more than one round of revision is necessary, so a small proportion of papers have quite long publication times. Publication times as short as 3 days from receipt to online availability have occasionally been achieved.

Over these years the greatest proportion of published papers has originated in the People's Republic of China, reaching 38.9% in 2004; the next highest proportions in 2004 were USA (7.7%), Turkey (6.8%), UK (6.4%) and India (5.7%).

Most published papers have a length of 2-3 pages. Each reports the structure of a single material; reports of multiple structures are not accepted, in order to achieve maximum automation in procedures and publishing efficiency.

The journal has two joint Section Editors, whose activities include providing advice to Co-editors, selecting monthly electronic cover illustrations for the journal's web site, and proof-reading all papers before publication to ensure consistency and conformity with journal policies. They also serve as Co-editors.

The number of Co-editors has risen each year in response to the growth of the journal itself: 19 in 2002, 25 in 2003, and 31 in 2004; more Co-editors have already been appointed early in 2005. Unfortunately, we have lost the services of one Co-editor, Professor Mario Nardelli, who had served from the very beginning of the journal; his death in 2004 was a significant loss to the IUCr as a whole. The distribution of Co-editors by country (at the end of 2004) is Australia (2), Austria (1), Canada (3), China (1), Croatia (1), France (1), Germany (2), India (1), Italy (1), Japan (2), Malaysia (1), New Zealand (1), Russia (2), Sweden (1), Switzerland (1), UK (3 plus 2 section editors), USA (5).

The journal is served mainly by two members of editorial staff in the Chester IUCr offices, Gillian Holmes and Sean Conway, under the guidance and supervision of Peter Strickland. This level of central editorial staffing has not changed during the lifetime of the journal, and the efficiency and dedication of the staff with their much increased workload are much appreciated.

The basic manuscript submission, handling and editorial procedures set up at the launch of the journal have remained broadly the same during this period, though there have been a number of changes and improvements in response to the increasing number of papers. These include some streamlining of e-mail and other correspondence with authors; significant development of web resources for Co-editors including online status lists and access to the documents associated with each paper (a very positive development for the Section Editors at the proof-reading stage); a two-stage proof checking procedure (Section Editors make some corrections and raise queries before the proofs are made available to authors); the automatic return of submissions to authors for correction before formal receipt and allocation to a Co-editor if serious problems are detected in the automatic checking process; and automated Section Editor feedback to Co-editors from the proof-reading.

More significant developments in the manuscript submission procedure are currently underway, for implementation during 2005, and will be presented in the next annual and triennial reports.

Improvements in services for authors over the three-year period include the release (and later update) of the CIF editing tool enCIFer, provided by the Cambridge Crystallographic Data Centre, and a preliminary version of a utility for editing CIF-based submissions through Microsoft Word, using a template with embedded macros developed in the IUCr editorial office. A wide range of web-based author interfaces for submission, proofs and electronic reprints is provided in a single location on the journal's home-page, together with access for readers and subscribers, only one step away from the main Crystallography Journals Online web site.

The journal has proved very popular with authors, especially those in countries of the Middle and Far East. Attractive features are the rapid publication, the ease of submission, availability of useful author services, full-colour publication with no charge, and the opportunity to publish crystal structures without an extended discussion of the results. It is also widely appreciated that Section E, along with other IUCr journals, maintains very high technical standards of production and encourages rigour and care in the determination of crystal structures.

Section E provides a complementary service to that of Section C, where a more substantial discussion of results is required, and where papers can be published describing two or more related structures. Its rapid growth has eased

pressure on Section C, while at the same time leading to a substantial increase overall in the publication of crystal structures in the IUCr journals, and it has attracted many new authors.

The journal received ISI accreditation within one year of its launch; papers published in it are thus certified as undergoing peer review, and they are fully indexed and used in citation analyses, which is an important consideration for many authors.

Although the journal's impact factor, calculated for the first time in 2004, is rather low at 0.453, this is to be expected from the nature of the journal and its relationship to Section C (which has a higher value of 0.828, climbing from its previous value of 0.659, possibly due in some measure to the launch of Section E), and it is higher than those of other journals with a similar remit (*J. Chem. Crystallogr.* at 0.400 and *Z. Kristallogr. New Cryst. Struct.* at 0.349).

**D.G. Watson and W. Clegg**, Editors

### **Acta Crystallographica Section F**

Discussions for a new Section of Acta Crystallographica catering for high-throughput crystallization communications started in about 1997. As structural genomics programmes became funded in the early 2000s the issue broadened as to how to handle high-throughput, short, structural biology communications. In terms of quantity approximately half of any single issue of Acta Crystallographica Section D had become regularly devoted to crystallization communications. The structural genomics funding, in addition, was very healthy and a journal outlet might be optimized for them as well. Thus, through 2003 and 2004, the situations of crystallization and high-throughput structural biology/genomics reports were monitored carefully by IUCr journals staff and the Editor-in-Chief. In 2004 the final decision was taken to bud part of Acta D into a new Acta F by the IUCr Executive Committee. In the analyses similarities of Acta C budding into Acta E were also there and helpful. Acta F's launch was agreed in mid 2004 with a launch of January 2005. The name of Acta F was also finalized through 2004 but with the decisive seed made in Ventura California at a meeting of H.M. Einspahr, J.M. Guss and J.R. Helliwell, namely as Structural Biology and Crystallization Communications.

The new all-electronic Section F of Acta Crystallographica was launched in January 2005, making 2004 a very busy year for all concerned. A panel of distinguished and enthusiastic Co-editors has been appointed ensuring that the high scientific and production standards that characterize Acta Crystallographica will be maintained in the new journal.

Acta F aims to provide a home for short communications on the crystallization and structure of biological macromolecules. Structures determined through structural genomics initiatives or from iterative studies such as those used in the pharmaceutical industry are particularly welcomed.

An entirely new feature of Section F will be the close coordination of data submission to the Protein Data Bank (PDB) and preparation of mandatory items for inclusion in short structural papers. The preferred mode of data transfer from the database to the journal will be in the form of an mmCIF file. This will enable the generation of tables for publication and validation data for referees. One of the Section Editors (H.M. Einspahr) has worked closely with staff of the PDB (H.M. Berman and J.D. Westbrook) and the IUCr offices in Chester (Brian McMahon and Peter Strickland) to define the new mmCIF terms required for a complete description of a structure determination. Parallel efforts are being made to improve the communication between Co-editors, referees and authors.

The first issue of the new journal looks very good and our thanks go to the technical staff in Chester, especially to Louise Jones.

**H.M. Einspahr and J.M. Guss**, Editors

### **Journal of Applied Crystallography**

JAC published 760 pages in 2002, 1,009 pages in 2003 (plus 496 pages of Conference Proceedings of the 12th International Conference on Small-Angle Scattering held in Venice, Italy, in 2002), and 1,041 pages in 2004. The increase in the number of pages (small-angle scattering not included) is due to an increase in the number of articles, but also, to a lesser extent (~7%), to the increased length of individual articles. The increase in the number of papers reflects the appointment of very successful new Co-editors in the USA, but among the main subscriber countries, more papers may still be desirable from the USA and Japan. There was a further decrease of the average publication time (from 7.1 to 6.7 months) owing to the reduction of editing time, while the average review time remained constant at about 4.5 months. Manuscripts are now almost exclusively submitted and reviewed electronically. The combined rejection and withdrawal rate remained at 25 to 27% (without small-angle scattering). The impact factor continues at a high level, among the IUCr journals only second to Acta B, and JAC was ranked fifth in crystallography journals (2003).

A relatively large number of Co-editors will retire this year; the great service to the journal by S. S. Hasnain, J. R. Helliwell, A. M. Moore, Å. Oskarsson, D. Pandey, and H. Zimmermann is highly appreciated. Some new appointments will be considered during the current and the forthcoming years.

**G. Kostorz**, Editor

## **Journal of Synchrotron Radiation**

October 2004 marked the 10th anniversary of JSR. A total of 230 research articles comprising 1,265 pages were published during the period 2002-2004. This is less than past three-year periods reflecting a change in emphasis of the journal from publishing large proceedings from major synchrotron radiation conferences to more focused, special editions with focused themes. Although this approach reduces the total number of pages published per year, we believe the quality of the papers has increased. During this time the impact factor rose from 0.885 in 2002 to 1.144 in 2003. We hope that this trend continues during the upcoming years. The average publication time has been sporadic during this three-year period, starting with 6.6 months in 2002, shooting upwards to 8.2 months in 2003, and recovering to 6.5 months in 2004. This seems to be driven in large part to an increase in review time during this triennium. We, as Main Editors, will have to be increasingly vigilant to ensure that all editors encourage rapid reviewing by referees and timely editing by authors.

In the next triennium we expect the interest in this field will continue to grow as new approaches to the generation of radiation in the range from VUV to hard X-rays, such as energy recover linacs (ERLs) and free electron lasers (FELs), are developed. We fully expect that JSR will remain the pre-eminent journal dedicated to reporting scientific and instrument advancements, regardless of the source technology, in the years to come.

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

## APPENDIX C

### Review documents

#### Journal of Applied Crystallography - notes for referees

The task of a referee involves three main components: speed, confidentiality and thoroughness. These are, to some extent, conflicting, and the following notes may be of assistance.

##### 1. Speed

Unless the paper is of exceptional length or complexity, your report should be despatched within two weeks of receipt of the paper. If you are unable to act, please let the Co-editor know immediately, with the suggestion of an alternative referee.

##### 2. Confidentiality

In exceptional cases you may find it desirable to discuss the paper with one of your associates; if you do this it is your responsibility to ensure that the information spreads no further. Under no circumstances should the paper or any copy of it be retained.

The Editors do not reveal the identity of referees to authors. If, nevertheless, you wish to correspond directly with the author, the first contact should be made through the Editor or Co-editor.

##### 3. Thoroughness

It will be helpful if you keep the following points in mind both in reading the paper and in writing your report:

- (a) Is the work original and new?
- (b) Is the work sound and technically up-to-date? Are the conclusions firmly based on the observations or reasoning given?
- (c) Are there any aspects of the paper for which you would like to suggest another referee? (Referees are not expected to accept responsibility for the correctness of every detail of mathematical derivations, calculations, and the like.)
- (d) Is the abstract an adequate summary of the paper? Abstracts should, as far as practicable, be 'informative' rather than 'indicative'; that is, they should contain the most-important numerical and other results, and not merely state that such results are given in the paper.
- (e) Is the literature adequately and correctly referenced?
- (f) Is the journal for which the paper has been submitted the most appropriate?
- (g) If the paper has been offered to the appropriate journal, and the results are worthy of publication, is the presentation the most efficient possible? The 'information density' should be high and uniform throughout, in view of the volume of material submitted for publication.

The following additional points should also be considered with care:

- (h) Has the paper been submitted in the correct category, or should it be recast in a shorter form? For further details of the different categories of contributions, and for general information, see Notes for Authors.
- (i) Does the paper contain any tabular, illustrative or other lengthy matter which is, while worth preserving, likely to be of interest only to a very few readers? The IUCr has a Supplementary Publication Scheme which provides for the preservation and future availability of such material.
- (j) Is the language usage satisfactory? Suggestions for minor corrections may be made when returning your review report. Obscure passages, if any, should be identified for the author to improve.

#### Journal of Applied Crystallography - referee's report form

##### 1. Is the manuscript worthy of publication?

- Yes, as it is
- Yes, with minor revision
- Yes, but with major revision
- No, not at all

##### 2. Is the work technically sound?

- Does the evidence presented justify the conclusions drawn?
- If not, please specify.

##### 3. Is the presentation as efficient as possible?

- Can any material be omitted or deposited?

Please specify.

4. Is the choice of journal correct?
5. Have the requirements of Notes for Authors been met?
6. Is the Literature adequately cited?
7. Revisions to be made by the author:

## APPENDIX D

### Abstracts of Open Commission presentations

#### Overview of IUCr Journals

John R. Helliwell\*, Peter R. Strickland, School of Chemistry, The University of Manchester, M13 9PL, UK, CCLRC, Daresbury Laboratory, Warrington WA4 4AD, UK, and IUCr Journals, 5 Abbey Square, Chester CH1 2HU, UK. E-mail: [john.helliwell@manchester.ac.uk](mailto:john.helliwell@manchester.ac.uk)

Comparing the year ends of the last three triennia, 11728 journal pages were published in 2004, compared with 9215 in 2001 and 7937 in 1998. This increase in the number of pages has been accompanied by a major reduction in publication times for all sections of Acta Cryst., J. Appl. Cryst. and J. Synchrotron Rad. In the most recent triennium, an electronic submission system was introduced and has been very popular with Co-editors and authors. The journals continued to be the most cited in crystallography; Acta Cryst. B currently has the highest impact factor (3.643). The overall withdrawal plus rejection rate for Acta Cryst. was 26% in 2004, up compared with 2002 (18%). For Acta Cryst. A, special issues based on workshop "hot topics" have been introduced, similar to the strategy in recent years for J. Synchrotron Rad. An open-access option was introduced for authors in 2004; grants have allowed all UK papers to be published open access in 2004/2005. Acta Cryst. E has been very successful in attracting ever increasing numbers of electronic structure reports. Acta Cryst. C is increasingly the home of the most important and high-quality crystal structure communications; its impact factor rising from 0.571 in 2001 to 0.828 in 2003. In 2004 we launched Acta Cryst. F: Structural Biology and Crystallization Communications (Editors H. Einspahr and M. Guss); extensive work with the PDB has been made by H. Einspahr on the streamlining of deposition-to-publication methodologies. Finally, a review is currently being made of Education papers within IUCr Journals.

#### Acta Crystallographica Section A: Foundations of Crystallography

Dieter Schwarzenbach\*, Lab. de cristallographie, EPFL, BSP, CH-1015 Lausanne, Switzerland. E-mail: [dieter.schwarzenbach@epfl.ch](mailto:dieter.schwarzenbach@epfl.ch)

In the triennium 2002-2004, Section A has published 18 bimonthly issues comprising 2585 pages, including the abstracts of the IUCr Geneva congress and the ECM22 meeting. The number of published research papers and short communications+letters was 201 and 27, respectively, comprising 1648 pages. These numbers are roughly on the level of the 18 regular issues of the period 1999-2001. From year to year, there are notable fluctuations but the average level is stable. Rejection and withdrawal rates fluctuate around 33%. The geographical origin of the articles, summed as integral and half-integral numbers, is over 50% Europe, about 25% the Americas and under 25% Asia+Australia. The subject matters may be grouped into ad-hoc categories with comparable number of papers: (1) geometry, twinning; (2) algorithms, ab initio calculations, experimental set-ups; (3) diffraction theory, imaging methods, diffuse scattering; (4) structure determination, electron crystallography; (5) electron densities. A highlight was the special issue on "New information from modern charge density methods" which appeared as the September 2004 issue under the responsibility of F. K. Larsen, and comprises 21 articles presented at the ECDM-III meeting in Denmark. Section A covers a broad interdisciplinary spectrum of the exact sciences. It is the leading journal for work in Foundations of Crystallography, with impact factors fluctuating between 1.42 and 1.75 over the past 5 years (latest value 1.558). Two special issues and three Lead articles/Topical reviews are presently planned. Thanks are due to authorship, referees, co-editors and IUCr staff for their high-quality work.

#### Acta Crystallographica Section B: Structural Science

Carolyn P. Brock, Department of Chemistry, University of Kentucky, Lexington KY, 40506-0055, USA. E-mail: [cpbrock@uky.edu](mailto:cpbrock@uky.edu)

During the triennium 2002-2004 Section B of Acta Crystallographica published 2672 pages that included 280 full Research Papers, 27 Short Communications, and one Topical Review. In 2002 a special issue on Crystallographic Databases was published jointly with Section D of Acta (13 articles from Section B). The ratio of papers in Section B that discussed inorganic and molecular compounds was about 35:65 during the triennium, but the ratio varies from year to year. A very positive development is the continuing increase of the impact factor from 1.73 for 2000 to 3.64 for 2003 (announced in 2004). This increase has brought Section B greater visibility and very favorable publicity. The heavily cited 2002 special issue on databases was an important factor in the rise of the impact factor. Challenges to the competitive position of Section B have been identified. Section B must now compete for papers with the new journals CrystEngComm (started in 1999 by the Royal Society of Chemistry in Great Britain) and Crystal Growth & Design (started in 2001 by the American Chemical Society). Technical changes during the triennium include an almost fully automated electronic submission and processing system that has lowered the time from submission to publication from

7.2 mo in 2001 to 4.8 mo in 2004. Color figures have become so common that the journal pages look quite different than they were three years ago.

### **Acta Crystallographica Section C: Crystal Structure Communications**

G. Ferguson, School of Chemistry, University of St. Andrews, St. Andrews, Fife, KY16 9ST Scotland and Chemistry Department, University of Guelph, Guelph, Ontario, Canada N1G 2W1. E-mail: [✉actac@uoguelph.ca](mailto:actac@uoguelph.ca)

Acta Crystallographica Section C continues to specialize in the rapid publication of high-quality studies of novel and challenging crystal and molecular structures. In 2003 Section C published 478 papers (49 inorganic, 186 metal-organic and 243 organic) in a total of 1482 pages. In 2004, Section C published 554 papers (42 inorganic, 227 metal-organic, 285 organic) in a total of 1686 pages. Publication times continue their downward trend, while the citation impact has risen from 0.571 in 2001, to 0.659 in 2002 and 0.828 in 2003. There has been a significant increase in the number of submissions to Section C in the last triennium and this has resulted in a major increase in editorial workload. Some 39% of original technically correct submissions to Section C in 2003 were subsequently withdrawn or rejected; this withdrawal/rejection rate climbed to 48% in 2004. The principal reasons for this significant increase in the withdrawal/rejection rate were either that the text in the Comment section of the CIF was deemed not to provide the "significant added value to the numerical data freely available in the CIF", or (increasingly) that the text in the Comment section was very poorly crafted and difficult to understand. Changes made to the 2005 Notes for authors to improve the quality of initial submissions will be described. Keywords: IUCr journals, Acta Crystallographica C

### **Acta Crystallographica Section D: Biological Crystallography, 2002-2004**

E. N. Baker, Z. Dauter, School of Biological Sciences, University of Auckland, Auckland, New Zealand and Biosciences Division, Argonne National Laboratory, Argonne IL60439, USA.

Acta D was established as a journal dedicated to the expanding field of biological crystallography. The last triennium has seen the celebration of 10 years' publication, the retirement of the founding Editor, Jenny Glusker, to whom great thanks are due, and the appointment of Ted Baker and Zbyszek Dauter as new joint Editors. The journal has grown steadily, from 2243 pages in 2002 to 2406 in 2004. Average publication times have decreased from 5.2 to 4.3 months, but the impact factor has remained at around 2. Reflecting the current surge in methods development, Acta D has published many important methodological papers in the past 3 years, both in regular issues and in the special issues dedicated to the standout CCP4 study weekend series. The number of structural papers has remained steady at about 10 per issue, but the number of crystallization papers has increased to the point where they constitute 60% of papers in the journal. From 2005, however, these will be published in the all-electronic sister journal Acta F. Acta D will then focus on crystallographic methods and new protein structures, aiming to attract more high profile structural papers, and will seek to increase the number of topical reviews and commentaries.

### **Structure Reports Online(Acta E): rapid growth 2001-2004**

William Clegg\*, David G. Watson, School of Natural Sciences (Chemistry), University of Newcastle upon Tyne NE1 7RU, UK and Cambridge Crystallographic Data Centre, Cambridge CB2 1EZ, UK. E-mail: [✉w.clegg@ncl.ac.uk](mailto:w.clegg@ncl.ac.uk) and [✉watson@ccdc.cam.ac.uk](mailto:watson@ccdc.cam.ac.uk)

Acta Crystallographica Section E: Structure Reports Online was launched in 2001 as the first purely electronic journal of the IUCr. Its purpose is the rapid publication of individual results of crystal structure determination, with an emphasis on brevity, high technical quality, and high speed. Between its launch and the end of 2004, the journal has grown steadily and massively. In terms of both papers and pages, the 2004 journal is more than double the size of that in 2001. Over the same period, the average publication time has been slightly reduced from 1 month to 0.8 months. Each year a substantial number of new Co-editors have been appointed, reaching over 30 by the end of 2004. Procedures for submission and handling of papers have been refined and substantial further improvements are currently underway. Authors are provided with a number of tools to aid them in the preparation and checking of manuscripts; they have the opportunity of incorporating a wide range of full-colour graphics and supplementary material; communication with editorial staff, proof-reading, and the provision of free reprints are all carried out electronically, through web interfaces and e-mail. The journal has proved very popular and is an excellent medium for the publication of individual crystal structures for which detailed discussion is not required, complementing Section C with its requirement for significant discussion of results and its acceptance of multiple-structure papers.

### **Acta Crystallographica Section F, launch year report**

H. M. Einspahr, J. M. Guss, Lawrenceville, New Jersey, USA and University of Sydney, Australia.

The new all-electronic Section F of Acta Crystallographica was launched in January 2005. This new journal aims to

provide a home for short communications on the crystallization and structure of biological macromolecules. Structures determined through structural genomics initiatives or from iterative studies such as those used in the pharmaceutical industry are particularly welcome. A panel of distinguished Co-editors will ensure that the high scientific and production standards of Acta Crystallographica are maintained. An entirely new feature of Section F will be the close coordination of data submission to the Protein Data Bank and preparation of mandatory items for inclusion in short structural papers. The preferred mode of data transfer from the database to the journal will be in the form of an mmCIF file. This will enable the generation of tables for publication and validation data for referees. One of the section editors has been working closely with staff of the PDB and the IUCr offices in Chester to define the new mmCIF terms required for a complete description of a structure determination. Parallel efforts are being made to improve the communication between Co-editors, referees and authors.

### **Journal of Applied Crystallography**

Gernot Kostorz, ETH Zürich, Applied Physics, 8093 Zürich, Switzerland. E-mail: ✉ [kostorz@iap.phys.ethz.ch](mailto:kostorz@iap.phys.ethz.ch)

In its thirty-seventh year, the Journal of Applied Crystallography continues to serve a broad readership by providing an international forum for the coverage of all topics related to the development and application of crystallographic methods all across the basic and applied natural sciences. The main subject areas and major developments during the last three years will be reviewed, and the strength and potential for future improvements of the journal will be assessed. There will be ample time for the discussion of points raised at the session.

### **Journal of Synchrotron Radiation: Current status and issues**

Dennis M. Mills, Åke Kvick, Toshiaki Ohta, Advanced Photon Source, Argonne National Laboratory, Argonne, IL, USA, European Synchrotron Radiation Facility, Grenoble CEDEX, France, and University of Tokyo, Tokyo, Japan.

The Journal of Synchrotron Radiation (JSR) continues to provide the synchrotron radiation research community a venue for publication of important research and instrumentation/technique development. For the calendar years 2002, 2003, and 2004 the overall number of articles published was 320, comprising 1400 pages. Based on discussions from the last editors meeting (due in part to the adverse effect of conference proceedings in the calculation of the journal impact factor), major conference proceedings are no longer sought after by the journal. Rather, the main editors believe that special issues focused on a particular topic (often the highlights of a larger conference) provide the synchrotron radiation community with high quality summaries of important developments in the field. In the last three years five Special Issues of the journal were published. We see this as a growth area as we already have commitments for 5 Special Issues in 2005. In 2004 Facility Information pages, one page per issue is devoted to each of the three third-generation hard X-ray sources (APS, ESRF, and Spring-8), were initiated. These pages provide an opportunity for these facilities to communicate important news and updates to the international community of synchrotron radiation users. The content of these pages, along with expansion of information pages to other facilities will be discussed.

### **Getting the best out of IUCr journals (practical advice and demonstrations)**

Peter Strickland, Gillian Holmes, Louise Jones, Brian McMahon, IUCr Journals, 5 Abbey Square, Chester CH1 2HU, UK. E-mail: ✉ [ps@iucr.org](mailto:ps@iucr.org)

This second Commission on Journals session concentrates on providing all those who use IUCr Journals, including authors, reviewers, editors and readers, with practical advice on how to get the best out of the journals. So, if you ever wondered what happens to your article during the submission, review and production stages, want to know more about current publication and editorial procedures, or wish to discover quick ways of accessing and searching the journals, then you should attend this session. Various live demonstrations of the work of the IUCr Editorial Office will be included, with opportunities to ask questions throughout the session. The topics will include: (a) article submission tips; (b) figure and scheme preparation for publication - figure resolution, use of colour, accurate colour reproduction; (c) using the submission and review system; (d) using checkCIF; (e) demonstration of tools for editing and viewing CIFs, and advice on preparing CIFs for publication; (f) demonstration of editorial systems and production processes; (g) article viewing and navigation; (h) searching Crystallography Journals Online; (i) linking - description of the creation of links to bibliographic and structural databases; (j) article distribution - e-mail alerting, metadata delivery to third parties, search engines and databases, RSS feeds; (k) tracking your paper; (l) future developments.

# **Acta A agenda**

## **Grand Hotel Panoramic, Montecatini Terme, Italy**

22 August, 13:45-14:55 (Editors are encouraged to join a meeting for another journal after this meeting)

### **CHAIR: Dieter Schwarzenbach**

Attendees: Acta A Editors and Co-editors, and any other interested Editors

IUCr staff attending: Sue Barnes

## **1. GENERAL**

This item is intended cover general matters and to give the Editor or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

## **2. JOURNAL DEVELOPMENT**

### 2.1. Scientific development

Are there any new related scientific areas that are developing that the journal should cover?

If yes, should an appointment be made to the Board to cover this area?

Would a special issue on such developments be worthwhile?

Are there other areas on which special issues should be commissioned?

Does the expertise on the Board cover the aims and scope of the journal well, or are new appointments needed?

### 2.2. Submissions

How can we encourage more submissions to Section A?

Are there any ideas on how an increase in submissions might be achieved?

What sort of papers should we be trying to attract and how can we encourage their submission?

### 2.3. Impact factor

Is there any way that the journal impact factor can be increased?

Are there particular categories of paper that should be encouraged/discouraged?

Are there particular topics that are more highly cited?

Are there particular authors that should be encouraged to write for the journal?

### 2.4. Lead articles/topical reviews

What topics should be considered?

Who are potential candidate authors?

### 2.5. Publication speed

Are there any ways in which we can increase publication speed or otherwise improve services to authors?

## **3. SUBMISSION AND REVIEW**

Are the status pages useful?

What new submission system features would be useful for Co-editors?

How can the Notes for referees be improved?

How can the review form be improved before it is implemented online?

Are there any measures that would improve the consistency of the review process?

Are the documentation and help pages for authors, editors and referees clear?

Should Section A continue to allow hard-copy submission?

Above what number of authors would it be reasonable to ask for the roles of the authors?

## **4. JOURNAL PROMOTION AND SPONSORSHIP**

### 4.1. Promoting the journal using a marketing leaflet

The Journals Working Group would like comments on the leaflet promoting Section A. A specific question they have is: do the references in the leaflet need to be updated?

### 4.2. In what other ways can Section A be promoted?

### 4.3. How can advertising/sponsorship revenues be increased?

## **5. JOURNAL DESIGN**

### **5.1. PRINT:**

Is the present design of the journal satisfactory?

Are there any items (e.g. mathematical appendices) that can be removed from the print version of the journal?

### **5.2. ONLINE:**

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

## **6. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors.

## **7. USE OF COLOUR**

Should the Notes for Authors be made stricter on the use of colour?

Should the Notes for Reviewers be modified to emphasize restrictions in the use of colour to reviewers?

Should Main and Section Editors review all colour at the proof stage?

Should colour only be allowed online?

If so, can the caption in the printed journal refer to colour?

Should the journal charge for colour?

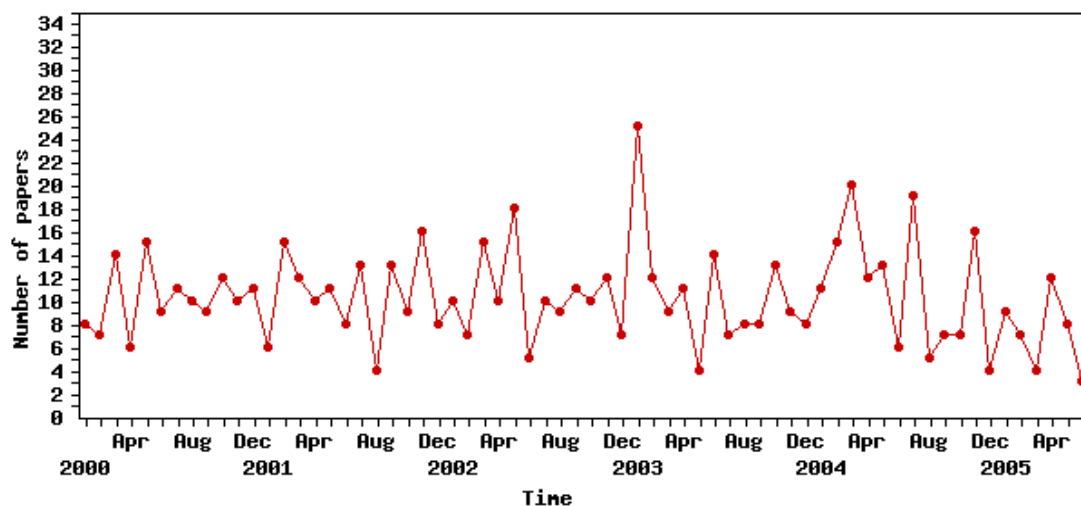
## **8. MATTERS ARISING FROM THE GENERAL AGENDA**

## APPENDIX - Background information on Section A

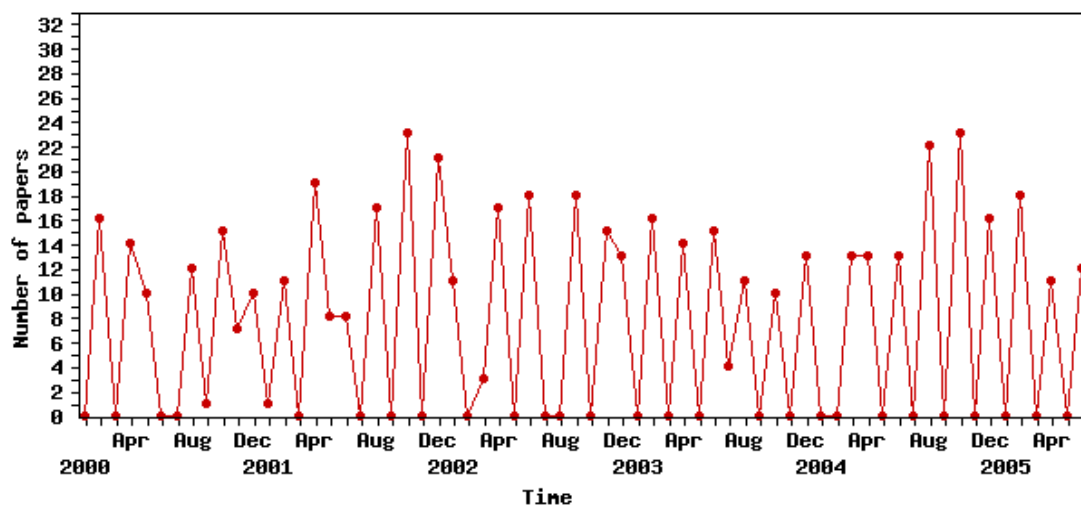
### Aims and scope

Acta Crystallographica Section A: Foundations of Crystallography publishes papers reporting fundamental advances in all areas of crystallography in the broadest sense. The central themes are, on the one hand, experimental and theoretical studies of the properties and arrangements of atoms, ions and molecules in condensed matter, ideal or real, and of their symmetry and, on the other, the theoretical and experimental aspects of the various methods to determine these arrangements.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Acta Crystallographica Section A

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1744  |
| Institutional subscribers | 657   |
| Individual subscribers    | 74    |
| Impact Factor (2004)      | 1.829 |
| Ranking (2004)            | 6/24  |

### Acta Crystallographica Section A - competing journals based on citing

Number of times articles published in 2003 (in journals below) cited articles published in *Acta Crystallographica Section A*

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 9521    | 42   | 122  | 132  | 145  |                      |
| ACTA CRYSTALLOGR E | 840     | 0    | 1    | 0    | 0    | 0.453                |
| ACTA CRYSTALLOGR D | 402     | 2    | 8    | 7    | 8    | 2.208                |
| ACTA CRYSTALLOGR A | 332     | 14   | 33   | 29   | 22   | 1.558                |
| ACTA CRYSTALLOGR C | 308     | 0    | 0    | 0    | 0    | 0.828                |
| J BIOL CHEM        | 292     | 0    | 0    | 0    | 0    | 6.482                |
| Z KRISTALLOGR      | 287     | 2    | 15   | 9    | 15   | 1.266                |
| J MOL BIOL         | 251     | 0    | 0    | 0    | 0    | 5.239                |
| INORG CHEM         | 221     | 0    | 1    | 1    | 1    | 3.389                |
| J APPL CRYSTALLOGR | 196     | 1    | 9    | 5    | 9    | 2.324                |

### Acta Crystallographica Section A - list of cited journals

Number of times articles published in journals below (in years below) were cited in *Acta Crystallographica Section A* in 2003

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 1618    | 60   | 115  | 108  | 92   |                      |
| ACTA CRYSTALLOGR A | 332     | 14   | 33   | 29   | 22   | 1.558                |
| Z KRISTALLOGR      | 71      | 0    | 5    | 1    | 6    | 1.266                |
| ACTA CRYSTALLOGR D | 69      | 5    | 15   | 6    | 8    | 2.208                |
| J APPL CRYSTALLOGR | 66      | 3    | 7    | 3    | 5    | 2.324                |
| PHYS REV B         | 59      | 0    | 0    | 5    | 3    | 2.962                |
| ACTA CRYSTALLOGR   | 57      | 0    | 0    | 0    | 0    |                      |
| ACTA CRYSTALLOGR B | 48      | 0    | 2    | 1    | 3    | 3.643                |
| PHYS REV LETT      | 37      | 0    | 2    | 6    | 3    | 7.035                |
| NATURE             | 35      | 1    | 1    | 0    | 2    | 30.979               |

### Acta Crystallographica Section A - citation report by issue

| 2001  |      |                                  |                        |                         | 2002  |      |                                  |                        |                         | 2003  |      |                                  |                        |                         |
|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|
| Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 17                               | 2.8                    | 0                       | 1     | 0    | 16                               | 1.8                    | 0                       | 1     | 0    | 11                               | 3.0                    | 0                       |
| 2     | 0    | 11                               | 2.7                    | 0                       | 2     | 0    | 14                               | 3.3                    | 0                       | 2     | 0    | 14                               | 2.8                    | 0                       |
| 3     | 0    | 16                               | 3.1                    | 0                       | 3     | 0    | 13                               | 1.6                    | 0                       | 3     | 0    | 14                               | 2.6                    | 0                       |
| 4     | 0    | 14                               | 4.1                    | 0                       | 4     | 0    | 14                               | 1.7                    | 0                       | 4     | 0    | 11                               | 3.0                    | 0                       |
| 5     | 0    | 16                               | 3.4                    | 0                       | 5     | 0    | 16                               | 1.4                    | 0                       | 5     | 0    | 8                                | 2.5                    | 0                       |
| 6     | 0    | 17                               | 2.3                    | 0                       | 6     | 0    | 14                               | 1.4                    | 0                       | 6     | 0    | 8                                | 2.2                    | 0                       |
|       |      |                                  |                        |                         | s1    | 0    | 0                                | 0                      | 0                       |       |      |                                  |                        |                         |

## Acta Crystallographica Section A - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| research papers                        | 75              | 75                              | 0                           | 3.4                    | 65              | 65                              | 0                           | 2.2                    | 58              | 58                              | 0                           | 3.0                    |
| short communications                   | 12              | 12                              | 0                           | 1.6                    | 11              | 11                              | 0                           | 1.7                    | 6               | 6                               | 0                           | 0.8                    |
| lead articles                          | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| topical reviews                        | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| letters to the editor                  | 0               | 0                               | 0                           | 0.0                    | 3               | 2                               | 1                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| addenda and errata                     | 2               | 2                               | 0                           | 0.5                    | 6               | 6                               | 0                           | 0.2                    | 2               | 2                               | 0                           | 0.0                    |
| book reviews                           | 3               | 0                               | 3                           | 0.0                    | 8               | 0                               | 8                           | 0.0                    | 5               | 0                               | 5                           | 0.0                    |
| books received                         | 3               | 0                               | 3                           | 0.0                    | 3               | 0                               | 3                           | 0.0                    | 3               | 0                               | 3                           | 0.0                    |
| editorial                              | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue preface                          | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| international union of crystallography | 3               | 0                               | 3                           | 0.0                    | 4               | 0                               | 4                           | 0.0                    | 5               | 0                               | 5                           | 0.0                    |
| meeting reports                        | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| notes and news                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| new commercial products                | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| obituaries                             | 2               | 2                               | 0                           | 0.0                    | 3               | 3                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 1487            | 0                               | 1487                        | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Acta Crystallographica Section A - 2001 |      |            |                 |              |                             |  |  |
|---|------|------------|-----------------|--------------|-----------------------------|--|--|
| Issue                                   | Part | First page | Paper category  | ISI citation | Total IUCr citation to date | Authors  | Title  |
| 5                                       | 0    | 576        | research papers | 18           | 1                           | <b>Takakura, H.</b> , Yamamoto, A., Tsai, A.P.                         | The structure of a decagonal <a href="#">Al<sub>72</sub>Ni<sub>20</sub>Co<sub>8</sub></a> quasicrystal   |
| 6                                       | 0    | 663        | research papers | 12           | 2                           | <b>Kirfel, A.</b> , Krane, H.-G., Blaha, P., Schwarz, K., Lippmann, T. | Electron-density distribution in stishovite, <a href="#">SiO<sub>2</sub></a> : a new high-energy synchrotron-radiation study                                 |
| 3                                       | 0    | 272        | research papers | 10           | 7                           | Volkov, A., Abramov, Y.A., <b>Coppens, P.</b>                          | Density-optimized radial exponents for X-ray charge-density refinement from ab initio crystal calculations   |
| 1                                       | 0    | 40         | research papers | 10           | 11                          | <b>Giacovazzo, C.</b> , Siliqi, D.                                     | The method of joint probability distribution functions applied to the one-wavelength anomalous-scattering (OAS) case   |
| 2                                       | 0    | 176        | research papers | 9            | 6                           | <b>Sowa, H.</b>  | On the transition from the wurtzite to the <a href="#">NaCl</a> type   |
| 4                                       | 0    | 395        | research papers | 9            | 6                           | Volkov, A., <b>Coppens, P.</b>   | Critical examination of the radial functions in the Hansen-Coppens multipole model through topological analysis of primary and refined theoretical densities |
| 3                                       | 0    | 333        | research papers | 8            | 4                           | <b>Steurer, W.</b> , Cervellino, A.                                    | Quasiperiodicity in decagonal phases forced by inclined net planes?  |

| 6  | 0    | 700        | research papers      | 8            | 7                           | <b>Giacovazzo, C.</b> , Siliqi, D.  | The method of joint probability distribution functions applied to MAD techniques. The two-wavelength case for acentric crystals |
|--|------|------------|----------------------|--------------|-----------------------------|---|---|
| 1  | 0    | 76         | research papers      | 7            | 6                           | <b>Jayatilaka, D.</b> , Grimwood, D.J.  | Wavefunctions derived from experiment. I. Motivation and theory   |
| 1  | 0    | 87         | research papers      | 7            | 5                           | <b>Grimwood, D.J.</b> , Jayatilaka, D.  | Wavefunctions derived from experiment. II. A wavefunction for oxalic acid dihydrate   |
| 4  | 0    | 378        | research papers      | 7            | 7                           | <b>Janner, A.</b>   | Introduction to a general crystallography   |
| 4  | 0    | 389        | research papers      | 7            | 9                           | <b>Thorkildsen, G.</b> , Larsen, H.B., Weckert, E.  | Approximate solution of the Takagi-Taupin equations for a semi-infinite crystal in the three-beam Laue-Laue case                |
| 5  | 0    | 604        | research papers      | 6            | 7                           | <b>Scardi, P.</b> , Leoni, M.   | Diffraction line profiles from polydisperse crystalline systems   |
| 2  | 0    | 163        | research papers      | 6            | 1                           | Shneerson, V.L., Wild, D.L., <b>Saldin, D.K.</b>  | An exponential modeling algorithm for protein structure completion by X-ray crystallography                                     |
| 3  | 0    | 359        | research papers      | 6            | 5                           | <b>Stetsko, Yu.P.</b> , Juretschke, H.J., Huang, Y.-S., Lee, Y.-R., Lin, T.-C., Chang, S.-L.  | Polarization-resolved output analysis of X-ray multiple-wave interaction  |
| 4  | 0    | 369        | research papers      | 6            | 3                           | <b>Gertsman, V.Y.</b>   | Geometrical theory of triple junctions of CSL boundaries  |
| 1  | 0    | 112        | short communications | 6            | 6                           | <b>Voytekhovsky, Y.L.</b>   | On the symmetry of 4- to 11-hedra   |
| <b>Acta Crystallographica Section A - 2002</b> |      |            |                      |              |                             |   |   |
| Issue  | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors   | Title   |
| 2  | 0    | 133        | research papers      | 21           | 6                           | Kim, C.D., Pillet, S., Wu, G., Fullagar, W.K., <b>Coppens, P.</b>   | Excited-state structure by time-resolved X-ray diffraction  |
| 2  | 0    | 190        | research papers      | 10           | 6                           | <b>Scardi, P.</b> , Leoni, M.   | Whole powder pattern modelling  |
| 2  | 0    | 180        | research papers      | 5            | 3                           | Cervellino, A., <b>Steurer, W.</b>  | General periodic average structures of decagonal quasicrystals  |
| 1  | 0    | 33         | research papers      | 5            | 5                           | Chao, C.-H., Hung, C.-Y., Huang, Y.-S., Ching, C.-H., Lee, Y.-R., Jean, Y.-C., Lai, S.-C., Stetsko, Y.P., Yuan, H., <b>Chang, S.-L.</b> | Multiple diffraction data analysis for macromolecular crystals in stereoscopic multibeam imaging                                |
| 4  | 0    | 346        | research papers      | 5            | 1                           | <b>Wooten, F.</b>   | Structure, odd lines and topological entropy of disorder of amorphous silicon   |
| 1  | 0    | 4          | research papers      | 4            | 2                           | <b>Jiang, B.</b> , Zuo, J.M., Chen, Q., Spence, J.C.H.  | Orbital ordering in <a href="#">LaMnO<sub>3</sub></a> : estimates of structure factors and comparison of measurement methods    |
| 1  | 0    | 72         | short communications | 4            | 5                           | Fokine, A., <b>Urzhumtsev, A.</b>   | On the use of low-resolution data for translation search in molecular replacement   |
| 3  | 0    | 232        | research papers      | 4            | 3                           | Bytheway, I., Grimwood, D.J., <b>Jayatilaka, D.</b>   | Wavefunctions derived from experiment. III. Topological analysis of crystal fragments   |
| <b>Acta Crystallographica Section A - 2003</b> |      |            |                      |              |                             |   |   |
| Issue  | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors   | Title   |
| 2  | 0    | 143        | research papers      | 20           | 6                           | He, H., Marchesini, S., Howells, M., Weierstall, U., Hembree, G., <b>Spence, J.C.H.</b>   | Experimental lensless soft-X-ray imaging using iterative algorithms: phasing diffuse scattering                                 |
| 1  | 0    | 22         | research papers      | 18           | 4                           | Delgado Friedrichs, O., <b>O'Keeffe, M.</b> , Yaghi, O.M.   | Three-periodic nets and tilings: regular and quasiregular nets  |

|   |   |     |                 |    |    |   |  |
|---|---|-----|-----------------|----|----|---|--|
| 4 | 0 | 327 | research papers | 10 | 10 | Olczak, A., Cianci, M., Hao, Q., Rizkallah, P.J., Raftery, J., <b>Helliwell, J.R.</b>                         | S-SWAT (softer single-wavelength anomalous technique): potential in high-throughput protein crystallography  |
| 5 | 0 | 437 | research papers | 9  | 3  | <b>Lippmann, T.</b> , Blaha, P., Andersen, N.H., Poulsen, H.F., Wolf, T., Schneider, J.R., Schwarz, K.-H.     | Charge-density analysis of <a href="#">YBa2Cu3O6.98</a> . Comparison of theoretical and experimental results   |
| 5 | 0 | 459 | research papers | 9  | 2  | <b>Smaalen, S. van</b> , Palatinus, L., Schneider, M.   | The maximum-entropy method in superspace   |
| 4 | 0 | 317 | research papers | 9  | 7  | <b>Sowa, H.</b> , Koch, E., Fischer, W.   | Hexagonal and trigonal sphere packings. I. Invariant and univariant lattice complexes  |
| 3 | 0 | 228 | research papers | 7  | 4  | <b>Otwinowski, Z.</b> , Borek, D., Majewski, W., Minor, W.  | Multiparametric scaling of diffraction intensities   |
| 2 | 0 | 168 | research papers | 5  | 0  | <b>Xu, F.-F.</b> , Bando, Y.  | Structures of a hollow filamentary conical helix   |
| 1 | 0 | 7   | research papers | 5  | 1  | <b>Sondhauss, P.</b> , Wark, J.S.   | Extension of the time-dependent dynamical diffraction theory to 'optical phonon'-type distortions: application to diffraction from coherent acoustic and optical phonons |
| 4 | 0 | 341 | research papers | 5  | 3  | <b>Jiang, B.</b> , Zuo, J.M., Jiang, N., O'Keeffe, M., Spence, J.C.H.   | Charge density and chemical bonding in rutile, <a href="#">TiO2</a>  |
| 3 | 0 | 201 | research papers | 5  | 3  | <b>Elser, V.</b>  | Solution of the crystallographic phase problem by iterated projections   |
| 6 | 0 | 515 | research papers | 5  | 3  | Delgado Friedrichs, O., <b>O'Keeffe, M.</b> , Yaghi, O.M.   | Three-periodic nets and tilings: semiregular nets  |
| 3 | 0 | 235 | research papers | 4  | 3  | <b>Okitsu, K.</b>   | X-ray Takagi-Taupin dynamical theory generalized to n-beam diffraction cases   |
| 6 | 0 | 560 | research papers | 4  | 4  | Burla, M.C., Carrozzini, B., Caliendo, R., Cascarano, G.L., De Caro, L., <b>Giacovazzo, C.</b> , Polidori, G. | Ab initio protein phasing at 1.4 Å resolution: the new phasing approach of SIR2003-N   |
| 3 | 0 | 255 | research papers | 4  | 1  | <b>Spence, J.C.H.</b> , Wu, J.S., Giacovazzo, C., Carrozzini, B., Cascarano, G.L., Padmore, H.A.              | Solving non-periodic structures using direct methods: phasing diffuse scattering   |
| 4 | 0 | 351 | research papers | 4  | 2  | <b>Delgado Friedrichs, O.</b> , O'Keeffe, M.  | Identification of and symmetry computation for crystal nets  |

## Acta Crystallographica Section A - sales and circulation figures

### Institutional and consortial circulation totals

|                             | 2003 | 2004 |
|-----------------------------|------|------|
| Consortia site access       |      | 1744 |
| 1. Europe                   |      | 882  |
| 2. USA                      |      | 206  |
| 3. Canada                   |      | 32   |
| 4. Aus/NZ                   |      | 83   |
| 5. Japan                    |      | 86   |
| 6. Rest of World            |      | 455  |
| Institutional subscriptions | 688  | 657  |
| Online                      | 37   | 60   |
| Standard                    | 649  | 593  |
| Online Collection           | 2    | 4    |
| Personal subscriptions      | 88   | 74   |

## Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 9          | 16         |
|                               | Standard          | 233        | 212        |
|                               | Online Collection | 2          | 2          |
| <b>1. Europe Total</b>        |                   | <b>244</b> | <b>230</b> |
| 2. North America              | Online            | 16         | 29         |
|                               | Standard          | 209        | 189        |
|                               | Online Collection | 0          | 2          |
| <b>2. North America Total</b> |                   | <b>225</b> | <b>220</b> |
| 3. Aus/NZ                     | Online            | 2          | 2          |
|                               | Standard          | 15         | 14         |
| <b>3. Aus/NZ Total</b>        |                   | <b>17</b>  | <b>16</b>  |
| 4. Japan                      | Online            | 7          | 10         |
|                               | Standard          | 101        | 90         |
| <b>4. Japan Total</b>         |                   | <b>108</b> | <b>100</b> |
| 5. Rest of World              | Online            | 3          | 3          |
|                               | Standard          | 91         | 88         |
|                               | Online Collection | 0          | 0          |
| <b>5. Rest of World Total</b> |                   | <b>94</b>  | <b>91</b>  |
| <b>Grand Total</b>            |                   | <b>688</b> | <b>657</b> |

# Acta B agenda

## Grand Hotel Panoramic, Montecatini Terme, Italy

22 August, 14:55-16:05 (Editors are encouraged to join the Acta B/C/E meeting before this meeting, and the Acta C/E meeting after this meeting)

### CHAIR: Carol Brock

Attendees: Acta B Editors and Co-editors, and any other interested Editors

IUCr staff attending: Jill Bradshaw

### 1. GENERAL

This item is intended cover general matters and to give the Editor or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

#### 1.1. Experimental Table (Table 1)

Crystallographers doing a multi-T study may now refine the structure at many more temperatures than they would have a few years ago. Is each refinement worth a column in Table 1? There have also been papers about toptactic solid-state reactions in which refinements of numerous intermediate mixed crystals were presented. Is each of those refinements worth a column in Table 1? If there are more refinements than can fit in a one-page Table then the other refinements should be described as deposited. All structural data would be equally available in the CIF. The actual number of columns that can be included is a judgement call. If a multi-T study turns up lots of different phases then the phases must all be listed in the printed Table 1, even if more than one page is required. If there is no phase change then five columns (at most) is probably sufficient. In helping authors make this decision please remember that a large Table 1 with lots of similar entries doesn't look very good. Authors can be assured that the supplementary material is now easily available to almost all readers.

### 2. JOURNAL DEVELOPMENT

#### 2.1. Scientific development

Are there any new related scientific areas that are developing that the journal should cover?

If yes, should an appointment be made to the Board to cover this area?

Would a special issue on such developments be worthwhile?

Are there other areas on which special issues should be commissioned?

Does the expertise on the Board cover the aims and scope of the journal well, or are new appointments needed?

#### 2.2. Submissions

How can we encourage more submissions to Section B?

Are there any ideas on how an increase in submissions might be achieved?

What sort of papers should we be trying to attract and how can we encourage their submission?

#### 2.3. Impact factor

Is there any way that the journal impact factor can be increased?

Are there particular categories of paper that should be encouraged/discouraged?

Are there particular topics that are more highly cited?

Are there particular authors that should be encouraged to write for the journal?

#### 2.4. Lead articles/topical reviews

What topics should be considered?

Who are potential candidate authors?

#### 2.5. Publication speed

Are there any ways in which we can increase publication speed or otherwise improve services to authors?

### 3. SUBMISSION AND REVIEW

Are the status pages useful?

What new submission system features would be useful for Co-editors?

How can the Notes for referees be improved?

How can the review form be improved before it is implemented online?

Are there any measures that would improve the consistency of the review process?

Are the documentation and help pages for authors, editors and referees clear?

Should Section B continue to allow hard-copy submission?

Above what number of authors would it be reasonable to ask for the roles of the authors?

Comments (see APPENDIX 2) have also been provided by Chris Glidewell on the Section B submission process from the point of view of an author. Does the submission process require modification based on these comments?

#### **4. JOURNAL PROMOTION AND SPONSORSHIP**

##### 4.1. Promoting the journal using a marketing leaflet

Would a leaflet promoting Section B be appropriate? If so, ideas for the content of the leaflet are welcomed.

##### 4.2. In what other ways can Section B be promoted?

##### 4.3. How can advertising/sponsorship revenues be increased?

#### **5. JOURNAL DESIGN**

##### 5.1. PRINT:

Is the present design of the journal satisfactory?

Are there any items that can be removed from the print version of the journal?

##### 5.2. ONLINE:

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

#### **6. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors.

#### **7. USE OF COLOUR**

Should the Notes for Authors be made stricter on the use of colour?

Should the Notes for Reviewers be modified to emphasize restrictions in the use of colour to reviewers?

Should Main and Section Editors review all colour at the proof stage?

Should colour only be allowed online?

If so, can the caption in the printed journal refer to colour?

Should the journal charge for colour?

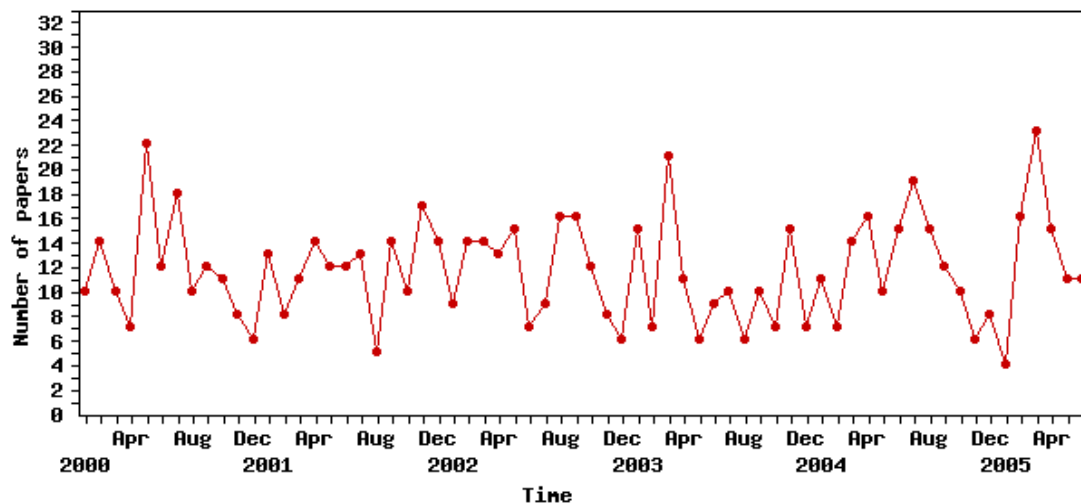
#### **8. MATTERS ARISING FROM THE GENERAL AGENDA**

## APPENDIX 1 - Background information on Section B

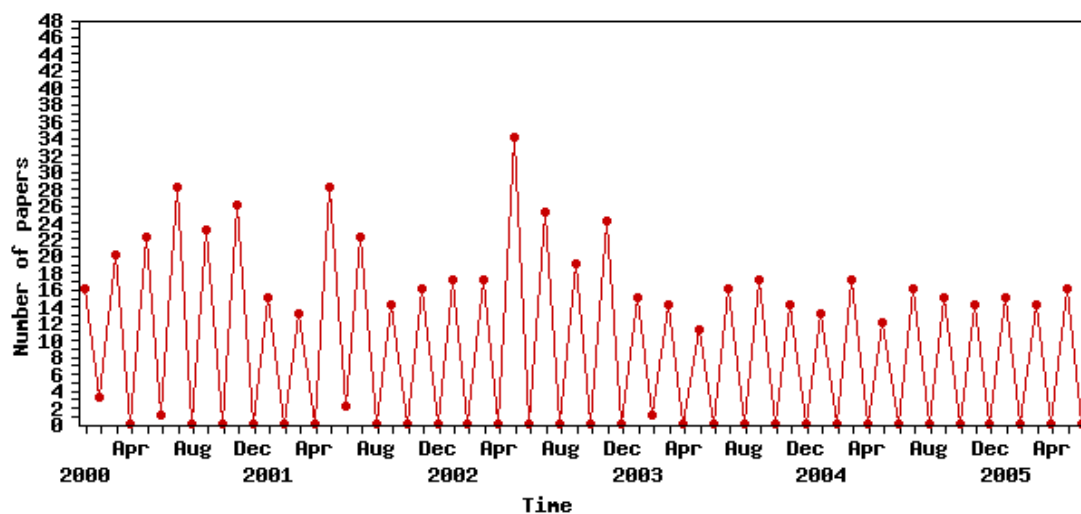
### Aims and scope

Acta Crystallographica Section B: Structural Science publishes papers in which structure is the primary focus of the work reported. The central themes of Structural Science are the acquisition of structural knowledge from novel experimental observations or from existing data, the correlation of structural knowledge with physico-chemical and other properties, and the application of this knowledge to solve problems in the structural domain. Structural Science has broad chemical coverage, encompassing metals and alloys, inorganics and minerals, metal-organics and purely organic compounds.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Acta Crystallographica Section B

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1740  |
| Institutional subscribers | 627   |
| Individual subscribers    | 58    |
| Impact factor (2004)      | 5.418 |
| Ranking                   | 1/24  |

### Acta Crystallographica Section B - competing journals based on citing

Number of times articles published in 2003 (in journals below) cited articles published in *Acta Crystallographica Section B*

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 9372    | 32   | 609  | 196  | 233  |                      |
| ACTA CRYSTALLOGR E | 553     | 1    | 153  | 11   | 12   | 0.453                |
| ACTA CRYSTALLOGR C | 495     | 7    | 149  | 18   | 29   | 0.828                |
| ACTA CRYSTALLOGR B | 326     | 10   | 31   | 21   | 22   | 3.643                |
| INORG CHEM         | 314     | 0    | 7    | 10   | 1    | 3.389                |
| J SOLID STATE CHEM | 284     | 1    | 1    | 5    | 5    | 1.413                |
| J MOL STRUCT       | 228     | 0    | 9    | 11   | 7    | 1.021                |
| PHYS REV B         | 198     | 0    | 4    | 4    | 3    | 2.962                |
| J AM CHEM SOC      | 187     | 0    | 10   | 5    | 4    | 6.516                |
| J PHYS CHEM B      | 183     | 0    | 6    | 2    | 7    | 3.679                |

### Acta Crystallographica Section B - list of cited journals

Number of times articles published in journals below (in years below) were cited in *Acta Crystallographica Section B* in 2003

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 2631    | 68   | 150  | 153  | 166  |                      |
| ACTA CRYSTALLOGR B | 326     | 10   | 31   | 21   | 22   | 3.643                |
| ACTA CRYSTALLOGR A | 140     | 0    | 5    | 7    | 8    | 1.558                |
| J APPL CRYSTALLOGR | 115     | 7    | 3    | 5    | 4    | 2.324                |
| J AM CHEM SOC      | 96      | 0    | 2    | 4    | 4    | 6.516                |
| ACTA CRYSTALLOGR C | 79      | 1    | 13   | 5    | 4    | 0.828                |
| ACTA CRYSTALLOGR   | 70      | 0    | 1    | 0    | 0    |                      |
| J SOLID STATE CHEM | 61      | 1    | 5    | 5    | 10   | 1.413                |
| Z KRISTALLOGR      | 58      | 1    | 3    | 3    | 6    | 1.266                |
| INORG CHEM         | 51      | 1    | 0    | 3    | 4    | 3.389                |

### Acta Crystallographica Section B - citation report by issue

Special issues are shaded.

| 2001  |      |                                  |                        |                         | 2002  |      |                                  |                        |                         | 2003  |      |                                  |                        |                         |
|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|
| Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 13                               | 5.8                    | 0                       | 1     | 0    | 15                               | 4.6                    | 0                       | 1     | 0    | 16                               | 3.9                    | 0                       |
| 2     | 0    | 13                               | 4.4                    | 0                       | 2     | 0    | 17                               | 3.2                    | 0                       | 2     | 0    | 13                               | 2.7                    | 0                       |
| 3     | 0    | 28                               | 4.5                    | 0                       | 3     | 1    | 13                               | 48.5                   | 0                       | 3     | 0    | 11                               | 2.1                    | 0                       |
|       |      |                                  |                        |                         | 3     | 2    | 20                               | 1.7                    | 0                       |       |      |                                  |                        |                         |
| 4     | 0    | 20                               | 4.2                    | 0                       | 4     | 0    | 21                               | 4.0                    | 0                       | 4     | 0    | 14                               | 3.3                    | 0                       |
| 5     | 0    | 13                               | 2.5                    | 0                       | 5     | 0    | 19                               | 2.1                    | 0                       | 5     | 0    | 17                               | 1.8                    | 0                       |
| 6     | 0    | 16                               | 4.2                    | 0                       | 6     | 0    | 21                               | 1.9                    | 0                       | 6     | 0    | 14                               | 1.9                    | 0                       |

## Acta Crystallographica Section B - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| research papers                        | 97              | 97                              | 0                           | 4.2                    | 118             | 118                             | 0                           | 8.0                    | 78              | 78                              | 0                           | 2.7                    |
| short communications                   | 3               | 3                               | 0                           | 5.0                    | 1               | 1                               | 0                           | 1.0                    | 4               | 4                               | 0                           | 1.8                    |
| lead articles                          | 1               | 1                               | 0                           | 6.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| topical reviews                        | 1               | 1                               | 0                           | 18.0                   | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| letters to the editor                  | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| addenda and errata                     | 0               | 0                               | 0                           | 0.0                    | 7               | 7                               | 0                           | 0.3                    | 3               | 3                               | 0                           | 1.0                    |
| book reviews                           | 1               | 0                               | 1                           | 0.0                    | 3               | 0                               | 3                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| books received                         | 5               | 0                               | 5                           | 0.0                    | 5               | 0                               | 5                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| editorial                              | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue preface                          | 0               | 0                               | 0                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| international union of crystallography | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| meeting reports                        | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| notes and news                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| new commercial products                | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| obituaries                             | 1               | 1                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Acta Crystallographica Section B - 2001 |      |            |                      |              |                             |  |  |
|---|------|------------|----------------------|--------------|-----------------------------|--|--|
| Issue                                   | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors  | Title  |
| 1                                       | 0    | 1          | topical reviews      | 18           | 2                           | Rao, C.N.R., Natarajan, S., Choudhury, A., Neeraj, S., Vaidyanathan, R.  | Synthons and design in metal phosphates and oxalates with open architectures   |
| 3                                       | 0    | 435        | research papers      | 17           | 5                           | Wilson, C.C.   | Migration of the proton in the strong O-H...O hydrogen bond in urea-phosphoric acid (1/1)  |
| 6                                       | 0    | 725        | research papers      | 17           | 5                           | Lufaso, M.W., Woodward, P.M.   | Prediction of the crystal structures of perovskites using the software program SPuDS   |
| 1                                       | 0    | 103        | short communications | 15           | 3                           | Steiner, T.  | Competition of hydrogen-bond acceptors for the strong carboxyl donor   |
| 3                                       | 0    | 317        | research papers      | 12           | 13                          | Low, J.N., Moreno Sanchez, J.M., Arranz Mascaros, P., Godino Salido, M.L., Lopez Garzon, R., Cobo Domingo, J., Glidewell, C. | Hydrated metal complexes of N-(6-amino-3,4-dihydro-3-methyl-5-nitroso-4-oxopyrimidin-2-yl) glycinate: interplay of molecular, molecular-electronic and supramolecular structures       |
| 4                                       | 0    | 520        | research papers      | 12           | 11                          | Cai, J., Chen, C.-H., Liao, C.-Z., Feng, X.-L., Chen, X.-M.  | Solid-state structures of group 1 and group 2 metal 1,5-naphthalenedisulfonates: systematic investigation of lamellar three-dimensional networks constructed by metal arenedisulfonate |

|   |   |     |                 |    |    |   |   |
|---|---|-----|-----------------|----|----|---|---|
| 4 | 0 | 591 | research papers | 11 | 10 | <b>Bertolasi, V.</b> , Gilli, P., Ferretti, V., Gilli, G.   | General rules for the packing of hydrogen-bonded crystals as derived from the analysis of squaric acid anions: aminoaromatic nitrogen base co-crystals  |
| 2 | 0 | 201 | research papers | 11 | 11 | <b>Burchell, C.J.</b> , Glidewell, C., Lough, A.J., Ferguson, G.  | Salts of 3,5-dinitrobenzoic acid with organic diamines: hydrogen-bonded supramolecular structures in one, two and three dimensions  |
| 6 | 0 | 800 | research papers | 10 | 9  | <b>Marsh, R.E.</b> , Spek, A.L.   | Use of software to search for higher symmetry: space group C2   |
| 4 | 0 | 531 | research papers | 10 | 4  | <b>Dova, E.</b> , Stassen, A.F., Driessen, R.A.J., Sonneveld, E., Goubitz, K., Peschar, R., Haasnoot, J.G., Reedijk, J., Schenk, H. | Structure determination of the [Fe(teec) <sub>6</sub> ](BF <sub>4</sub> ) <sub>2</sub> metal complex from laboratory and synchrotron X-ray powder diffraction data with grid-search techniques  |
| 3 | 0 | 288 | research papers | 10 | 2  | Yasui, M., Ishikawa, Y., Akiyama, N., Ishida, T., Nogami, T., <b>Iwasaki, F.</b>  | Dipyrimidine-copper(II) dinitrate complexes showing magnetic interactions   |
| 1 | 0 | 95  | research papers | 9  | 2  | Wheatley, P.S., Lough, A.J., Ferguson, G., Burchell, C.J., <b>Glidewell, C.</b>   | Ethane-1,2-diphosphonic acid as a building block in supramolecular chemistry; a pillared-layer framework and framework-encapsulated cations   |
| 1 | 0 | 27  | research papers | 9  | 1  | <b>Lebrun, N.</b> , Mahe, F., Lamiot, J., Foulon, M., Petit, J.C., Prevost, D.  | Kinetic behaviour investigations and crystal structure of nitric acid dihydrate   |
| 4 | 0 | 471 | research papers | 9  | 6  | <b>Elcoro, L.</b> , Perez-Mato, J.M., Withers, R.L.   | Intergrowth polytypoids as modulated structures: a superspace description of the Sr <sub>n</sub> (Nb,Ti) <sub>n</sub> O <sub>3n+2</sub> compound series   |
| 4 | 0 | 491 | research papers | 8  | 1  | Magyari-Kope, B., <b>Vitos, L.</b> , Johansson, B., Kollar, J.  | Parametrization of perovskite structures: an ab initio study  |
| 2 | 0 | 178 | research papers | 8  | 2  | <b>Goubitz, K.</b> , Capkova, P., Melanova, K., Molleman, W., Schenk, H.  | Structure determination of two intercalated compounds VOPO <sub>4</sub> ·(CH <sub>2</sub> ) <sub>4</sub> O and VOPO <sub>4</sub> ·OH·(CH <sub>2</sub> ) <sub>2</sub> -O·(CH <sub>2</sub> ) <sub>2</sub> -OH; synchrotron powder diffraction and molecular modelling |
| 3 | 0 | 359 | research papers | 8  | 2  | Zhurava, E.A., <b>Pinkerton, A.A.</b>   | Chemical bonding in energetic materials: [beta]-NTO   |
| 3 | 0 | 278 | research papers | 8  | 2  | <b>Adams, St.</b>   | Relationship between bond valence and bond softness of alkali halides and chalcogenides   |

#### Acta Crystallographica Section B - 2002

| Issue | Part | First page | Paper category  | ISI citation | Total IUCr citation to date | Authors   | Title   |
|-------|------|------------|-----------------|--------------|-----------------------------|---|---|
| 3     | 1    | 380        | research papers | 496          | 800                         | <b>Allen, F.H.</b>  | The Cambridge Structural Database: a quarter of a million crystal structures and rising   |
| 3     | 1    | 389        | research papers | 73           | 130                         | Bruno, I.J., Cole, J.C., Edgington, P.R., Kessler, M., Macrae, C.F., <b>McCabe, P.</b> , Pearson, J., <b>Taylor, R.</b>   | New software for searching the Cambridge Structural Database and visualizing crystal structures                                     |
| 4     | 0    | 647        | research papers | 31           | 15                          | <b>Motherwell, W.D.S.</b> , Ammon, H.L., Dunitz, J.D., Dzyabchenko, A., Erk, P., Gavezzotti, A., Hofmann, D.W.M., Leusen, F.J.J., Lommerse, J.P.M., Mooij, W.T.M., Price, S.L., Scheraga, H., Schweizer, B., Schmidt, M.U., Eijck, B.P. van, Verwer, P., Williams, D.E. | Crystal structure prediction of small organic molecules: a second blind test  |
| 3     | 1    | 407        | research papers | 24           | 12                          | <b>Allen, F.H.</b> , Motherwell, W.D.S.   | Applications of the Cambridge Structural Database in organic chemistry and crystal chemistry  |
| 2     | 0    | 198        | research papers | 17           | 1                           | <b>Ilyushin, G.D.</b> , Blatov, V.A.  | Crystal chemistry of zirconosilicates and their analogs: topological classification of MT frameworks and suprapolyhedral invariants |
| 1     | 0    | 8          | research papers | 15           | 3                           | Cervellino, A., Haibach, T., <b>Steurer, W.</b>   | Structure solution of the basic decagonal Al-Co-Ni phase by the atomic surfaces modelling method                                    |

|   |   |     |                 |    |    |  |   |
|---|---|-----|-----------------|----|----|--|---|
| 2 | 0 | 300 | research papers | 13 | 15 | Quesada, A., Marchal, A., Melguizo, M., Noguera, M., Sanchez, A., Low, J.N., Cannon, D., Farrell, D.M.M., <b>Glidewell, C.</b> | Amino-substituted O6-benzyl-5-nitrosopyrimidines: interplay of molecular, molecular-electronic and supramolecular structures                        |
| 1 | 0 | 62  | research papers | 12 | 6  | Marsh, R.E., Kapon, M., Hu, S., <b>Herbstein, F.H.</b>   | Some 60 new space-group corrections   |
| 1 | 0 | 94  | research papers | 11 | 16 | Kelly, C.J., Skakle, J.M.S., Wardell, J.L., Wardell, S.M.S.V., Low, J.N., <b>Glidewell, C.</b>                                 | Iodo-nitroarenesulfonamides: interplay of hard and soft hydrogen bonds, I...O interactions and aromatic [bold pi]...[bold pi] stacking interactions |

#### Acta Crystallographica Section B - 2003

| Issue | Part | First page | Paper category  | ISI citation | Total IUCr citation to date | Authors   | Title   |
|-------|------|------------|-----------------|--------------|-----------------------------|---|---|
| 4     | 0    | 463        | research papers | 22           | 3                           | <b>Howard, C.J.</b> , Kennedy, B.J., Woodward, P.M.   | Ordered double perovskites - a group-theoretical analysis   |
| 1     | 0    | 1          | research papers | 13           | 3                           | <b>White, T.J.</b> , Dong, Z.L.   | Structural derivation and crystal chemistry of apatites   |
| 5     | 0    | 634        | research papers | 11           | 7                           | Pidcock, E., <b>Motherwell, W.D.S.</b> , Cole, J.C.   | A database survey of molecular and crystallographic symmetry  |
| 4     | 0    | 512        | research papers | 8            | 0                           | Ouvrard, C., Le Questel, J.-Y., Berthelot, M., <b>Laurence, C.</b>  | Halogen-bond geometry: a crystallographic database investigation of dihalogen complexes   |
| 1     | 0    | 100        | research papers | 8            | 4                           | Bowes, K.F., Ferguson, G., Lough, A.J., <b>Glidewell, C.</b>  | Salts of maleic and fumaric acids with organic polyamines: comparison of isomeric acids as building blocks in supramolecular chemistry  |
| 4     | 0    | 479        | research papers | 7            | 2                           | <b>Marchivie, M.</b> , Guionneau, P., Letard, J.-F., Chasseau, D.   | Towards direct correlations between spin-crossover and structural features in iron(II) complexes  |
| 2     | 0    | 287        | research papers | 7            | 1                           | Giastas, P., Yannakopoulou, K., <b>Mavridis, I.M.</b>   | Molecular structures of the inclusion complexes [beta]-cyclodextrin-1,2-bis(4-aminophenyl)ethane and [beta]-cyclodextrin-4,4'-diaminobiphenyl; packing of dimeric [beta]-cyclodextrin inclusion complexes |
| 6     | 0    | 687        | research papers | 6            | 0                           | Aubert, E., Porcher, F., Souhassou, M., <b>Lecomte, C.</b>  | Characterization of intra-framework and guest/host interactions in the AlPO4-15 molecular sieve by charge-density analysis  |
| 6     | 0    | 794        | research papers | 6            | 0                           | <b>Cowan, J.A.</b> , Howard, J.A.K., <b>McIntyre, G.J.</b> , Lo, S.M.-F., Williams, I.D.  | Variable-temperature neutron diffraction studies of the short, strong N...O hydrogen bonds in the 1:2 co-crystal of benzene-1,2,4,5-tetracarboxylic acid and 4,4'-bipyridyl                               |
| 1     | 0    | 87         | research papers | 6            | 4                           | Bowes, K.F., Ferguson, G., Lough, A.J., Zakaria, C.M., <b>Glidewell, C.</b>   | Phosphonoacetic acid as a building block in supramolecular chemistry: salts with organic polyamines   |
| 3     | 0    | 393        | research papers | 6            | 0                           | <b>Hoshino, A.</b> , Takenaka, Y., Miyaji, H.   | Redetermination of the crystal structure of [alpha]-copper phthalocyanine grown on KCl  |
| 1     | 0    | 43         | research papers | 6            | 1                           | Clemente, D.A., <b>Marzotto, A.</b>   | 22 Space-group changes  |
| 5     | 0    | 670        | research papers | 6            | 3                           | <b>Turowska-Tyrk, I.</b>  | Monitoring structural transformations in crystals. 5.Part 4: Turowska-Tyrk et al. (2003). A topotactic [2 + 2]-photodimerization reaction   |
| 2     | 0    | 209        | research papers | 5            | 0                           | <b>Hoche, T.</b> , Esmailzadeh, S., Uecker, R., Lidin, S., Neumann, W.  | (3 + 1)-Dimensional structure refinement of the fresnoite framework-structure type compound <a href="#">Ba2TiGe2O8</a>  |
| 1     | 0    | 132        | research papers | 5            | 5                           | Sorensen, H.O., <b>Larsen, S.</b>   | Hydrogen bonding in enantiomeric versus racemic mono-carboxylic acids; a case study of 2-phenoxypropionic acid  |
| 1     | 0    | 28         | research papers | 5            | 0                           | <b>Woike, T.</b> , Petricek, V., Dusek, M., Hansen, N.K., Fertey, P., Lecomte, C., Arakcheeva, A., Chapuis, G., Imlau, M., Pankrath, R. | The modulated structure of Ba0.39Sr0.61Nb2O6. I. Harmonic solution  |

|   |   |     |                 |   |   |                   |   |
|---|---|-----|-----------------|---|---|-------------------|---|
| 1 | 0 | 149 | research papers | 5 | 2 | Ohba, S., Ito, Y. | Single-crystal-to-single-crystal photodimerization of 4-chlorocinnamoyl-O,O'-dimethyldopamine |
|---|---|-----|-----------------|---|---|-------------------|---|

## Acta Crystallographica Section B - sales and circulation figures

### Institutional and consortial circulation totals

|                             | 2003 | 2004 |
|-----------------------------|------|------|
| Consortia site access       |      | 1740 |
| 1. Europe                   |      | 882  |
| 2. USA                      |      | 202  |
| 3. Canada                   |      | 32   |
| 4. Aus/NZ                   |      | 83   |
| 5. Japan                    |      | 86   |
| 6. Rest of World            |      | 455  |
| Institutional subscriptions | 663  | 627  |
| Online                      | 35   | 52   |
| Standard                    | 626  | 571  |
| Online Collection           | 2    | 4    |
| Personal subscriptions      | 67   | 58   |

### Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 10         | 15         |
|                               | Standard          | 232        | 214        |
|                               | Online Collection | 2          | 2          |
| <b>1. Europe Total</b>        |                   | <b>244</b> | <b>231</b> |
| 2. North America              | Online            | 16         | 24         |
|                               | Standard          | 213        | 190        |
|                               | Online Collection | 0          | 2          |
| <b>2. North America Total</b> |                   | <b>229</b> | <b>216</b> |
| 3. Aus/NZ                     | Online            | 2          | 2          |
|                               | Standard          | 14         | 13         |
| <b>3. Aus/NZ Total</b>        |                   | <b>16</b>  | <b>15</b>  |
| 4. Japan                      | Online            | 6          | 9          |
|                               | Standard          | 93         | 83         |
| <b>4. Japan Total</b>         |                   | <b>99</b>  | <b>92</b>  |
| 5. Rest of World              | Online            | 1          | 2          |
|                               | Standard          | 74         | 71         |
|                               | Online Collection | 0          | 0          |
| <b>5. Rest of World Total</b> |                   | <b>75</b>  | <b>73</b>  |
| <b>Grand Total</b>            |                   | <b>663</b> | <b>627</b> |

## APPENDIX 2 - Comments on submission to Section B

The following are comments by Chris Glidewell.

1. For papers reporting structure determinations and analyses, Sections B, C and E should be regarded as domains in a continuum, dealing respectively with contributions that can crudely be categorised as large, medium and small. In e-mails concerning a paper (see point 3 below) the author quoted the Section B editor thus "For the record, Carol says that any paper with four or more related structures probably belongs in B." Clearly, Section B in particular carries a lot of material which does not fall into this pattern, but that need not negate the following remarks.
2. Accepting the above notion, it follows that transfers of the appropriate types of submission need to be readily transferable between sections according to the judgements of referees and Co-editors.
3. At present, quite a few papers submitted originally to Section C end up in Section E; although a few papers take the opposite route, these are comparatively few in number, probably because all concerned with Section E simply do not have the time to make the necessary transfer judgements. Although less common, transfers between Sections B and C do occur, and I have recently dealt with papers going in both directions: one example is a paper originally submitted to Section B, but declined on the grounds that it was too slight for B, while another was, after consultation with the Section B editor, withdrawn from Section C in order to be recast for Section B.
4. For the B/C transfers referred to in 3 above, it is clear that neither set of authors was very enthusiastic about the change of Section, in view of the substantial amount of work involved in recasting their papers. When Section E was initiated, there were a number of e-mail exchanges between Co-Editors, attempting to establish how B, C and E were related: quoting from memory, a comment from Sandy Blake seems as apposite now as it did then "Preparation of a Section E submission might take a few hours, preparation of a Section C submission might take a few days, but preparation of a Section B submission takes much, much longer." The production of a Section B paper is no easier than it was ten years ago, and that is what needs to be addressed.
5. There are several aspects of Section B submissions which for papers reporting structure determinations and analyses are likely to act as deterrents to potential authors when compared with the comparable aspects for Sections C and E: preparation of the material, submission of the material, and publication times. For Sections C and E, the use of Checkcif (and EnCIFer, for those who need it) makes production of a submission-quality CIF straightforward; the electronic upload system can scarcely be simpler; and, in my experience at least, the reviewing is very quick, and the speed of production, of both proofs and final published paper, are exemplary. Contrasted with this, the production of a Section B paper, requiring manual generation of the formatted text and Tables consistent with the CIFs, is not a light task [see, for example, Table 2 in B61 (2005) 103-114, which required manual production, checking & proof-reading]. The submission process, as laid down in the Online submission instructions, is vastly more complex than the corresponding procedures for Section C and E: many potential authors simply do not have the capacity (or the time) to combine into a single document source files in Word, .rtf, Postscript and .pdf (and possibly other) formats. This is done with admirable efficiency by the Editorial Office for Sections C and E: why cannot this be routine for Section B also? While review of Section C and E papers is generally fast, it cannot be regarded as satisfactory to wait four months for Section B referee reports which then say, in effect, accept without change.
6. The consequence from point 5 above is that, without change, there is likely to be a continued decline in Section B as compared with Sections C and E. Like many other authors I should prefer to submit a higher proportion of my work to Section B: as it happens, several papers lately containing four or five structures (cf. the Brock comment in 1 above) have been sent to Section C for reasons which should now be obvious.
7. What to do to facilitate Section B submissions, and to facilitate transfers between Sections B and C?
  - (a) Incorporate into the Section B submission process as much as possible of the CIF-based process used by C and E, i.e. full text to be in the CIF, not as a separate document; ALL Tables to be generated from the CIF, not made by hand (and to be checkable by [CheckCif](#) #); formatting, with section and sub-section headers, to be possible from CIF.

# It appears that Tables introduced via `_publ_manuscript_incl_extra_item` loops are not currently subject to checking by [CheckCif](#): for multi-structure papers, such Tables are often essential.
  - (b) Adopt a submission procedure identical to that used for Sections C and E.
  - (c) Overall, make the Section B process as near as possible a mimic of the C/E process, at least for papers which could, in principle, go to any one of these Sections: transfers might then be simple.

# Acta B/C/E agenda

## Grand Hotel Panoramic, Montecatini Terme, Italy

22 August, 13:45-14:55 (Editors are encouraged to join the Acta B or Acta C/E meeting after this meeting)

### CHAIR: to be announced

Attendees: Acta B/C/E Editors and Co-editors, and any other interested Editors

IUCr staff attending: Sean Conway, Gillian Holmes, Jill Bradshaw

### 1. GENERAL

This item is intended to cover general matters related to Acta B, C and E and to give the Editors or Co-editors the chance to raise important issues related to the journals that are not covered elsewhere in the agenda.

### 2. PUBLISHED DATA

An approximate listing of the data published in B/C/E papers is given in the table below.

What information might be removed (e.g. could the hkl ranges and the density be removed)?

The CSD have asked whether we might report melting point and recrystallization solvent information. What are the views of the meeting on this?

Are there any ways in which we could combine items so that the display of information in the journal is more efficient?

### Data currently published

| Crystal data                                    | Data collection                          | Refinement                   |
|---|--|------------------------------|
| Chemical formula                                | Diffractometer                           | Refinement on F <sup>2</sup> |
| Mr  | Mode of intensity measurement and scan   | $R[F_2 > 2\sigma(F_2)]$      |
| Crystal system, space group                     | Absorption correction                    | wR(F <sub>2</sub> )          |
| Unit-cell lengths                               | Tmin, Tmax                               | S                            |
| Unit-cell angles                                | No. of measured reflections              | No. of reflections           |
| V   | No. of independent reflections           | No. of parameters            |
| Z   | No. of reflections with $I > 2\sigma(I)$ | H-atom treatment             |
| Dx  | Rint                                     | w                            |
| Radiation type                                  | theta max                                | ( $\Delta\sigma$ )max        |
| Number of reflections used to measure unit cell | hkl ranges                               | Delta rho max                |
| Theta range                                     |  | Delta rho min                |
| Mu  |  | Absolute structure           |
| T   |  | Flack parameter              |
| Crystal habit                                   |  |                              |
| Crystal colour                                  |  |                              |
| Crystal dimensions                              |  |                              |

### 3. JOURNAL IDENTITY AND PROMOTION

3.1. How can the identities of Sections B/C/E be made more distinct?

3.2. Do authors clearly understand the distinctions between the journals when submitting papers?

3.3. How could the joint promotional leaflet for Acta Cryst. B, C and E be improved?

3.4. Where can B, C and E be promoted?

3.5. In what other ways can Acta B, C and E be promoted?

Should there be additions to ealerts, proofs message etc.? Do these get noticed?

#### 4. POWDER DIFFRACTION GUIDELINES

The information available on the web about powder CIF submissions has been recently updated; the revised guidelines are given in the APPENDIX to these agenda notes.

Are there any additional points that should be included in the guidelines?

What steps are required to publicise powder CIF submissions? Is the information easy to find?

Should there be additional validation procedures for these papers?

#### 5. PREVIOUSLY PUBLISHED STRUCTURES

This item is intended to allow discussion of the circumstances under which previously published structures may be published in the journals.

A comment concerning Acta C policy on this subject is as follows:

"I think that the Acta C policy on this is fairly clear. The Comment section must provide significant added value to the numerical data which are freely available at the CCDC. The sort of thing that I envisage is a case where the 'synthetic chemists' (for want of a better descriptor) have published a paper which included an ORTEP plot to establish connectivity - and there is no discussion of the structure at all. Most reputable journals will require that a CIF for the compound be deposited with the CCDC. If the crystallographers then feel that an additional "structural" paper is warranted, all that they have to do for an Acta C submission is make it clear that the Comment section does provide the required 'significant added value'."

It would be useful to clarify the policies of B/C/E on this matter.

#### 6. FIGURES

Figures published in Section C are currently relabelled in nearly all cases by the Editorial Office, whereas for Sections B and E relabelling is less common. It is proposed that the amount of relabelling done for Section C is reduced. This means that clearer instructions for authors on labelling of diagrams may be required. It might also be helpful to provide instructions for authors that relate the size of the lettering to the length of a standard C-C bond in the finished diagram, as the final size of the diagram is generally based on the final C-C lengths in the published diagram.

Editors' views on what should be included in such guidelines are welcomed.

Note that Section E has a flexible approach to this matter:

"The labelling of symmetry-generated atoms in Figures and text needs to be handled with some flexibility. In tables (geometry and H-bonds), symmetry codes are generated automatically and superscript i, ii, iii, iv, etc are used. Ideally the same style should be used in text and Figures, but this is not easy (or maybe not possible) with some widely used graphics programs. Where another style is used, it should be consistent (e.g. not upper case letters in the Figures and lower-case letters in the text), it must be defined (e.g. in Figure captions), and preferably it should be related to the Tables (e.g. "The suffix A corresponds to symmetry code (i) in Table 1.')."

#### 7. MATTERS ARISING FROM THE GENERAL AGENDA

## APPENDIX

### Guidelines for authors of Rietveld refinement papers

These notes are provided for authors who wish to submit a paper describing the results of Rietveld refinement of a structural model against powder diffraction data to any of the IUCr journals. They should be read in conjunction with the current version of the Notes for Authors for the relevant journal.

### Powder CIFs

The results of the Rietveld refinement and the powder diffraction data should be provided in Crystallographic Information File (CIF) format. For Acta Crystallographica Sections C and E, enter the text of your paper in the CIF that contains the results. For other journals, prepare your paper as directed by the relevant Notes for Authors and submit the CIFs containing the results of the Rietveld refinement and the powder diffraction data when you are asked to do so during the online submission procedure.

### How to prepare your CIF

A CIF contains a list of data items and their associated values. The formal definition of each data item is given in a CIF dictionary. The data items that are specific to powder studies all start `_pd` (for example, `_pd_proc_ls_profile_function`) and are defined in the powder CIF dictionary. Data items that can be used to describe a single-crystal or a powder study (for example, `_cell_length_a`) are defined in the core CIF dictionary. Data items that are not relevant to the study do not need to be included in the CIF.

The following items are provided to help you prepare a powder CIF for a Rietveld study:

- Powder CIF template files and example powder CIFs:
  - Template for a powder CIF for describing the results of a Rietveld refinement
  - Template for a powder CIF containing powder diffraction data
  - Example of a powder CIF describing the results of a Rietveld refinement
  - Example of a powder CIF containing powder diffraction data
  - Example of a powder CIF for a multiple phase/multiple data set refinement.
- List of data items to include in a powder CIF
- Powder CIF dictionary (containing the definitions of all powder CIF data names used in the template files and examples)
- Core CIF dictionary (containing the definitions of all core CIF data names used in the template files and examples)
- Search for a CIF data name
- Programs that can read and/or write powder CIFs

### Figures

Figures which present the experimental and calculated diffraction profiles of the material studied should also contain the difference between these profiles. Your paper should include a figure with the experimental, calculated and difference profiles and the corresponding data should be supplied in CIF format. Where a large number of refinements with similar data are presented, a single figure for a typical fit may be provided.

### Powder diffraction data

The primary diffraction data (i.e. the numerical intensity or counts at each measured point on the profile as a function of scattering angle or time-of-flight) should be supplied in CIF format. If the data set was reduced in size by summing together multiple measurements before it was analysed, the reduced data set (together with computed and difference values) should also be supplied. If the data have been scaled or do not follow pulse-counting statistics (for example, data from image-plate detectors), please include standard intensities. The diffraction data will be used during the review process and will be made available to readers through Crystallography Journals Online when your paper is published. They will also be archived by the IUCr.

We recommend that the data you submit include information corresponding to each item (1) to (5) in the following list:

(1) The data corresponding to the ordinate of your Rietveld refinement plot (e.g. two theta values, neutron time of flight etc.). Note that two theta values can be listed in full or can be specified by giving two theta(min), two theta(max) and the step size.

(a) CIF data names suitable for diffractometer data are:

`_pd_meas_2theta_range_min`, `_pd_meas_2theta_range_max`, `_pd_meas_2theta_range_inc`

`_pd_meas_2theta_scan`  
`_pd_proc_2theta_range_min`, `_pd_proc_2theta_range_max`, `_pd_proc_2theta_range_inc`  
`_pd_proc_2theta_corrected`  
`_pd_proc_d_spacing`  
`_pd_proc_recip_len_Q`

(Two theta values must be given. d-spacings and Q values are not required, but it can be helpful to readers to include them.)

(b) CIF data names suitable for time-of-flight data are:

`_pd_meas_time_of_flight`  
`_pd_proc_wavelength`  
`_pd_proc_d_spacing`  
`_pd_proc_recip_len_Q`

(The use of `_pd_meas_time_of_flight` and either `_pd_proc_d_spacing` or `_pd_proc_recip_len_Q` is strongly recommended.)

(c) CIF data names for other kinds of data (energy-dispersive, camera etc.) include:

`_pd_meas_position`  
`_pd_proc_energy_incident`  
`_pd_proc_d_spacing`  
`_pd_proc_recip_len_Q`

(The use of `_pd_proc_d_spacing` or `_pd_proc_recip_len_Q` in addition to `_pd_meas_position` or `_pd_proc_energy_incident` is strongly recommended.)

(2) The observed (or processed) intensity values. CIF data names are:

`_pd_meas_counts_total`  
`_pd_meas_intensity_total`  
`_pd_proc_intensity_total`  
`_pd_proc_intensity_net`

(If `_pd_meas_counts_total` is not used, standard uncertainties should be specified or least-squares weights should be included.)

(3) Details of the background. CIF data names are:

`_pd_meas_counts_background`  
`_pd_meas_counts_container`  
`_pd_meas_intensity_background`  
`_pd_meas_intensity_container`  
`_pd_proc_intensity_bkg_calc`  
`_pd_proc_intensity_bkg_fix`

(4) Rietveld refinements are almost always weighted by the reciprocal of the intensity values or the reciprocal of the intensity standard uncertainties squared (used the code 'sigma' for `_refine_ls_weighting_scheme` to indicate this). If any other weighting has been used, this should be specified by using the code 'calc' for `_refine_ls_weighting_scheme` and details of the scheme used should be given in `_refine_ls_weighting_details`.

(5) The calculated pattern (CIF data names `_pd_calc_intensity_net` or `_pd_calc_intensity_total`).

# Acta C/E agenda

## Grand Hotel Panoramic, Montecatini Terme, Italy

22 August, 14:55-17:25 (Editors are encouraged to join the Acta B/C/E meeting before this meeting)

### **CHAIR: to be announced**

Attendees: Acta C/E Editors and Co-editors, and any other interested Editors

IUCr staff attending: Sean Conway, Gillian Holmes

## **1. ACTA C AND E**

### **1.1. GENERAL**

This item is intended to cover general matters related to Acta C and E and to give the Editors or Co-editors the chance to raise important issues related to the journals that are not covered elsewhere in the agenda.

### **1.2. REPORT OF SECTION C/E MEETING**

The Section C and E Editors met with Chester staff in May. Notes on the meeting are attached as APPENDIX 2, together with comments and recommendations by John Helliwell. A number of the issues (the new submission system, transfer of papers from C to E, and poor quality papers) are discussed in agenda items below. Co-editors are invited to comment on any of the issues.

Marilyn Olmstead has commented:

“The suggestion to make the location of maximum and minimum electron density peaks a new CIF data item was discussed in Switzerland three years ago. I don't know if anything has happened since then, but I definitely think this should be done, rather than having the Co-Editors have to insist on it all the time.”

### **1.3. SUBMISSION AND REVIEW**

#### 1.3.1. New submission system

The new submission system for Sections C and E will be demonstrated. By the time of the meeting, it is hoped that the system will be operational and that a number of Co-editors will have started to receive submissions via the system.

Authors will upload their CIF, structure factors and other files via the web; duplication checking and copyright transfer will be carried out during the submission process. Co-editors will be informed by email when new paper has arrived and given a URL to view the paper. Revisions can also be uploaded via the system. The status system is to be extended to allow access to the paper, and to provide the Co-editor with the ability to contact authors and reviewers. Decisions (e.g. accept, reject etc.) and their associated emails can also be recorded via the interface.

#### 1.3.2. Transfer of papers from C to E

A pilot scheme is to be undertaken for the transfer of papers from C to E with same Co-editor handling the paper through to acceptance. This means that Acta C Co-editors taking part in such a scheme would need to (a) make an early decision as to whether the paper should be in C or E (so as not to waste referees time); (b) if considered appropriate for transfer, consult with the author about the transfer; (c) make sure that the paper was acceptable for Section E before completing the transfer and accepting the paper for Section E. The scheme will be voluntary.

#### 1.3.4. Validation procedures

When the new submission system is introduced, the arrangements for validation will be revised. The handling of papers with A alerts and a completed VRF will be made the same for Acta C and E. It is planned that a subset of Co-editors will handle such papers, and will refer to the Data-Validation Editors as necessary to ensure consistency of handling such papers.

Editors' views on this change and on validation procedures are welcomed.

### **1.4. POOR QUALITY PAPERS**

Ideas for handling poor quality papers will be discussed.

The Editorial Office have developed a new tool (pubCIF) for viewing and preparing CIFs for publication. It will be demonstrated at the meeting. This has a number of features to make writing of papers easier, including a publication wizard that allows an author to write the first version of the Abstract and a short Comment section by selecting sentences

from an interactive form. The program also includes a feature for shortening badly written Comment sections.

It is expected that the program will be available in the next few weeks; Co-editors who would like to try a copy should contact [support@iucr.org](mailto:support@iucr.org).

Ricardo Baggio has asked about handling of symmetry codes in tables. publCIF remembers the coding applied in Table 1 when processing Table2; it is planned that the online printCIF service will be based on publCIF in due course.

### 1.5. MERGING FRIEDELS

In the case of a light-atom non-chiral molecule in a crystal system which yields Friedel and Bijvoet pairs, it is proposed that these reflections should be merged as nothing stereochemical results from their inclusion.

On the other hand when we have a light-atom chiral molecule in a crystal system which yields Friedel and Bijvoet pairs, it may be that there IS information there - but we are not smart enough to know how to use it. In such cases, it is proposed that we would not ask that Friedel and Bijvoet pairs be merged.

### 1.6. ABSORPTION CORRECTION REPORTING

It is proposed that the numbers given for T<sub>min</sub> and T<sub>max</sub> should represent the range of transmission factors actually applied to the diffraction pattern during an absorption correction as follows:

- (1) Reserve the current T<sub>min</sub>, T<sub>max</sub> entries in the CIF, to be listed in Table 1 under the heading 'Absorption Correction' for the actual correction range as applied to the intensities. These numbers would not be modified in the editorial office as is currently the practice since there is no justification for the editor changing the description of an experiment unless requested to do so by the author.
- (2) Add an additional entry in Table 1 for the 'expected range'. Those values are probably best calculated by the PRINTCIF software from the crystal size dimensions provided in the CIF
- (3) Store values for the expected range under new datanames in the CIF.

Thus the information given in the paper would change from

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

T<sub>min</sub> = 0.053, T<sub>max</sub> = 0.632

to something like

Absorption correction: multi-scan (SADABS; Sheldrick, 2003)

T<sub>min</sub> = 0.053, T<sub>max</sub> = 0.632; expected range 0.048-0.580

The wording within checkCIF (and any alert levels) will need to accommodate the suggested change.

This change will not only clear up any ambiguity about what is to be reported under T<sub>min</sub> and T<sub>max</sub> but will allow the reader to assess the adequacy of an absorption correction, e.g. in a case where the experimentally applied transmission factors are reported as 0.43 and 1.00 and the expected range is reported as 0.008 and 0.010.

### 1.7. DV TESTS

Are the current tests adequate?

Is the information easy to find? Should it be more prominent?

### 1.8. SINGLE STRUCTURE POLICY (TONY LINDEN)

Acta E has a policy of only publishing single-structure papers. Is this restriction bound in limitations in the way the technical processing of papers for the journal has been set up or is it merely a policy decision? Can the policy be changed? Do we need to? Or do we need to develop guidelines to indicate to authors how intimately related structures might be published in Acta E?

If a multi-structure paper submitted to Acta C is recommended for transfer to E, this is not so easily accomplished unless the Comment section is substantially rewritten for each individual paper to take account of the fact that the structures are now all in different papers. That makes a lot of extra effort for the authors and can lead to diminution of the impact of each individual report.

Allowing for multi-structure papers in E would make the transfer from C an easier process for all concerned. It might also attract more comprehensive papers directly to E (although some of these might then qualify for transfer to C!).

It has been suggested that the way to overcome the need for a multi-structure paper in E is to write the Comment for the

paper containing the first structure as if it was a multi-structure paper and then put the remaining structures in the subsequent papers (which should all be sequential in the journal) without any information in the Comment section other than an indicator to refer to the first paper in the series. This is one possibility, but is it realistic in practice, particularly for citation and citation index purposes.

Are there other options available to deal with this issue?

## **2. ACTA C**

### **2.1. GENERAL**

This item is intended cover general matters related to Acta C and to give the Editors or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

### **2.2. JOURNAL DEVELOPMENT**

What sort of papers should we be trying to attract and how can we encourage their submission?

How can the science impact of papers be increased?

Are there particular authors that should be encouraged to write for the journal?

Are there any ways in which we can increase publication speed or otherwise improve services to authors?

### **2.3. JOURNAL DESIGN**

#### **2.3.1. PRINT:**

Is the present design of the journal satisfactory?

Are there any items that can be removed from the print version of the journal?

#### **2.3.2. ONLINE:**

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

### **2.4. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors.

### **2.5. USE OF COLOUR**

Is the present policy (the print journal is black and white and the online journal is colour) working satisfactorily?

Do any guidelines need to be given to authors on the use of colour?

## **3. ACTA E**

### **3.1. GENERAL**

This item is intended cover general matters related to Acta E and to give the Editors or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

### **3.2. JOURNAL GROWTH**

The chief problem facing the journal has been its success in attracting papers. This matter is discussed in APPENDIX 3, where an upper limit on the number of pages is suggested.

Editors' views on strategies to cope with the growth of the journal are welcomed.

### **3.3. JOURNAL DEVELOPMENT**

Is there any way that the journal impact factor can be increased?

Are there particular authors that should be encouraged to write for the journal?

Are there any ways in which we can improve services to authors?

### **3.4. JOURNAL DESIGN**

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

Do the arrangements for the covers need to be modified?

### **3.5. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors. NB the Notes for Authors for Section E were not updated for 2005.

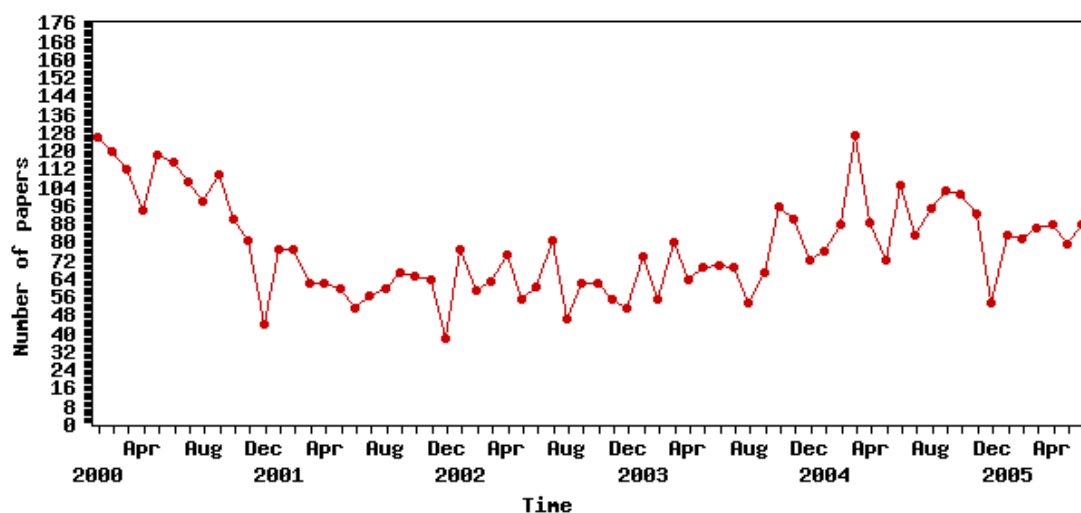
## APPENDIX 1 - Background information on Section C

### Aims and scope

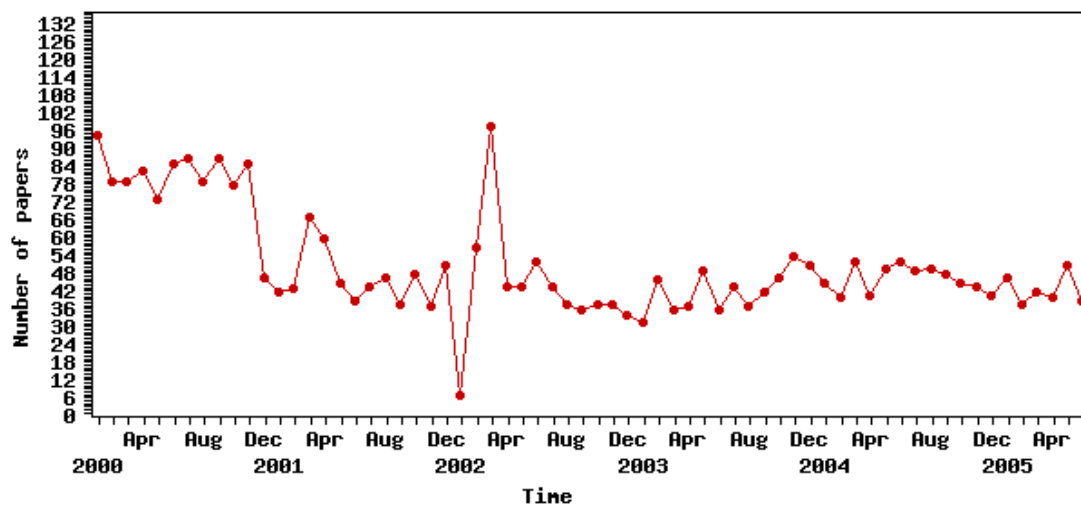
Acta Crystallographica Section C: Crystal Structure Communications is a rapid communication journal for the publication of concise reports on crystal and molecular structures. The numerical and text descriptions of each structure are submitted to the journal electronically as a Crystallographic Information File (CIF) and are checked and typeset automatically prior to peer review. The published paper contains an encapsulation of the data that are essential to understanding the main features of the study.

The journal is aimed primarily at the structural sciences community, but also meets the needs of molecular and solid-state chemists, materials scientists and those working in other disciplines.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Acta Crystallographica Section C

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1740  |
| Institutional subscribers | 605   |
| Individual subscribers    | 43    |
| Impact factor (2004)      | 0.728 |
| Ranking (2004)            | 17/24 |

### Acta Crystallographica Section C - competing journals based on citing

Number of times articles published in 2003 (in journals below) cited articles published in *Acta Crystallographica Section C*

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 7074    | 116  | 391  | 497  | 479  |                      |
| ACTA CRYSTALLOGR E | 1103    | 44   | 80   | 83   | 87   | 0.453                |
| ACTA CRYSTALLOGR C | 607     | 45   | 103  | 76   | 51   | 0.828                |
| INORG CHEM         | 274     | 1    | 3    | 18   | 8    | 3.389                |
| J MOL STRUCT       | 216     | 3    | 15   | 19   | 17   | 1.021                |
| DALTON T           | 201     | 2    | 6    | 12   | 22   | 2.908                |
| Z ANORG ALLG CHEM  | 177     | 2    | 3    | 10   | 10   | 1.127                |
| INORG CHIM ACTA    | 176     | 0    | 6    | 4    | 19   | 1.578                |
| POLYHEDRON         | 143     | 0    | 7    | 6    | 10   | 1.584                |
| EUR J INORG CHEM   | 138     | 1    | 2    | 2    | 8    | 2.48                 |

### Acta Crystallographica Section C - list of cited journals

Number of times articles published in journals below (in years below) were cited in *Acta Crystallographica Section C* in 2003

| Citing Journal      | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|---------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS        | 7868    | 340  | 636  | 555  | 530  |                      |
| ACTA CRYSTALLOGR C  | 607     | 45   | 103  | 76   | 51   | 0.828                |
| ACTA CRYSTALLOGR B  | 495     | 7    | 149  | 18   | 29   | 3.643                |
| J APPL CRYSTALLOGR  | 454     | 104  | 2    | 0    | 22   | 2.324                |
| ACTA CRYSTALLOGR A  | 308     | 0    | 0    | 0    | 0    | 1.558                |
| J AM CHEM SOC       | 262     | 0    | 12   | 11   | 9    | 6.516                |
| INORG CHEM          | 256     | 3    | 16   | 27   | 22   | 3.389                |
| SHELXL97            | 201     | 0    | 0    | 1    | 0    |                      |
| DALTON T            | 173     | 6    | 17   | 12   | 27   | 2.908                |
| ANGEW CHEM INT EDIT | 162     | 5    | 7    | 7    | 8    | 8.427                |

### Acta Crystallographica Section C - citation report by issue

| 2001  |      |                                  |                        |                         | 2002  |      |                                  |                        |                         | 2003  |      |                                  |                        |                         |
|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|
| Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 49                               | 2.6                    | 1                       | 1     | 0    | 53                               | 1.6                    | 2                       | 1     | 0    | 32                               | 1.4                    | 0                       |
| 2     | 0    | 36                               | 2.2                    | 1                       | 2     | 0    | 51                               | 1.6                    | 0                       | 2     | 0    | 31                               | 1.2                    | 0                       |
| 3     | 0    | 42                               | 2.7                    | 0                       | 3     | 0    | 56                               | 1.0                    | 0                       | 3     | 0    | 45                               | 1.5                    | 2                       |
| 4     | 0    | 66                               | 2.6                    | 2                       | 4     | 0    | 48                               | 0.8                    | 1                       | 4     | 0    | 35                               | 1.2                    | 2                       |
| 5     | 0    | 59                               | 1.9                    | 0                       | 5     | 0    | 43                               | 1.2                    | 3                       | 5     | 0    | 36                               | 1.2                    | 0                       |
| 6     | 0    | 44                               | 1.7                    | 0                       | 6     | 0    | 43                               | 0.9                    | 6                       | 6     | 0    | 48                               | 1.2                    | 2                       |
| 7     | 0    | 38                               | 2.4                    | 1                       | 7     | 0    | 51                               | 0.7                    | 2                       | 7     | 0    | 35                               | 0.4                    | 1                       |
| 8     | 0    | 43                               | 2.2                    | 1                       | 8     | 0    | 43                               | 1.1                    | 0                       | 8     | 0    | 43                               | 0.7                    | 1                       |
| 9     | 0    | 46                               | 2.1                    | 0                       | 9     | 0    | 37                               | 0.5                    | 1                       | 9     | 0    | 36                               | 0.8                    | 0                       |
| 10    | 0    | 37                               | 1.6                    | 4                       | 10    | 0    | 35                               | 1.1                    | 0                       | 10    | 0    | 41                               | 0.9                    | 0                       |
| 11    | 0    | 47                               | 1.6                    | 1                       | 11    | 0    | 38                               | 0.5                    | 0                       | 11    | 0    | 46                               | 1.3                    | 0                       |
| 12    | 0    | 36                               | 2.1                    | 0                       | 12    | 0    | 36                               | 0.6                    | 0                       | 12    | 0    | 53                               | 1.0                    | 0                       |

## Acta Crystallographica Section C - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| inorganic compounds                    | 41              | 41                              | 0                           | 2.2                    | 61              | 61                              | 0                           | 0.8                    | 49              | 49                              | 0                           | 0.5                    |
| organic compounds                      | 293             | 293                             | 0                           | 2.3                    | 249             | 249                             | 0                           | 1.0                    | 243             | 243                             | 0                           | 1.0                    |
| metal-organic compounds                | 207             | 207                             | 0                           | 2.0                    | 221             | 221                             | 0                           | 1.1                    | 186             | 186                             | 0                           | 1.3                    |
| addenda and errata                     | 2               | 2                               | 0                           | 0.0                    | 2               | 2                               | 0                           | 0.5                    | 2               | 2                               | 0                           | 0.0                    |
| letters to the editor                  | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| editorial                              | 1               | 0                               | 1                           | 0.0                    | 1               | 1                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 0.0                    |
| issue preface                          | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| international union of crystallography | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| notes and news                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Acta Crystallographica Section C - 2001 |      |            |                         |              |                             |  |  |
|---|------|------------|-------------------------|--------------|-----------------------------|--|--|
| Issue                                   | Part | First page | Paper category          | ISI citation | Total IUCr citation to date | Authors  | Title  |
| 9                                       | 0    | 1120       | organic compounds       | 20           | 11                          | <b>Janczak, J.</b> , Perpetuo, G.J.  | Melaminium chloride hemihydrate  |
| 8                                       | 0    | 939        | organic compounds       | 20           | 1                           | Mattheus, C.C., Dros, A.B., Baas, J., Meetsma, A., Boer, J.L. de, <b>Palstra, T.T.M.</b> | Polymorphism in pentacene  |
| 1                                       | 0    | 123        | organic compounds       | 19           | 12                          | <b>Janczak, J.</b> , Perpetuo, G.J.  | Melaminium phthalate   |
| 7                                       | 0    | 873        | organic compounds       | 18           | 11                          | <b>Janczak, J.</b> , Perpetuo, G.J.  | Melaminium bis(4-hydroxybenzenesulfonate) dihydrate  |
| 3                                       | 0    | 271        | metal-organic compounds | 17           | 4                           | <b>Yilmaz, V.T.</b> , Andac, O., Topcu, Y., Harrison, W.T.A.                             | trans-Bis(ethanolamine-N,O)bis(saccharinato-N) copper(II)  |
| 12                                      | 0    | 1431       | organic compounds       | 17           | 9                           | <b>Janczak, J.</b> , Perpetuo, G.J.  | Bis(melaminium) sulfate dihydrate  |
| 4                                       | 0    | 459        | organic compounds       | 14           | 9                           | Prabakaran, P., Robert, J.J., <b>Thomas Muthiah, P.</b> , Bocelli, G., Righi, L.         | Aminopyrimidine-carboxyl(ate) interactions in trimethoprim maleate, an antifolate drug                               |
| 3                                       | 0    | 230        | inorganic compounds     | 14           | 4                           | Aken, B.B. van, <b>Meetsma, A.</b> , Palstra, T.T.M.                                     | Hexagonal $Y\text{MnO}_3$  |
| 2                                       | 0    | 216        | organic compounds       | 14           | 14                          | Cannon, D., <b>Glidewell, C.</b> , Low, J.N., Quesada, A., Wardell, J.L.                 | Hydrogen bonding in C-methylated nitroanilines: three triclinic examples with $Z' = 2$ or 4                          |
| 3                                       | 0    | 315        | organic compounds       | 13           | 12                          | Ferguson, G., <b>Glidewell, C.</b> , Low, J.N., Skakle, J.M.S., Wardell, J.L.            | Hydrogen bonding in C-methylated nitroanilines: the three-dimensional framework structure of 2-methyl-4-nitroaniline |
| 4                                       | 0    | 377        | metal-organic compounds | 13           | 4                           | <b>Nather, C.</b> , Greve, J.  | Poly[copper(I)-[bold mu]-bromo-[bold mu]-2,3-dimethylpyrazine-N:N']  |

|   |   |     |                         |    |    |   |  |
|---|---|-----|-------------------------|----|----|---|--|
| 8 | 0 | 942 | organic compounds       | 13 | 17 | <a href="#">McWilliam</a> , S.A., Skakle, J.M.S., Low, J.N., Wardell, J.L., Garden, S.J., Pinto, A.C., Torres, J.C., <a href="#">Glidewell</a> , C. | Triclinic and orthorhombic polymorphs of 2-iodo-4-nitroaniline: interplay of hydrogen bonds, nitro...I interactions and aromatic [bold pi]-[bold pi]-stacking interactions |
| 7 | 0 | 870 | organic compounds       | 12 | 3  | Collings, J.C., <a href="#">Batsanov</a> , A.S., Howard, J.A.K., Marder, T.B.   | Octafluoronaphthalene-diphenylacetylene (1/1)  |
| 4 | 0 | 347 | inorganic compounds     | 12 | 2  | Becker, M., <a href="#">Jansen</a> , M.   | Zinc cyanamide, Zn(CN <sub>2</sub> )   |
| 1 | 0 | 117 | organic compounds       | 12 | 6  | <a href="#">Hokelek</a> , T., Isiklan, M., Kilic, Z.  | 4-[[1E)-(2-Hydroxyphenyl)methylidene]amino]-1,5-dimethyl-2-phenyl-2,3-dihydro-1H-pyrazol-3-one   |
| 1 | 0 | 70  | organic compounds       | 11 | 2  | <a href="#">Thuery</a> , P., Nierlich, M., Vicens, J., Masci, B.  | A 1:1:1 chloroform/tetrahydrofuran solvate of p-tert-butyltetrahomodioxacalix[4]arene  |
| 1 | 0 | 115 | organic compounds       | 11 | 8  | Subha Nandhini, M., Krishnakumar, R.V., <a href="#">Natarajan</a> , S.  | Glycinium oxalate  |
| 1 | 0 | 26  | metal-organic compounds | 10 | 0  | Stahler, R., Nather, C., <a href="#">Bensch</a> , W.  | Tris{bis[N-(2-aminoethyl)-1,2-ethanediamine-[bold kappa]3N]nickel(II)} bis(tetrathioantimonate)  |

#### Acta Crystallographica Section C - 2002

| Issue | Part | First page | Paper category          | ISI citation | Total IUCr citation to date | Authors   | Title   |
|-------|------|------------|-------------------------|--------------|-----------------------------|---|---|
| 2     | 0    | o112       | organic compounds       | 9            | 6                           | Perpetuo, G.J., <a href="#">Janczak</a> , J.  | Melaminium acetate acetic acid solvate monohydrate  |
| 5     | 0    | o289       | organic compounds       | 9            | 9                           | Low, J.N., Quesada, A., Marchal, A., Melguizo, M., Nogueras, M., <a href="#">Glidewell</a> , C. | Hydrogen bonding in 2-amino-4,6-dimethoxypyrimidine, 2-benzylamino-4,6-bis(benzyloxy)pyrimidine and 2-amino-4,6-bis(N-pyrrolidino)pyrimidine: chains of fused rings and a centrosymmetric dimer           |
| 3     | 0    | m158       | metal-organic compounds | 7            | 11                          | Zhu, M.-L., Lu, L.-P., Jin, X.-L., <a href="#">Yang</a> , P.                                    | Trichloro(1,1-dimethylbiguanidium-[bold kappa]N <sub>3</sub> )zinc(II)  |
| 2     | 0    | m124       | metal-organic compounds | 7            | 5                           | <a href="#">Kooijman</a> , H., Spek, A.L., Albada, G.A. van, Reedijk, J.                        | catena-Poly[[dicyanamido(5,5'-dimethyl-2,2'-bipyridine-[bold kappa]2N,N')copper(II)]-[bold mu]-dicyanamido-[bold kappa]2N1:N5]  |
| 1     | 0    | m17        | metal-organic compounds | 7            | 3                           | Andac, O., Guney, S., Topcu, Y., <a href="#">Yilmaz</a> , V.T., Harrison, W.T.A.                | Bis(pyridine-2,6-dimethanol-N,O,O')cobalt(II) and -copper(II) disaccharinate dihydrate: three-dimensional structures with extensive hydrogen bonds and aromatic [bold pi]-[bold pi]-stacking interactions |
| 1     | 0    | m1         | metal-organic compounds | 7            | 5                           | Zakaria, C.M., Ferguson, G., Lough, A.J., <a href="#">Glidewell</a> , C.                        | Hydrogen-bonded adducts of ferrocene-1,1'-diylbis(diphenylmethanol): monomeric and polymeric adducts with 1,2-bis(4-pyridyl)ethene and 1,6-diaminohexane  |
| 1     | 0    | m12        | metal-organic compounds | 6            | 4                           | <a href="#">Cheng</a> , Y.-Q., Hu, M.-L., Wang, S., Ye, M.-D.                                   | [bold mu]1,3-Azido-diazidotetrakis(1,10-phenanthroline)dicationic copper(II) azide tetrahydrate   |
| 2     | 0    | m77        | metal-organic compounds | 6            | 7                           | <a href="#">Vega</a> , D., Fernandez, D., Ellena, J.A.  | Disodium pamidronate  |
| 2     | 0    | m129       | metal-organic compounds | 6            | 2                           | <a href="#">Bats</a> , J.W., Ma, K., Wagner, M.   | Isomorphism and phase transition in triferrocenylboroxine and triferrocenylborazine   |
| 6     | 0    | o355       | organic compounds       | 6            | 6                           | Quesada, A., Low, J.N., Melguizo, M., Nogueras, M., <a href="#">Glidewell</a> , C.              | 2-Amino-4,6-bis(benzyloxy)-5-nitrosopyrimidine: chains built from three-centre N-H...N(O) and N-H...[bold pi](arene) hydrogen bonds   |
| 8     | 0    | m427       | metal-organic compounds | 6            | 2                           | <a href="#">Yilmaz</a> , V.T., Guney, S., Andac, O., Harrison, W.T.A.                           | Bis(2-pyridylmethanol)bis(saccharinato)zinc(II) and -cadmium(II) at 120 K: three-dimensional structures containing both N- and O-coordinated ambidentate saccharinate ligands                             |
| 7     | 0    | o421       | organic compounds       | 6            | 7                           | Hema, R., <a href="#">Parthasarathi</a> , V., Thamotharan, S., Dubey, S., Jindal, D.P.          | 16-(4-Cyanobenzylidene)-3[beta]-pyrrolidinoandrost-5-en-17[beta]-ol monohydrate   |

| Acta Crystallographica Section C - 2003 |      |            |                         |              |                             |  |   |
|---|------|------------|-------------------------|--------------|-----------------------------|--|---|
| Issue                                   | Part | First page | Paper category          | ISI citation | Total IUCr citation to date | Authors  | Title   |
| 5                                       | 0    | o234       | organic compounds       | 14           | 4                           | Odabasoglu, M., Albayrak, C., <b>Buyukgungor, O.</b> , Goesmann, H.              | 4-[(3-Chlorophenyl)diazenyl]-2-[[tris(hydroxymethyl)methyl]aminomethylene]cyclohexa-3,5-dien-1(2H)-one  |
| 11                                      | 0    | o616       | organic compounds       | 13           | 2                           | Odabasoglu, M., Albayrak, C., <b>Buyukgungor, O.</b> , Lonnecke, P.              | 2-[[Tris(hydroxymethyl)methyl]aminomethylene]cyclohexa-3,5-dien-1(2H)-one and its 6-hydroxy and 6-methoxy derivatives   |
| 12                                      | 0    | m516       | metal-organic compounds | 12           | 9                           | Ma, C.-B., Chen, F., Chen, C.-N., <b>Liu, Q.-T.</b>                              | trans-Diaquabis(1H-imidazole-4,5-dicarboxylate-[bold kappa]2N3,O4)manganese(II)   |
| 11                                      | 0    | m454       | metal-organic compounds | 11           | 9                           | <b>Hu, M.-L.</b> , Xiao, H.-P., Wang, S., Li, X.-H.                              | catena-Poly[[[(1,10-phenanthroline-[bold kappa]2N,N')copper(II)]-[bold mu]-(dihydrogen benzene-1,2,4,5-tetracarboxylato)-[bold kappa]2O1:O4]  |
| 6                                       | 0    | m218       | metal-organic compounds | 10           | 9                           | Zhu, H.-L., Usman, A., <b>Fun, H.-K.</b> , Wang, X.-J.                           | Bis(2-aminopyridine-[bold kappa]N1)(benzoato-[bold kappa]O)silver(I)  |
| 4                                       | 0    | m124       | metal-organic compounds | 9            | 4                           | Srinivasan, B.R., Dhuri, S.N., <b>Nather, C.</b> , Bensch, W.                    | 1,3-Propanediammonium tetrathiotungstate and N,N,N',N'-tetramethylethylenediammonium tetrathiotungstate   |
| 3                                       | 0    | o135       | organic compounds       | 8            | 7                           | Shan, S., <b>Xu, D.-J.</b> , Hung, C.-H., Wu, J.-Y., Chiang, M.Y.                | Benzaldehyde 2,4-dinitrophenylhydrazone   |
| 3                                       | 0    | m97        | metal-organic compounds | 7            | 7                           | Usman, A., <b>Fun, H.-K.</b> , Chantrapromma, S., Zhu, H.-L., Wang, X.-J.        | Polymeric structure of (ethylenediamine)silver(I) 3-nitrobenzoate monohydrate   |
| 6                                       | 0    | o349       | organic compounds       | 7            | 4                           | <b>Janczak, J.</b> , Perpetuo, G.J.  | Bis(melaminium) dl-malate tetrahydrate  |
| 11                                      | 0    | m473       | metal-organic compounds | 6            | 4                           | <b>Zhang, Y.-M.</b> , Xian, L., Wei, T.-B.                                       | Chlorobis[N'-ethoxycarbonyl-N-(4-methylphenyl)thiourea-[bold kappa]S]copper(I)  |
| 3                                       | 0    | m79        | metal-organic compounds | 6            | 0                           | Alcantara-Flores, J.L., <b>Bernes, S.</b> , Reyes-Ortega, Y., Zamorano-Ulloa, R. | The triclinic polymorph of dibromo[(-)-sparteine-[bold kappa]2N,N']zinc(II)   |
| 1                                       | 0    | o14        | organic compounds       | 6            | 6                           | <b>Glidewell, C.</b> , Low, J.N., Melguizo, M., Quesada, A.                      | Hydrogen bonding in nitroaniline analogues: hydrogen-bonded sheets in 2-amino-4,6-dimethoxy-5-nitropyrimidine and [bold pi]-stacked hydrogen-bonded sheets in 4-amino-2,6-dimethoxy-5-nitropyrimidine |
| 12                                      | 0    | o703       | organic compounds       | 6            | 6                           | Hema, R., <b>Parthasarathi, V.</b> , Sarkunam, K., Nallu, M., Linden, A.         | 3-(4-Chlorobenzoyl)-7-(N,N-dimethylamino)-1-phenylindolizine and 3-(2,4-dichlorobenzoyl)-7-(N,N-dimethylamino)-1-phenylindolizine   |

## Acta Crystallographica Section C - sales and circulation figures

### Institutional and consortial circulation totals

|                             | 2003 | 2004 |
|-----------------------------|------|------|
| Consortia site access       |      | 1740 |
| 1. Europe                   |      | 882  |
| 2. USA                      |      | 202  |
| 3. Canada                   |      | 32   |
| 4. Aus/NZ                   |      | 83   |
| 5. Japan                    |      | 86   |
| 6. Rest of World            |      | 455  |
| Institutional subscriptions | 643  | 605  |
| Online                      | 32   | 49   |

|                        |     |     |
|------------------------|-----|-----|
| Standard               | 609 | 552 |
| Online Collection      | 2   | 4   |
| Personal subscriptions | 49  | 43  |

### Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 11         | 15         |
|                               | Standard          | 224        | 205        |
|                               | Online Collection | 2          | 2          |
| <b>1. Europe Total</b>        |                   | <b>237</b> | <b>222</b> |
| 2. North America              | Online            | 14         | 23         |
|                               | Standard          | 206        | 183        |
|                               | Online Collection | 0          | 2          |
| <b>2. North America Total</b> |                   | <b>220</b> | <b>208</b> |
| 3. Aus/NZ                     | Online            | 1          | 1          |
|                               | Standard          | 15         | 14         |
| <b>3. Aus/NZ Total</b>        |                   | <b>16</b>  | <b>15</b>  |
| 4. Japan                      | Online            | 6          | 9          |
|                               | Standard          | 87         | 75         |
| <b>4. Japan Total</b>         |                   | <b>93</b>  | <b>84</b>  |
| 5. Rest of World              | Online            | 0          | 1          |
|                               | Standard          | 77         | 75         |
|                               | Online Collection | 0          | 0          |
| <b>5. Rest of World Total</b> |                   | <b>77</b>  | <b>76</b>  |
| <b>Grand Total</b>            |                   | <b>643</b> | <b>605</b> |

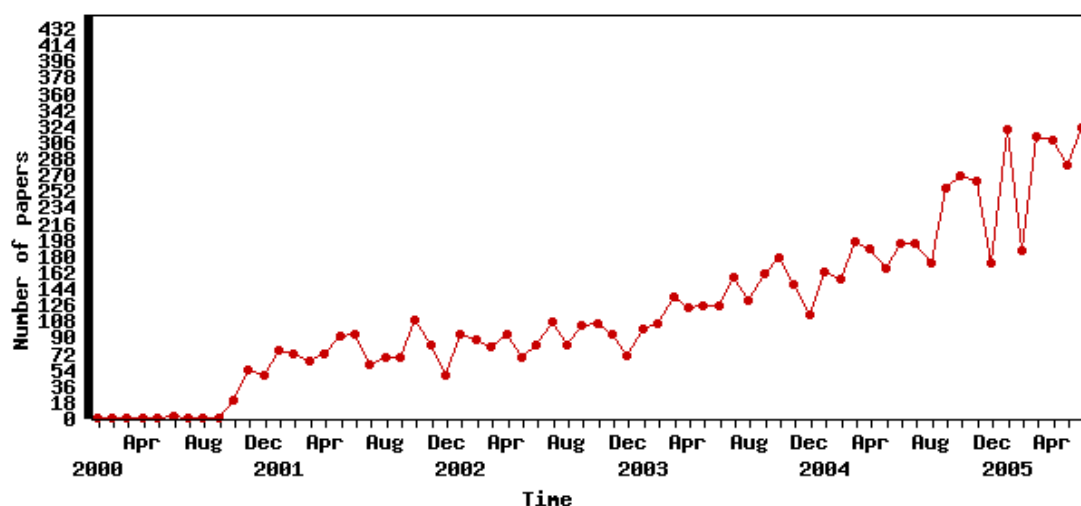
## APPENDIX 2 - Background information on Section E

### Aims and scope

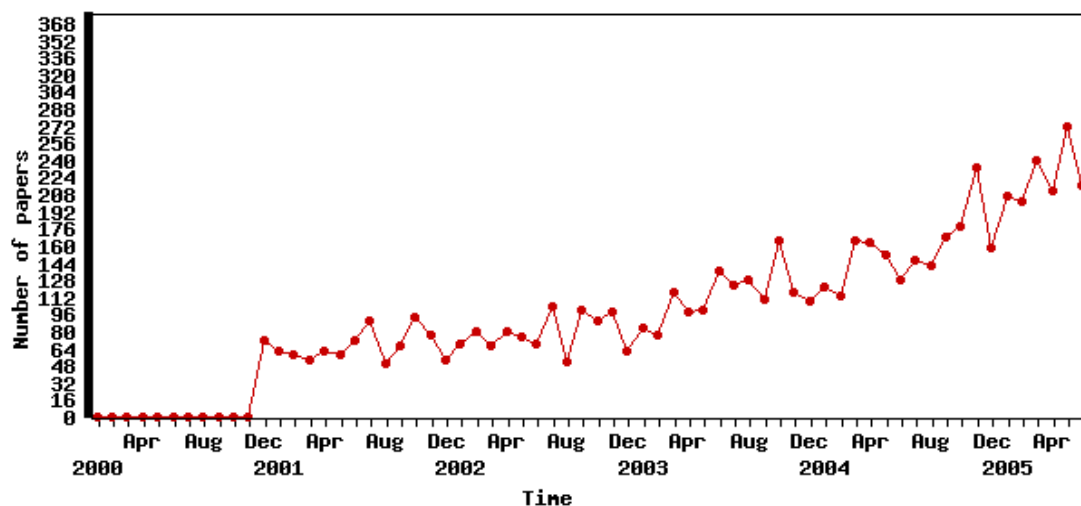
Structure Reports Online was launched in January 2001 as the IUCr's first electronic-only journal. It is a rapid communication journal for the publication of concise reports on inorganic, metal-organic and organic structures, and benefits from an enhanced electronic publication procedure. Each published report includes a set of key indicators, giving a summary of the main descriptors of the precision and completeness of the study, with indications of problems such as disorder. The publication of routine as well as more difficult structures is encouraged, with appropriate comment by authors on the problems encountered, and reflection of these in the key indicators.

Structure Reports Online is aimed primarily at the structural sciences community, but also meets the needs of molecular and solid-state chemists, materials scientists and those working in other disciplines. An average of 63 papers per month have been published in the journal since its launch, and the journal maintains impressive publication times with an average time from receipt to publication of less than one month. A reduced subscription rate is available to authors.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Acta Crystallographica Section E

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1734  |
| Institutional subscribers | 6     |
| Individual subscribers    | 3     |
| Impact factor (2004)      | 0.491 |
| Ranking                   | 23/24 |

### Acta Crystallographica Section E - citation report by issue

| 2001  |      |                                 |                        |                         | 2002  |      |                                 |                        |                         | 2003  |      |                                 |                        |                         |
|-------|------|---------------------------------|------------------------|-------------------------|-------|------|---------------------------------|------------------------|-------------------------|-------|------|---------------------------------|------------------------|-------------------------|
| Issue | Part | No. of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No. of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No. of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 70                              | 0.8                    | 0                       | 1     | 0    | 0                               | 0                      | 0                       | 1     | 0    | 59                              | 1.6                    | 2                       |
| 2     | 0    | 61                              | 0.8                    | 0                       | 2     | 0    | 0                               | 0                      | 0                       | 2     | 0    | 83                              | 1.4                    | 1                       |
| 3     | 0    | 58                              | 1.0                    | 1                       | 3     | 0    | 0                               | 0                      | 0                       | 3     | 0    | 75                              | 1.3                    | 4                       |
| 4     | 0    | 52                              | 1.0                    | 2                       | 4     | 0    | 0                               | 0                      | 0                       | 4     | 0    | 116                             | 0.9                    | 1                       |
| 5     | 0    | 60                              | 0.7                    | 3                       | 5     | 0    | 52                              | 0.8                    | 1                       | 5     | 0    | 98                              | 0.8                    | 5                       |
| 6     | 0    | 58                              | 0.8                    | 0                       | 6     | 0    | 74                              | 0.8                    | 1                       | 6     | 0    | 99                              | 1.6                    | 0                       |
| 7     | 0    | 70                              | 1.3                    | 2                       | 7     | 0    | 67                              | 0.7                    | 0                       | 7     | 0    | 136                             | 1.6                    | 0                       |
| 8     | 0    | 89                              | 1.0                    | 0                       | 8     | 0    | 102                             | 0.8                    | 2                       | 8     | 0    | 122                             | 1.1                    | 1                       |
| 9     | 0    | 49                              | 1.2                    | 0                       | 9     | 0    | 51                              | 0.5                    | 0                       | 9     | 0    | 126                             | 0.9                    | 0                       |
| 10    | 0    | 66                              | 1.4                    | 1                       | 10    | 0    | 99                              | 0.6                    | 0                       | 10    | 0    | 110                             | 0.8                    | 0                       |
| 11    | 0    | 89                              | 0.9                    | 1                       | 11    | 0    | 88                              | 1.0                    | 2                       | 11    | 0    | 164                             | 0.7                    | 2                       |
| 12    | 0    | 77                              | 1.4                    | 0                       | 12    | 0    | 100                             | 1.1                    | 1                       | 12    | 0    | 116                             | 0.7                    | 1                       |

### Acta Crystallographica Section E - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| inorganic compounds                    | 47              | 47                              | 0                           | 1.2                    | 49              | 37                              | 12                          | 0.7                    | 59              | 59                              | 0                           | 0.5                    |
| organic compounds                      | 508             | 508                             | 0                           | 1.0                    | 577             | 363                             | 214                         | 0.8                    | 792             | 792                             | 0                           | 1.1                    |
| metal-organic compounds                | 242             | 242                             | 0                           | 1.0                    | 295             | 232                             | 63                          | 0.9                    | 446             | 446                             | 0                           | 1.1                    |
| addenda and errata                     | 3               | 1                               | 2                           | 0.0                    | 2               | 1                               | 1                           | 0.0                    | 5               | 5                               | 0                           | 0.0                    |
| letters to the editor                  | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| editorial                              | 1               | 1                               | 0                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 2               | 2                               | 0                           | 0.0                    |
| issue preface                          | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| international union of crystallography | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| notes and news                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Acta Crystallographica Section E - 2001 |      |            |                         |              |                             |   |   |
|---|------|------------|-------------------------|--------------|-----------------------------|---|---|
| Issue                                   | Part | First page | Paper category          | ISI citation | Total IUCr citation to date | Authors   | Title   |
| 10                                      | 0    | o947       | organic compounds       | 21           | 19                          | Davies, J.E., <b>Bond, A.D.</b>   | Quinoline   |
| 9                                       | 0    | o901       | organic compounds       | 11           | 12                          | Jeyabharathi, A., Ponnuswamy, M.N., Amal Raj, A., Raghunathan, R., Razak, I.A., Usman, A., Chantrapromma, S., <b>Fun, H.-K.</b> | 3-Benzylidene-1'-methyl-4'-phenylcyclohexanespiro-3'-pyrrolidine-2'-spiro-3-indoline-2,2-dione  |
| 12                                      | 0    | m591       | metal-organic compounds | 10           | 11                          | Raj, S.B., <b>Muthiah, P.T.</b> , Bocelli, G., Righi, L.  | Tetraaqua(8-hydroxyquinoline-5-sulfonato-N,O)nickel(II) monohydrate   |
| 3                                       | 0    | m111       | metal-organic compounds | 9            | 3                           | Salami, T.O., Zavalij, P.Y., <b>Oliver, S.R.J.</b>  | BING-1: a tin-oxalate-sodium-fluoride framework, <a href="#">Na4Sn4(C2O4)3F6</a>  |
| 12                                      | 0    | o1179      | organic compounds       | 8            | 9                           | <b>Muthiah, P.T.</b> , Umadevi, B., Stanley, N., Shui, X., Eggleston, D.S.  | Hydrogen bonding patterns in trimethoprim sulfate trihydrate [trimethoprim = 2,4-diamino-5-(3,4,5-methoxybenzyl)pyrimidine]                 |
| 11                                      | 0    | o1100      | organic compounds       | 8            | 4                           | Jovanovic, J., Schurmann, M., <b>Preut, H.</b> , Spitteller, M.   | Second modification of (E)-2,3,2',3'-tetrahydro-[1,1']biindenyldiene  |
| 4                                       | 0    | m132       | metal-organic compounds | 8            | 1                           | Lucas, N.T., Notaras, E.G.A., <b>Humphrey, M.G.</b>   | <a href="#">W2Ir2(CO)10</a> ([bold eta]5- <a href="#">C5H4Me</a> )2   |
| 11                                      | 0    | o1029      | organic compounds       | 7            | 5                           | Zheng, Y., Zhuang, J.-P., <b>Zhang, W.-Q.</b> , Leng, X.-B., Weng, L.-H.  | r-1,c-2,t-3,t-4-1,3-Bis(4-methoxyphenyl)-2,4-bis(5-phenyl-1,3,4-oxadiazol-2-yl)cyclobutane 1,4-dioxane solvate                              |
| 12                                      | 0    | o1206      | organic compounds       | 7            | 6                           | Robert, J.J., Raj, S.B., <b>Muthiah, P.T.</b>   | N-H...O and O-H...O hydrogen bonds in crystal engineering: trimethoprim hydrogen glutarate  |
| 12                                      | 0    | o1242      | organic compounds       | 7            | 6                           | <b>Bond, A.D.</b> , Davies, J.E., Kirby, A.J.   | 2,6-Lutidine  |
| 6                                       | 0    | i38        | inorganic compounds     | 7            | 3                           | <b>Van Aken, B.B.</b> , Meetsma, A., Palstra, T.T.M.  | Hexagonal <a href="#">ErMnO3</a>  |
| 2                                       | 0    | m82        | metal-organic compounds | 7            | 3                           | Topcu, Y., Andac, O., <b>Yilmaz, V.T.</b> , Harrison, W.T.A.  | Bis(triethanolamine-N,O,O')nickel(II) bis(saccharinate)   |
| 8                                       | 0    | o751       | organic compounds       | 7            | 7                           | Rajagopal, K., Krishnakumar, R.V., Mostad, A., <b>Natarajan, S.</b>   | Glycinium maleate   |
| Acta Crystallographica Section E - 2002 |      |            |                         |              |                             |   |   |
| Issue                                   | Part | First page | Paper category          | ISI citation | Total IUCr citation to date | Authors   | Title   |
| 10                                      | 0    | m513       | metal-organic compounds | 9            | 9                           | Basker Raj, S., <b>Muthiah, P.T.</b> , Bocelli, G., Olla, R.  | Metal-binding modes in sulfoxines: supramolecular network in (8-hydroxyquinoline-5-sulfonato-N1,O8) sodium(I)                               |
| 12                                      | 0    | o1365      | organic compounds       | 7            | 3                           | <b>Wang, J.-L.</b> , Zhang, S.-M., Miao, F.-M.  | 4-[(2-Hydroxyphenylamino)phenylmethylene]-5-methyl-2-phenyl-2H-pyrazol-3(4H)-one  |
| 12                                      | 0    | o1333      | organic compounds       | 7            | 10                          | Shan, S., <b>Xu, D.-J.</b> , Wu, J.-Y., Chiang, M.Y.  | Acetophenone (2,4-dinitrophenyl)hydrazone   |
| 5                                       | 0    | m217       | metal-organic compounds | 6            | 7                           | Zhu, M., Lu, L., <b>Yang, P.</b> , Jin, X.  | Bis(1,1-dimethylbiguanido)copper(II) octahydrate  |
| 10                                      | 0    | o1142      | organic compounds       | 6            | 7                           | Stibrany, R.T., Schugar, H.J., <b>Potenza, J.A.</b>   | [bold kappa]2N13,N13'-Hydro-rac-2,2'-bis[2-(1-propylbenzimidazol-2yl)]biphenyl trifluoromethanesulfonate, the salt of a novel proton sponge |
| 6                                       | 0    | m272       | metal-organic compounds | 6            | 7                           | Zhu, M., Lu, L., <b>Yang, P.</b> , Jin, X.  | Bis(1,1-dimethylbiguanido)nickel(II)  |

|    |   |       |                         |   |   |   |   |
|----|---|-------|-------------------------|---|---|---|---|
| 12 | 0 | o1397 | organic compounds       | 6 | 6 | Bouchouit, K., <b>Benali-Cherif, N.</b> , Benguedouar, L., Bendheif, L., Merazig, H.            | Guaninium dinitrate dihydrate   |
| 11 | 0 | m622  | metal-organic compounds | 5 | 3 | Srinivasan, B.R., Dhuri, S.N., <b>Nather, C.</b> , Bensch, W.                                   | Ethylenediammonium tetrathiotungstate(VI)   |
| 12 | 0 | m691  | metal-organic compounds | 5 | 2 | Almeida Paz, F.A., Bond, A.D., Khimyak, Y.Z., <b>Klinowski, J.</b>                              | A one-dimensional CoII coordination polymer exhibiting an unusual conformation for 1,2-bis(4-pyridyl)ethane   |
| 6  | 0 | m287  | metal-organic compounds | 5 | 5 | <b>Okabe, N.</b> , Muranishi, Y.  | Aquaobis(quinoline-2-carboxylato-N,O)vanadium(IV) ethanol hemisolvate   |
| 11 | 0 | o1182 | organic compounds       | 5 | 3 | Yu, M., <b>Wang, J.-L.</b> , Miao, F.-M.  | 1,5-Dimethyl-4-[[ <i>(E)</i> -3-oxo-3-(2-thienyl)-1-(trifluoromethyl)-1-propenyl]amino]-2-phenyl-1,2-dihydro-3H-pyrazol-3-one                                   |
| 7  | 0 | o753  | organic compounds       | 5 | 6 | Vasuki, G., Thamotharan, S., <b>Parthasarathi, V.</b> , Ramamurthi, K., Dubey, S., Jindal, D.P. | 16-(2-Pyridylmethylene)androst-4-ene-3,17-dione   |
| 8  | 0 | o822  | organic compounds       | 5 | 6 | <b>Benali-Cherif, N.</b> , Benguedouar, L., Cherouana, A., Bendjeddou, L., Merazig, H.          | 1-Histidinium dinitrate   |
| 6  | 0 | o620  | organic compounds       | 5 | 4 | <b>Palusiak, M.</b> , Malecka, M., Grabowski, S.J., Epszajn, J., Bieniek, A., Kowalska, J.A.    | (3 <i>S</i> ,4 <i>R</i> )-4-(2,5-Dimethoxyphenyl)-8-methoxyisochroman-3-ol  |
| 9  | 0 | o994  | organic compounds       | 5 | 0 | <b>Coruh, U.</b> , Akdemir, N., Agar, E., Kim, Y., Erdonmez, A.                                 | Dimethyl 2,2'-(4,5-dicyano- <i>o</i> -phenylenedithio) diacetate  |
| 12 | 0 | m730  | metal-organic compounds | 5 | 0 | Almeida Paz, F.A., Bond, A.D., Khimyak, Y.Z., <b>Klinowski, J.</b>                              | catena-Poly[[[diaquacadmium(II)]-di- $\mu$ -4,4'-trimethylenedipyridine- $\kappa$ [2 <i>N</i> : <i>N'</i> ]] dinitrate 4,4'-trimethylenedipyridine monohydrate] |

#### Acta Crystallographica Section E - 2003

| Issue | Part | First page | Paper category          | ISI citation | Total IUCr citation to date | Authors   | Title   |
|-------|------|------------|-------------------------|--------------|-----------------------------|---|---|
| 3     | 0    | o378       | organic compounds       | 23           | 22                          | Vembu, N., <b>Nallu, M.</b> , Garrison, J., Youngs, W.J.            | 2,4-Dinitrophenyl 4-toluenesulfonate: molecular aggregation through weak C-H...O interactions                             |
| 11    | 0    | m1025      | metal-organic compounds | 20           | 18                          | You, Z.-L., Lin, Y.-S., Liu, W.-S., Tan, M.-Y., <b>Zhu, H.-L.</b>   | Bis[2-(cyclopropyliminomethyl)phenolato]zinc(II)  |
| 6     | 0    | o830       | organic compounds       | 20           | 19                          | Vembu, N., <b>Nallu, M.</b> , Garrison, J., Hindi, K., Youngs, W.J. | 4-Methoxyphenyl 4-toluenesulfonate: supramolecular aggregation through C-H...O and C-H... $\pi$ interactions              |
| 4     | 0    | o503       | organic compounds       | 20           | 20                          | Vembu, N., <b>Nallu, M.</b> , Garrison, J., Youngs, W.J.            | 2-Chlorophenyl 4-toluenesulfonate: molecular aggregation through weak C-H...O interactions                                |
| 6     | 0    | o776       | organic compounds       | 19           | 18                          | Vembu, N., <b>Nallu, M.</b> , Garrison, J., Youngs, W.J.            | Redetermination of 8-tosyloxyquinoline at 100 K: supramolecular aggregation through weak C-H...O and C-H...N interactions |
| 2     | 0    | o151       | organic compounds       | 15           | 15                          | <b>Yamin, B.M.</b> , Yusof, M.S.M.                                  | N-Benzoyl-N'-phenylthiourea   |
| 7     | 0    | o1009      | organic compounds       | 14           | 14                          | Vembu, N., <b>Nallu, M.</b> , Spencer, E.C., Howard, J.A.K.         | Methyl 4-tosyloxybenzoate: supramolecular aggregation through C-H...O, C-H... $\pi$ and $\pi$ - $\pi$ interactions        |
| 7     | 0    | o936       | organic compounds       | 14           | 14                          | Vembu, N., <b>Nallu, M.</b> , Garrison, J., Youngs, W.J.            | 4-Chlorophenyl 4-toluenesulfonate: supramolecular aggregation through C-H...O, C-H...Cl and C-H... $\pi$ interactions     |
| 7     | 0    | o1033      | organic compounds       | 13           | 13                          | Vembu, N., <b>Nallu, M.</b> , Spencer, E.C., Howard, J.A.K.         | 2-Naphthyl 4-toluenesulfonate: supramolecular aggregation through C-H...O and C-H... $\pi$ interactions                   |

|    |   |       |                         |    |    |   |  |
|----|---|-------|-------------------------|----|----|---|--|
| 1  | 0 | m38   | metal-organic compounds | 13 | 11 | Lyakhov, A.S., Gaponik, P.N., Degtyarik, M.M., <b>Ivashkevich, L.S.</b>                 | The chain structure of catena-poly[[2-tert-butyltetrazole-[bold kappa]N4)copper(II)]-di-[bold mu]-chloro]  |
| 11 | 0 | m1038 | metal-organic compounds | 12 | 12 | You, Z.-L., Qu, Y., Liu, W.-S., Tan, M.-Y., <b>Zhu, H.-L.</b>                           | trans-Bis{2-[3-(cyclohexylamino)propyliminomethyl]phenolato-[bold kappa]3O,N,N'}cobalt(III) perchlorate  |
| 7  | 0 | o1019 | organic compounds       | 12 | 12 | <b>Vembu, N.</b> , Nallu, M., Garrison, J., Youngs, W.J.                                | Benzene 1,3,5-tris(p-toluenesulfonate): supramolecular aggregation through extensive C-H...O, C-H...[bold pi] and [bold pi]-[bold pi] interactions   |
| 7  | 0 | o1000 | organic compounds       | 11 | 9  | <b>Ocak, N.</b> , Agar, A., Akdemir, N., Agar, E., Garcia-Granda, S., Erdonmez, A.      | 4,4'-(N-Phenyl-2,2'-iminodiethoxy)diphthalonitrile   |
| 8  | 0 | o1216 | organic compounds       | 11 | 11 | Vembu, N., <b>Nallu, M.</b> , Spencer, E.C., Howard, J.A.K.                             | Methyl 4-(3-nitrobenzenesulfonyloxy)benzoate   |
| 1  | 0 | m46   | metal-organic compounds | 10 | 10 | Raj, S.B., <b>Muthiah, P.T.</b> , Rychlewska, U., Warzajtis, B., Bocelli, G., O'lla, R. | The interplay of coordination, [bold pi]-[bold pi] stacking and hydrogen bonding in the supramolecular self-assembly of bis([bold mu]-7-iodo-8-hydroxyquinoline-5-sulfonato-[bold kappa]3N,O'O') bis[triaquanickel(II)] tetrahydrate |
| 8  | 0 | o1213 | organic compounds       | 10 | 12 | Vembu, N., <b>Nallu, M.</b> , Spencer, E.C., Howard, J.A.K.                             | Phenyl 3-nitrobenzenesulfonate   |

## Acta Crystallographica Section E - sales and circulation figures

### Institutional and consortial circulation totals

|                             | 2003 | 2004 |
|-----------------------------|------|------|
| Consortia site access       |      | 1734 |
| 1. Europe                   |      | 882  |
| 2. USA                      |      | 196  |
| 3. Canada                   |      | 32   |
| 4. Aus/NZ                   |      | 83   |
| 5. Japan                    |      | 86   |
| 6. Rest of World            |      | 455  |
| Institutional subscriptions | 5    | 6    |
| Online                      | 5    | 6    |
| Online Collection           | 0    | 0    |
| Personal subscriptions      | 2    | 3    |

### Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 2          | 0          |
|                               | Online Collection | 0          | 0          |
| <b>1. Europe Total</b>        |                   | <b>2</b>   | <b>0</b>   |
| 2. North America              | Online            | 2          | 3          |
|                               | Online Collection | 0          | 0          |
| <b>2. North America Total</b> |                   | <b>2</b>   | <b>3</b>   |
| 3. Aus/NZ                     | Online            | 0          | 1          |
| <b>3. Aus/NZ Total</b>        |                   | <b>0</b>   | <b>1</b>   |
| 4. Japan                      | Online            | 1          | 2          |

|                               |                   |          |          |
|-------------------------------|-------------------|----------|----------|
| <b>4. Japan Total</b>         |                   | <b>1</b> | <b>2</b> |
| 5. Rest of World              | Online            | 0        | 0        |
|                               | Online Collection | 0        | 0        |
| <b>5. Rest of World Total</b> |                   | <b>0</b> | <b>0</b> |
| <b>Grand Total</b>            |                   | <b>5</b> | <b>6</b> |

### APPENDIX 3 - Section C/E meeting, Chester, May 2005

#### Notes on Section C/E meeting

Monday 16 May, Chester

By Peter Strickland

Present: George Ferguson, Bill Clegg, David Watson, Peter Strickland, Sean Conway, Gillian Holmes, Brian [McMahon](#), Mike Hoyland

#### (1) Introduction of the new submission system for Sections C and E

The new submission system was demonstrated stage by stage and suggestions for improvements were discussed and a number of questions from the Chester staff answered.

(a) At stage 1 of submission, the authors should be offered only four paper categories: inorganic compounds, metal-organic compounds, organic compounds, and addenda and errata. Authors should have to explicitly choose a category in order to proceed.

(b) In-house CIF duplication checks during submission should be based on matching of the unit-cell parameters, symmetry and authors. Identical CIFs to those already uploaded should be stopped outright; resubmissions of the same paper should be sent to the Co-editor handling the paper; duplicate structures should be sent to the Co-editor handling the original paper; duplications of published papers should be sent to the original handling Co-editor if still active (or the Section Editor if not). Authors may be asked by the submission system to clarify their intentions in the above cases.

(c) Treatment of papers that are resubmitted very quickly after rejection with minimal changes and which then appear again after being rejected a second or third time - authors should be allowed a limited number of resubmissions of a paper. At some stage they need to be informed that no future submissions of a particular structure will be reviewed. This matter requires rewording of the Notes for Authors and should be discussed at JComm. It might also require a new database status of "permanently rejected".

(d) During submission and before Co-editor assignment, authors need to agree that they have complied with the ethical standards of the journal, i.e. that all authors have contributed to the work reported and that all those who have been involved with or provided funding for the work have been acknowledged. This would be on a combined page with copyright transfer. The wording on the page will make it clear that the crystallographic data should not be submitted elsewhere whilst under consideration for publication in an IUCr journal. Ideally, no items should be pre-bulleted and authors should be made to specifically select copyright transfer, etc. It is intended that acceptance of the ethical statement by the authors will obviate the need to ask the authors at a later stage if an acknowledgement section is required in their paper. Authors who do not agree with the ethical standards will not be able to complete their submission.

(e) At stage 4, the CONTINUE button should convey the following meaning: "when the Figures, Schemes and Structure Factors have been uploaded, click here to CONTINUE".

(f) At stage 4, structure factors should only be uploadable for structural datablocks present in the CIF. In the case of Section E where all papers are single structure, this means that authors should only be allowed to upload a single structure-factor file for the structural datablock.

(g) Authors and Co-editors need to be given instructions on handling series of papers by authors for Section E. The authors should give a general descriptive text in part 1 of a series and then have a shortened Comment section in subsequent papers. This should be added to Notes for authors. Quotas within the submission system may make it difficult for such series all to be handled by one Co-editor; the online submission instructions should let authors know what to do about this.

(h) The mechanism for deciding which Co-editors will be offered to the authors was discussed. One suggestion was that Co-editors who were furthest away from reaching their quota should be offered as default choice. Papers containing

VRFs for A alerts will be sent to a subset of Co-editors. Lists of Co-editors who would handle such papers were agreed.

- (i) At stage 5, the words "areas of expertise" should be removed; only the Co-editors names should be given here.
- (j) The submission instructions should make it clear that if an author wishes to abort a submission before it has been assigned to a Co-editor, then they need to contact [support@iucr.org](mailto:support@iucr.org). Chester will check papers that have been incompletely submitted on a regular basis and alert authors to this.
- (k) The words on the button for completion of a revision need to be reviewed.
- (l) Authors will only be able to upload revisions when explicitly allowed to do so by the Co-editor. The upload page for revisions will ask authors to contact the Co-editor if they wish to upload a revision.
- (m) Chester intend to put a series of papers through the system manually for Bill, David and George to test the system, before it is released to authors and Co-editors.
- (n) Co-editors will need to access their review pages via the status system. They will see new papers on their status pages, but will also be alerted to new papers by an email which gives the new Co-editor code. The options allowed for Section C and E Co-editors from their pages should include:

- (i) accept
- (ii) withdraw/reject
- (iii) simple revision (involving only email clarification)
- (iv) minor revision (involving uploading of some replacement files, but not a replacement CIF)
- (v) major revision (involving uploading of a new CIF).
- (vi) accept and transfer (initially an option for Section C Co-editors only to complete the paper and transfer it to Section E)

Each of the options will require email templates. George, Bill and David will send Chester suggested messages for this.

In the case of acceptance, the final edited CIF should be attached to the email message sent to the authors. This should include the standard phrasing noting that the proofs will be seen by the Section Editor and that further changes may be requested at this stage.

In case (v) the CIF should be checked as usual and any new A alerts handled by the authors.

(o) Full submission instructions are in the process of being written for the submission system. It was suggested that, depending on time constraints, a flyer might be produced about the new system for the summer meetings. In addition, the system will be demonstrated at the second open JComm meeting.

(p) The submission system needs to identify and return multi-structure E submissions.

## **(2) Co-editor workload**

It was agreed that we should go ahead with a pilot scheme for the transfer of papers from C to E with same Co-editor handling the paper through to acceptance. This means that Acta C Co-editors would need to (a) make an early decision as to whether the paper should be in C or E (so as not to waste referees time); (b) if considered appropriate for transfer, consult with the author about the transfer; (c) make sure that the paper was acceptable for Section E before completing the transfer and accepting the paper for Section E. In cases of poorly written articles this might include requesting the author to cut or drastically shorten the Comment and to rewrite the Abstract. If the author is unable to comply with this request or if the Co-editor judges at stage (a) that the paper is not suitable for either journal, then the paper should be swiftly rejected and no further submissions to C or E considered [see point 1(c)]. Chester will consider including a template mechanism within pubCIF to aid authors in writing Abstracts and short Comment sections, and also to aid authors in shortening their article.

George, Bill and David agreed to draft a joint letter to be sent to all Section C Co-editors to ask them whether they will take part in the above procedure as it would involve more work on their part, but would cut down the overall workload on the C and E boards.

Multistructure papers recommended for transfer would still probably need to go through a rejection cycle, as the papers would need to be split into multiple papers for Section E. Chester will try to think about the best procedure for such papers.

Conversely, Section E Co-editors made aware of the possibility that papers can potentially be transferred to Section C. The procedure would be for the Section E Co-editor to first contact George Ferguson, get his opinion and then ask the authors whether they would like to transfer the paper. This matter can be discussed further at the JComm meeting this summer.

It was agreed that publCIF would be a good tool for final viewing and editing of papers, particularly for Section E Co-editors. It would be helpful if publCIF could check (i) the alphabetic order of references, (ii) whether citations in the text were included in the reference list, and (iii) whether the reference was missing final page numbers. To aid B authors, George asked if publCIF could be used to output geometry and hydrogen-bond tables for inclusion in the submission pdf.

The possibility of including an extra plot in the checkCIF report to help with the review process was discussed. George Ferguson described how this is done manually: "As part of my proof-checking process I always generate a default PLUTON plot showing the labelled unit-cell box and then type in the command ARU NONE at the bottom of the PLATON screen. This shows the bare labelled asymmetric-unit atoms in the unit cell. It is then easy to compare this with whatever diagrams are in the paper." Chester will investigate whether an automated diagram can be produced in this way to aid the work of Co-editors.

### **(3) Section Editor workload**

Changes that are required on a frequent basis at the proof stage should be reported to Chester, as these might potentially be handled by software in Chester or by validation alerts. Bill will talk at the second open JComm meeting on frequent problems with Section E papers.

Stylistic points were discussed. It was agreed that if moiety formulae are split at the dot at the end of a line, then insertion of a hyphen was appropriate. It was noted that "b" and "alpha" are incorrectly reported for trigonal structures.

It was also noted that the program to generate key indicators does not work correctly for powder papers. It also misses some cases of disorder and no H atoms found gives a key indicator of 1% completeness, not 0%.

It was discussed if the locations of maximum and minimum electron-density peaks greater than  $1 \text{ e } \text{\AA}^{-3}$ , since they are required by Notes for Authors and their absence queried by the Section Editors, could be made new data items. Another approach would be to make Co-editors more aware of this requirement.

### **(4) Planning**

#### **(a) Planning for further growth**

Projections of possible growth were considered. The growth of Section C seems to be under control and there were no concerns about this. The growth of Section E appears to be out of control and the situation will require discussion at JComm in the summer when various scenarios need to be put forward to the Co-editors (these should also be put to Section E Co-editors who are not attending JComm). The Chester view was that growth above 8000 pages would require a rethink of the journal policy, e.g. a shorter article format to allow quicker reviewing.

#### **(b) Long-term planning**

George, Bill and David plan to continue until 2008, but ways should be found to keep the workload within reason.

George has a number of potential names of successors. He will talk to these candidates in the summer to see if they would be interested in taking on the position after 2008.

Bill and David were encouraged to think about potential candidates, and to ask some of these to help with sharing their current workload on proofs (perhaps in the role of Deputy Section Editor). The downside could potentially be lower consistency in the way in which the proofs are handled.

### **(5) Poorly written articles**

It was agreed that there should be a discussion at JComm about language of publication, and whether only English should be supported in future.

The Section E Notes for authors will be changed to put the emphasis on the authors for correcting poorly written articles.

Co-editors will be encouraged to look at requesting the shortening of poorly written articles as a possible way to allow acceptance. This would require asking the authors to rewrite the Abstract and to remove some/all of the Comment. Poorly written text might be moved to special details fields in the CIF. Chester will consider how publCIF might be used in this process.

Reintroduction of a "Related Literature" section or the use of a standard sentence about related literature could facilitate the deletion of Comment text without leaving trailing references or risking reducing the number of citations to our journals.

## **(6) Change in page design to allow automatic, or more automatic make up**

Chester will put forward any ideas on this in the summer. The online date will be removed from the PDF version of the article to allow increased automation.

## **(7) Financing the growth of Sections C and E**

The possibilities for financing the growth of the journals were discussed. No conclusions were reached.

## **(8) External duplication checking**

Chester will follow up the matter of real-time duplication checking with CCDC. This could potentially be used to give A alerts for duplication on submission.

A case had been discovered where a Cambridge duplication check had not given a hit against a pre-release structure; David will investigate this.

## **(9) Handling papers with a large number of authors**

Papers with six or more authors will in future generate an A alert. In the VRF the author will be asked to define the role of each coauthor in contributing to the paper.

## **(10) Preparation of the agenda items relating to Sections C and E for the closed JComm meeting**

It was agreed that it would be appropriate to have a B/C/E meeting, followed by a joint C/E meeting to fill the rest of the time allocated for individual journal meetings on the afternoon of 22 August. Bill reiterated the need for the differences between the journals to be clear.

The agenda for the 2002 B/C/E meeting was reviewed and items appropriate for inclusion in the agenda this summer were selected.

## **(11) Any other business**

It would be useful if the Section E cover could be generated so that molecules with crystallographic symmetry could be included. Chester might consider the use of Mercury for generating the cover and will check when they next meet with CCDC whether there is now a command-line interface for Mercury that would allow automated scripts to be written.

## **Comments on the Acta C/E Meeting**

By John R Helliwell

The purpose of this summary is to present feedback to the IUCr Finance Committee the results of the meeting they requested in March 2005. It is accompanied by the detailed notes drawn up by IUCr Chester.

The aims of the meeting were to address the situations of:

- (i) Large numbers of poorly written articles submitted to Acta C and E
- (ii) An exponential rise of Acta E submissions
- (iii) Continuing the development of the distinct identities of Acta C and E alongside Acta Cryst B of course (see the B/C/E current promotional leaflet for IUCr Florence Congress, also available now for FC members)

Specifically the context of the meeting was:

- (i) Acta C and E are receiving large numbers of poorly written articles especially from China.
- (ii) Acta E's total number of pages published is now very large; as one measure of this after only 2.5 years its annual number of pages is at a level of being a large fraction of all of Acta Cryst published pages (46% in 2004).
- (iii) Acta C is developing a distinct identity from Acta E, and B, and it has been agreed that the science impact of each of its papers should be increased with an early objective of an average impact factor for the Journal of >1.0.

Recommendations:

- (i) A streamlined submission system could assist authors both in number of submissions and especially those with an inadequate command of the English language. A streamlined submission system might also be devisable to assist Co-editors. The latter benefit would lead to some extra capacity in number of submissions which could be handled by E Co-editors on the one hand and freeing up time for C Co-editors to concentrate on science impact of papers on the other hand. Such a system has been worked on by Chester over the last two years and is ready for implementation in the next two months. It is described in detail here in the accompanying Notes.
- (ii) In spite of Recommendation (i) it is agreed that there is very little new staff capacity left and specifically 8000 pages is the absolute maximum possible publishable number of pages per year for Acta E from the points of view of (a) Chester staff levels (b) number of E Co-editors and (c) Section Editor workload. In any case there are also no new

business models offered which would substantially increase either the Chester staffing or the number of E Co-editor numbers. Nb the estimate of 8000 pages maximum is a preliminary one and whereby a detailed mapping of Acta E Co-editors' and Chester staff time with the new submission system and with the efficiency gains identified has yet to be done. In particular there has been very little chance yet to discuss these plans with the E Co-editors.

(iii) A significant gain in the operational smoothness would be had if Acta C Co-editors might agree to accept for E those C submissions better suited for Acta E. A major problem category within this group of C-transfer-to-E submissions is the poorly written articles. New measures are proposed for this sub-group where authors will be invited to considerably shorten their comment sections and also rewrite their science descriptions. These major revisions would be supervised by their C Co-editor on a maximum of two occasions only i.e. after that the paper would have to be declared rejected. Nb the purpose of this approach, which will be at the expense of some Acta C Co-editors' time, is to foster the role of IUCr to be helpful to a global cohort of authors i.e. including China. It is not at all an ideal solution and indeed might be perceived by some C Co-editors as a distraction from their main mission, which should be science impact and detailed molecular structure quality in C papers. Thus C Co-editors will be invited to volunteer for this extra workload. It should be stressed as well that this is not a full solution to the problem; methods must be found by the journal and in the countries themselves to solve these problems.

(iv) After rejection a lot of authors are immediately resubmitting, hoping for a new Co-editor. New duplication checks will avoid this. In cases of genuine attempts to revise articles a maximum number of only two resubmissions will be allowed is recommended.

(v) A significant, albeit smaller problem, is the one of following ethical guidelines. Specifically there are a sizeable number of submissions where the number of authors is too large to be credible. The C and E Co-editors are then left with 'arguing' with authors to shorten the authors' list. Instead the submission system in future will require each author's role to be declared for papers with six or more authors. There will not be roles for e.g. honorary co-authorship situations like 'Head of Department' or for multiple responsible authors for 'data collection' or 'chemical synthesis'. A safety valve will have to be planned for where the Section Editors can be contacted in special cases. The converse ethical problem (i.e. ensuring all those that have taken part are acknowledged) will also be handled in the submission system.

(vi) An efficiency gain would stem from the use of a related literature paragraph within a condensed Comment section. Moreover this will improve the ethical aspect of the (many) cases where relevant papers are not referenced. Chester offer creation of this paragraph within a new CIF submission tool.

(vii) There may be an efficiency gain, albeit small, in allowing only English language submissions. There are very few non-English language submissions but they do cause significant extra amount of work for Chester. It is recommended that for Acta E especially, but also Acta C, that English be the sole allowed language.

(viii) Extending real time duplication checking to the CSD would result in more timely reports. A reduction in the number of duplicate structures submitted is possible only if we can persuade authors to search the relevant database and make an honest assessment of whether their proposed paper adds anything of significance to what has already been published.

# Acta D/F agenda

Grand Hotel Panoramic, Montecatini Terme, Italy

22 August, 13:45-17:25

**CHAIR: Ted Baker**

Attendees: Acta D/F Editors and Co-editors, and any other interested Editors

IUCr staff attending: Louise Jones

## 1. ACTA D AND F

### 1.1. GENERAL

This item is intended to cover general matters related to Acta D and F and to give the Editors or Co-editors the chance to raise important issues related to the journals that are not covered elsewhere in the agenda.

Some general points for discussion are as follows:

#### 1.1.1. Scope of D/F

Is the division between D/F clear?

Are any measures required to make the division clearer?

#### 1.1.2. NMR

Should D and F cover NMR?

If so, should a joint Co-editor be appointed?

Who would be an appropriate candidate?

#### 1.1.3. Should we publish sequences?

#### 1.1.4. Should we ask for EC numbers?

#### 1.1.5. How should stereoviews best be rendered in the online journals?

#### 1.1.6. How can we make sure authors deposit structure factors as well as coordinates?

### 1.2. ACTABIOSTANDARDS

The Actabiostandards mailing list has been set up to discuss matters relating to Acta D and F. Topics that have been under discussion are given below. Editors' views on these issues will be welcome at the meeting.

#### 1.2.1. Should Crystallization Communications contain information on electron density, refinement, final R, etc.?

#### 1.2.2. What should be the criterion for assigning the resolution limit of a diffraction data set?

1.2.3. An incorrect Rmerge formula is regularly appearing in manuscripts. Authors in D and F sometimes use erroneous formulae for Rmerge that are apparently copies from other Acta D (or F) papers (often the error is in the wrong denominator).

#### 1.2.4. Repetition of data: unit-cell parameters and other data are often described in the text and listed in the Table(s).

1.2.5. Sometimes descriptions of sample preparation in Crystallization Communications are replaced by references to other publications. This may mean that key data are missing for the reader or referee and they will have to track down that reference to know the actual sequence of the object of study or the actual composition of the protein solution.

1.2.6. A significant fraction of crystallization communications have initial trials which use commercial kits, where optimization is said to have occurred, but where optimized conditions are not specified. We should encourage authors to specify all of these conditions.

### 1.3. SUBMISSION AND REVIEW

Are the status pages useful?

What new submission system features would be useful for Co-editors?

How can the Notes for referees be improved?

How can the review form be improved before it is implemented online?

Are there any measures that would improve the consistency of the review process?

Are the documentation and help pages for authors, editors and referees clear?

Above what number of authors would it be reasonable to ask for the roles of the authors?

Some more specific D/F points are as follows:

A pilot scheme is currently being set up for the transfer of papers from Section C to Section E with same Co-editor handling the paper through to acceptance. More details of this are given in the Section C/E agenda notes. Would it be useful to have the same mechanism for the D/F borderline?

Are the current procedures for handling "crystallization" papers working?

Work has been carried out by Howard Einspahr, the PDB and the Editorial Office on a new submission mechanism that involves predeposition at the PDB, followed by submission of an mmCIF file to Chester. This more automated procedure opens up a number of possibilities including providing the authors with tabular material derived from the mmCIF and also allows validation reports to be created for reviewers. The first stage of the process has been to develop a list of recommended information for inclusion in the journals. The list will be useful for authors of Acta D or F. We expect to start to implement the submission procedure over the coming months and will need testers for this. So far we have identified a number of potential testers: Paula Fitzgerald, Ryan Kniewel, Gideon Davies, Marc Whitlow, Mark Chance, Tom Terwilliger, Sun-ho Kim and Andrzej Joachimiak. Do Editors have any other suggestions for testers?

Should validation reports be available for all structural papers in both journals i.e. should authors of Acta D papers also be encouraged to provide an mmCIF?

Should structure factors also be available for Editors and reviewers?

## **1.4. JOURNAL PROMOTION AND SPONSORSHIP**

### **1.4.1. Promoting the journals using a marketing leaflet**

Leaflets for both journals have been created. Do you have any suggestions for improvement? Do they target the correct audience?

### **1.4.2. Where can D and F be promoted?**

The journals have been promoted at a number of recent meetings: ISGO, ICCBM10, West Coast Protein Crystallography Workshop, Recent Advances in Macromolecular Crystallization, ACA. Where else should we advertise? Which future meetings should be covered?

### **1.4.3. In what other ways can Acta D and F be promoted?**

Should we have additions to ealerts, proofs message etc.? Do these get noticed?

### **1.4.4. How can advertising/sponsorship revenues be increased?**

Are there any companies you think would advertise in the journals or on the web pages?

Acta F is sponsored by Molecular Dimensions, Jena Bioscience, Greiner Bo-one; is there anyone else who would be interested in sponsoring Acta D or F?

## **2. ACTA D**

### **2.1. GENERAL**

This item is intended cover general matters related to Acta D and to give the Editors or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

### **2.2. JOURNAL DEVELOPMENT**

#### **2.2.1. Scientific development**

Are there any new related scientific areas that are developing that the journal should cover?

If yes, should an appointment be made to the Board to cover this area?

Would a special issue on such developments be worthwhile?

Are there other areas on which special issues should be commissioned?

Does the expertise on the Board cover the aims and scope of the journal well, or are new appointments needed?

How can we ensure good editors for conference proceedings?

#### **2.2.2. Submissions**

How can we encourage more submissions to Section D?

Are there any ideas on how an increase in submissions might be achieved?

What sort of papers should we be trying to attract and how can we encourage their submission?

#### **2.2.3. Impact factor**

Is there any way that the journal impact factor can be increased?

Are there particular categories of paper that should be encouraged/discouraged?

Are there particular topics that are more highly cited?

Are there particular authors that should be encouraged to write for the journal?

How successful have special issues been? Should we cover ICCBM11? Should we investigate covering the Gordon Research Conference on Diffraction Methods in Structural Biology (July 2006; Co-Chairs: Paul Adams & Elspeth Garman)? Should the journal (or JSR) cover the BIOXHIT meeting?

Should we try to commission papers on well known programs such as MOSFLM? (A number of authors will be present at the Biological Commission meeting during the Congress.)

2.2.4. Lead articles/topical reviews  
What topics should be considered?  
Who are potential candidate authors?

2.2.5. Publication speed  
Are there any ways in which we can increase publication speed or otherwise improve services to authors?

### **2.3. JOURNAL DESIGN**

2.3.1. PRINT:  
Is the present design of the journal satisfactory?  
Are there any items that can be removed from the print version of the journal?

2.3.2. ONLINE:  
Is the present design of the online journal satisfactory?  
Are there any areas that can be improved on or any items that need to be included or made more prominent?

### **2.4. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors.

### **2.5. USE OF COLOUR**

Should the Notes for Authors be made stricter on the use of colour?  
Should the Notes for Reviewers be modified to emphasize restrictions in the use of colour to reviewers?  
Should Main and Section Editors review all colour at the proof stage?  
Should colour only be allowed online?  
If so, can the caption in the printed journal refer to colour?  
Should the journal charge for colour?

## **3. ACTA F**

### **3.1. GENERAL**

This item is intended cover general matters related to Acta F and to give the Editors or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

#### 3.1.1. Review board

The idea of a review board (i.e. a set of reviewers who agree to handle a defined number of papers per year for a journal) has been suggested for Section F. The views of the meeting on this idea are welcomed. Any work in this area would most likely be a pilot project involving one or two Section F Editors, with the results reported back to JComm.

#### 3.1.2. Coverage by Medline

#### 3.1.3. "Commissioning" protein structure/genomics communications

The "commissioning" of protein structure/genomics communications should continue. Other sources of structural papers include unpublished structures already in the PDB. Should we invite depositors of such structures to write articles?

The Editors and the Editorial Office have been working with the New York Structural Genomics Research Consortium on their Autopublish program. If Editors are aware of similar projects for automated generation of protein structure/genomics papers, we would be happy to look into working with these.

#### 3.1.4. Other matters

Should two-structure articles be allowed?  
Should we be prepared to accept less than "fully refined" structures provided the degree of refinement is noted and the data (structure factors and coordinates are deposited in the PDB)?  
Should all/some/any items in the crystallization and/or structural data lists be made mandatory?  
How can the cover illustration be varied?

### **3.2. JOURNAL DEVELOPMENT**

#### 3.2.1. Scientific development

Are there any new related scientific areas that are developing that the journal should cover?  
If yes, should an appointment be made to the Board to cover this area?  
Does the expertise on the Board cover the aims and scope of the journal well, or are new appointments needed?

#### 3.2.2. Submissions

How can we encourage more submissions to Section F?  
Are there any ideas on how an increase in submissions might be achieved?

What sort of papers should we be trying to attract and how can we encourage their submission?

### 3.2.3. Publication speed

Are there any ways in which we can increase publication speed or otherwise improve services to authors?

### **3.3. JOURNAL DESIGN**

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

Do the arrangements for the covers need to be modified?

### **3.4. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors.

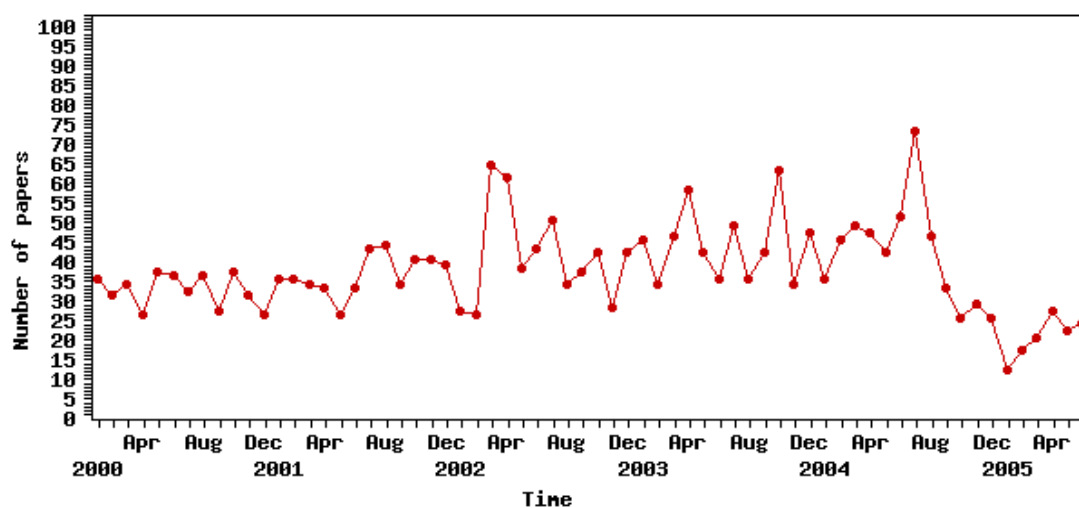
### **4. MATTERS ARISING FROM THE GENERAL AGENDA**

## APPENDIX - Background information on Section D

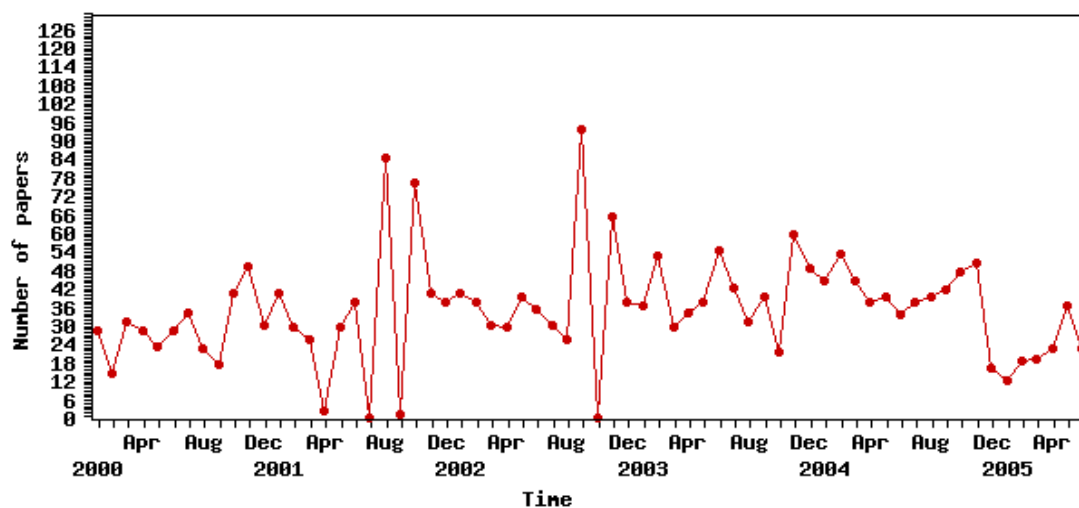
### Aims and scope

Acta Crystallographica Section D: Biological Crystallography welcomes the submission of papers covering any aspect of structural biology with a particular emphasis on the structures of biological macromolecules and the methods used to determine them. Reports on new protein structures are particularly encouraged, as are papers on crystallographic binding studies, structural analysis of mutants and other structure-function studies. Refinements of previously known structures may be published if sufficient new information is presented. Papers on crystallographic methods should be oriented towards biological crystallography, and may include new approaches to any aspect of structure determination or analysis. Papers on the crystallization of biological molecules will be accepted providing that these focus on new methods or other features that are of general importance or applicability.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Acta Crystallographica Section D

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1748  |
| Institutional subscribers | 576   |
| Individual subscribers    | 120   |
| Impact Factor (2004)      | 1.693 |
| Ranking (2004)            | 8/24  |

### Acta Crystallographica Section D - competing journals based on citing

Number of times articles published in 2003 (in journals below) cited articles published in *Acta Crystallographica Section D*

| Citing Journal      | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|---------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS        | 8527    | 207  | 873  | 946  | 725  |                      |
| ACTA CRYSTALLOGR D  | 1498    | 75   | 200  | 197  | 144  | 2.208                |
| J BIOL CHEM         | 1007    | 21   | 77   | 78   | 67   | 6.482                |
| J MOL BIOL          | 804     | 11   | 55   | 75   | 59   | 5.239                |
| BIOCHEMISTRY-US     | 463     | 2    | 24   | 39   | 20   | 3.922                |
| STRUCTURE           | 416     | 9    | 37   | 35   | 19   | 5.993                |
| METHOD ENZYMOL      | 297     | 6    | 47   | 43   | 34   | 1.618                |
| NAT STRUCT BIOL     | 238     | 6    | 14   | 25   | 13   | 11.579               |
| P NATL ACAD SCI USA | 238     | 5    | 11   | 22   | 11   | 10.272               |
| EMBO J              | 222     | 3    | 11   | 20   | 17   | 10.456               |

### Acta Crystallographica Section D - list of cited journals

Number of times articles published in journals below (in years below) was cited in *Acta Crystallographica Section D* in 2003

| Citing Journal      | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|---------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS        | 11364   | 289  | 780  | 983  | 909  |                      |
| ACTA CRYSTALLOGR D  | 1498    | 75   | 200  | 197  | 144  | 2.208                |
| J MOL BIOL          | 806     | 9    | 36   | 55   | 55   | 5.239                |
| J BIOL CHEM         | 584     | 17   | 62   | 54   | 49   | 6.482                |
| METHOD ENZYMOL      | 557     | 0    | 4    | 4    | 3    | 1.618                |
| BIOCHEMISTRY-US     | 433     | 4    | 26   | 42   | 35   | 3.922                |
| ACTA CRYSTALLOGR A  | 402     | 2    | 8    | 7    | 8    | 1.558                |
| J APPL CRYSTALLOGR  | 393     | 6    | 15   | 14   | 13   | 2.324                |
| P NATL ACAD SCI USA | 347     | 5    | 36   | 34   | 38   | 10.272               |
| NATURE              | 313     | 4    | 8    | 11   | 20   | 30.979               |

### Acta Crystallographica Section D - citation report by issue

Special issues are shaded.

| 2001  |      |                                  |                        |                         | 2002  |      |                                  |                        |                         | 2003  |      |                                  |                        |                         |
|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|
| Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 28                               | 9.0                    | 0                       | 1     | 0    | 36                               | 3.4                    | 0                       | 1     | 0    | 38                               | 4.4                    | 0                       |
| 2     | 0    | 40                               | 3.8                    | 0                       | 2     | 0    | 40                               | 2.8                    | 0                       | 2     | 0    | 36                               | 3.5                    | 0                       |
| 3     | 0    | 26                               | 5.0                    | 0                       | 3     | 0    | 37                               | 4.5                    | 0                       | 3     | 0    | 47                               | 2.9                    | 0                       |
| 4     | 0    | 26                               | 5.7                    | 0                       | 4     | 0    | 30                               | 2.3                    | 0                       | 4     | 0    | 31                               | 2.4                    | 0                       |
| 5     | 0    | 29                               | 4.1                    | 0                       | 5     | 0    | 29                               | 2.8                    | 0                       | 5     | 0    | 31                               | 2.2                    | 0                       |
| 6     | 0    | 37                               | 2.6                    | 0                       | 6     | 1    | 5                                | 15.6                   | 0                       | 6     | 0    | 37                               | 2.5                    | 0                       |
|       |      |                                  |                        |                         | 6     | 2    | 32                               | 2.8                    | 0                       |       |      |                                  |                        |                         |
| 7     | 0    | 20                               | 7.1                    | 0                       | 7     | 0    | 35                               | 3.0                    | 0                       | 7     | 0    | 54                               | 3.3                    | 0                       |
| 8     | 0    | 32                               | 5.9                    | 0                       | 8     | 0    | 30                               | 1.6                    | 0                       | 8     | 0    | 40                               | 1.8                    | 0                       |
| 9     | 0    | 31                               | 4.3                    | 0                       | 9     | 0    | 25                               | 2.0                    | 0                       | 9     | 0    | 31                               | 1.6                    | 0                       |
| 10    | 0    | 19                               | 13.9                   | 0                       | 10    | 1    | 52                               | 2.4                    | 0                       | 10    | 0    | 39                               | 1.8                    | 0                       |
|       |      |                                  |                        |                         | 10    | 2    | 31                               | 2.8                    | 0                       |       |      |                                  |                        |                         |
| 11    | 0    | 56                               | 2.5                    | 0                       | 11    | 0    | 12                               | 6.1                    | 0                       | 11    | 0    | 20                               | 4.0                    | 0                       |
| 12    | 0    | 40                               | 4.8                    | 0                       | 12    | 0    | 52                               | 1.9                    | 0                       | 12    | 0    | 58                               | 1.6                    | 0                       |

## Acta Crystallographica Section D - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| research papers                        | 142             | 142                             | 0                           | 9.8                    | 204             | 204                             | 0                           | 4.7                    | 168             | 168                             | 0                           | 4.2                    |
| crystallization papers                 | 207             | 207                             | 0                           | 1.8                    | 219             | 219                             | 0                           | 1.3                    | 247             | 247                             | 0                           | 1.4                    |
| short communications                   | 30              | 30                              | 0                           | 5.8                    | 17              | 17                              | 0                           | 2.1                    | 31              | 31                              | 0                           | 3.7                    |
| structural genomics papers             | 0               | 0                               | 0                           | 0.0                    | 2               | 2                               | 0                           | 8.0                    | 5               | 5                               | 0                           | 4.4                    |
| lead articles                          | 0               | 0                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 8.0                    | 0               | 0                               | 0                           | 0.0                    |
| topical reviews                        | 1               | 1                               | 0                           | 12.0                   | 0               | 0                               | 0                           | 0.0                    | 7               | 7                               | 0                           | 4.1                    |
| letters to the editor                  | 1               | 1                               | 0                           | 2.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| scientific comment                     | 1               | 1                               | 0                           | 1.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| addenda and errata                     | 1               | 1                               | 0                           | 1.0                    | 2               | 2                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 0.0                    |
| book reviews                           | 5               | 0                               | 5                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| books received                         | 1               | 0                               | 1                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 2               | 0                               | 2                           | 0.0                    |
| editorial                              | 0               | 0                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 0.0                    | 3               | 2                               | 1                           | 0.0                    |
| international union of crystallography | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 2               | 1                               | 1                           | 0.0                    |
| issue preface                          | 1               | 0                               | 1                           | 0.0                    | 3               | 0                               | 3                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| notes and news                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| new commercial products                | 0               | 0                               | 0                           | 0.0                    | 12              | 0                               | 12                          | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| meeting reports                        | 1               | 1                               | 0                           | 2.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| obituaries                             | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Acta Crystallographica Section D - 2001 |      |            |                      |              |                             |   |   |
|---|------|------------|----------------------|--------------|-----------------------------|---|---|
| Issue                                   | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors                                   | Title   |
| 1                                       | 0    | 122        | research papers      | 111          | 13                          | Winn, M.D., Isupov, M.N., Murshudov, G.N. | Use of TLS parameters to model anisotropic displacements in macromolecular refinement                                       |
| 10                                      | 0    | 1367       | research papers      | 103          | 34                          | Navaza, J.                                | Implementation of molecular replacement in <a href="#">AMoRe</a>  |
| 10                                      | 0    | 1373       | research papers      | 53           | 39                          | Read, R.J.                                | Pushing the boundaries of molecular replacement with maximum likelihood   |
| 8                                       | 0    | 1201       | short communications | 40           | 5                           | Harris, M., Jones, T.A.                   | Molray - a web interface between O and the POV-Ray ray tracer   |
| 12                                      | 0    | 1755       | research papers      | 40           | 17                          | Terwilliger, T.C.                         | Maximum-likelihood density modification using pattern recognition of structural motifs                                      |
| 3                                       | 0    | 401        | research papers      | 38           | 8                           | Harding, M.M.                             | Geometry of metal-ligand interactions in proteins   |
| 2                                       | 0    | 239        | research papers      | 30           | 14                          | Dauter, Z., Li, M., Wlodawer, A.          | Practical experience with the use of halides for phasing macromolecular structures: a powerful tool for structural genomics |

|    |   |      |                 |    |    |   |   |
|----|---|------|-----------------|----|----|---|---|
| 7  | 0 | 1013 | research papers | 29 | 21 | <b>Levitt, D.G.</b>   | A new software routine that automates the fitting of protein X-ray crystallographic electron-density maps   |
| 10 | 0 | 1445 | research papers | 29 | 13 | <b>Perrakis, A.</b> , Harkiolaki, M., Wilson, K.S., Lamzin, V.S.                    | ARP/wARP and molecular replacement  |
| 9  | 0 | 1230 | research papers | 26 | 27 | <b>Gordon, E.J.</b> , Leonard, G.A., <a href="#">McSweeney, S.</a> , Zagalsky, P.F. | The C1 subunit of [alpha]-crustacyanin: the de novo phasing of the crystal structure of a 40 kDa homodimeric protein using the anomalous scattering from S atoms combined with direct methods |
| 7  | 0 | 990  | research papers | 23 | 24 | <b>Dauter, Z.</b> , Adamiak, D.A.   | Anomalous signal of phosphorus used for phasing DNA oligomer: importance of data redundancy   |

#### Acta Crystallographica Section D - 2002

| Issue | Part | First page | Paper category             | ISI citation | Total IUCr citation to date | Authors   | Title  |
|-------|------|------------|----------------------------|--------------|-----------------------------|---|--|
| 6     | 1    | 899        | research papers            | 66           | 16                          | <b>Berman, H.M.</b> , Battistuz, T., Bhat, T.N., Bluhm, W.F., Bourne, P.E., Burkhardt, K., Feng, Z., Gilliland, G.L., Iype, L., Jain, S., Fagan, P., Marvin, J., Padilla, D., Ravichandran, V., Schneider, B., Thanki, N., Weissig, H., Westbrook, J., Zardecki, C.   | The Protein Data Bank  |
| 10    | 2    | 1772       | research papers            | 53           | 54                          | Schneider, T.R., <b>Sheldrick, G.M.</b>   | Substructure solution with SHELXD  |
| 3     | 0    | 494        | research papers            | 35           | 35                          | <b>Dauter, Z.</b> , Dauter, M., Dodson, E.J.  | Jolly SAD  |
| 6     | 2    | 968        | research papers            | 34           | 21                          | Morris, R.J., Perrakis, A., <b>Lamzin, V.S.</b>   | ARP/wARP's model-building algorithms. I. The main chain  |
| 11    | 0    | 1937       | research papers            | 31           | 13                          | <b>Terwilliger, T.C.</b>  | Automated structure solution, density modification and model building  |
| 1     | 0    | 21         | research papers            | 20           | 21                          | Micossi, E., Hunter, W.N., <b>Leonard, G.A.</b>   | De novo phasing of two crystal forms of tryptaredoxin II using the anomalous scattering from S atoms: a combination of small signal and medium resolution reveals this to be a general tool for solving protein crystal structures |
| 2     | 0    | 195        | research papers            | 17           | 6                           | <b>Schneider, T.R.</b>  | A genetic algorithm for the identification of conformationally invariant regions in protein molecules  |
| 7     | 0    | 1129       | research papers            | 17           | 0                           | Nureki, O., Shirouzu, M., Hashimoto, K., Ishitani, R., Terada, T., Tamakoshi, M., Oshima, T., Chijimatsu, M., Takio, K., Vassilyev, D.G., Shibata, T., Inoue, Y., Kuramitsu, S., <b>Yokoyama, S.</b>  | An enzyme with a deep trefoil knot for the active-site architecture  |
| 3     | 0    | 459        | research papers            | 15           | 11                          | Kriminski, S., Caylor, C.L., Nonato, M.C., Finkelstein, K.D., <b>Thorne, R.E.</b>   | Flash-cooling and annealing of protein crystals  |
| 1     | 0    | 70         | research papers            | 15           | 2                           | Hall, D.R., Hadden, J.M., Leonard, G.A., Bailey, S., Neu, M., Winn, M., <b>Lindley, P.F.</b>  | The crystal and molecular structures of diferric porcine and rabbit serum transferrins at resolutions of 2.15 and 2.60 Å, respectively   |
| 12    | 0    | 2109       | structural genomics papers | 15           | 11                          | Sulzenbacher, G., Gruez, A., Roig-Zamboni, V., Spinelli, S., Valencia, C., Pagot, F., Vincentelli, R., Bignon, C., Salomoni, A., Grisel, S., Maurin, D., Huyghe, C., Johansson, K., Grassick, A., Roussel, A., Bourne, Y., Perrier, S., Miallau, L., Cantau, P., Blanc, E., Genevois, M., Grossi, A., Zenatti, A., Campanacci, V., <b>Cambillau, C.</b> | A medium-throughput crystallization approach   |
| 1     | 0    | 39         | research papers            | 14           | 0                           | Benson, S.D., Bamford, J.K.H., Bamford, D.H., <b>Burnett, R.M.</b>  | The X-ray crystal structure of P3, the major coat protein of the lipid-containing bacteriophage PRD1, at 1.65 Å resolution   |

| 4  | 0    | 645        | research papers      | 14           | 6                           | Ng, J.D., Sauter, C., Lorber, B., Kirkland, N., Arnez, J., <b>Giege, R.</b>   | Comparative analysis of space-grown and earth-grown crystals of an aminoacyl-tRNA synthetase: space-grown crystals are more useful for structural determination              |
|--|------|------------|----------------------|--------------|-----------------------------|---|--|
| 3  | 0    | 441        | research papers      | 14           | 4                           | Berisio, R., Sica, F., Lamzin, V.S., Wilson, K.S., Zagari, A., <b>Mazzarella, L.</b>                                | Atomic resolution structures of ribonuclease A at six pH values  |
| <b>Acta Crystallographica Section D - 2003</b> |      |            |                      |              |                             |   |  |
| Issue  | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors   | Title  |
| 7  | 0    | 1131       | research papers      | 37           | 9                           | <b>Potterton, E.</b> , Briggs, P., Turkenburg, M., Dodson, E.   | A graphical user interface to the CCP4 program suite   |
| 1  | 0    | 38         | research papers      | 36           | 13                          | <b>Terwilliger, T.C.</b>  | Automated main-chain model building by template matching and iterative fragment extension  |
| 11   | 0    | 2023       | research papers      | 23           | 2                           | <b>Bricogne, G.</b> , Vornrhein, C., Flensburg, C., Schiltz, M., Paciorek, W.                                       | Generation, representation and flow of phase information in structure determination: recent developments in and around SHARP 2.0   |
| 6  | 0    | 1028       | research papers      | 18           | 6                           | Page, R., Grzechnik, S.K., Canaves, J.M., Spraggon, G., Kreuzsch, A., Kuhn, P., <b>Stevens, R.C.</b> , Lesley, S.A. | Shotgun crystallization strategy for structural genomics: an optimized two-tiered crystallization screen against the Thermotoga maritima proteome                            |
| 7  | 0    | 1206       | research papers      | 17           | 1                           | <b>Oefner, C.</b> , D'Arcy, A., Mac Sweeney, A., Pierau, S., Gardiner, R., Dale, G.E.                               | High-resolution structure of human apo dipeptidyl peptidase IV/CD26 and its complex with 1-[(2-[(5-iodopyridin-2-yl)amino]-ethyl)amino]-acetyl]-2-cyano-(S)-pyrrolidine      |
| 6  | 0    | 1020       | research papers      | 17           | 17                          | Ramagopal, U.A., Dauter, M., <b>Dauter, Z.</b>  | Phasing on anomalous signal of sulfurs: what is the limit?   |
| 1  | 0    | 45         | research papers      | 16           | 7                           | <b>Terwilliger, T.C.</b>  | Automated side-chain model building and sequence assignment by template matching   |
| 3  | 0    | 447        | research papers      | 15           | 0                           | Varrot, A., <b>Davies, G.J.</b>   | Direct experimental observation of the hydrogen-bonding network of a glycosidase along its reaction coordinate revealed by atomic resolution analyses of endoglucanase Cel5A |
| 4  | 0    | 688        | research papers      | 15           | 13                          | Debreczeni, J.E., Bunkoczi, G., Ma, Q., Blaser, H., <b>Sheldrick, G.M.</b>  | In-house measurement of the sulfur anomalous signal and its use for phasing  |
| 2  | 0    | 396        | short communications | 14           | 4                           | <b>D'Arcy, A.</b> , Mac Sweeney, A., Stihle, M., Haber, A.  | The advantages of using a modified microbatch method for rapid screening of protein crystallization conditions   |
| 1  | 0    | 194        | short communications | 14           | 2                           | Adachi, H., <b>Takano, K.</b> , Morikawa, M., Kanaya, S., Yoshimura, M., Mori, Y., Sasaki, T.                       | Application of a two-liquid system to sitting-drop vapour-diffusion protein crystallization  |
| 2  | 0    | 393        | short communications | 13           | 9                           | Debreczeni, J.E., Bunkoczi, G., Girmann, B., <b>Sheldrick, G.M.</b>   | In-house phase determination of the lima bean trypsin inhibitor: a low-resolution sulfur-SAD case  |
| 4  | 0    | 697        | research papers      | 13           | 8                           | Kriminski, S., Kazmierczak, M., <b>Thorne, R.E.</b>   | Heat transfer from protein crystals: implications for flash-cooling and X-ray beam heating   |

## Acta Crystallographica Section D - sales and circulation figures

### Institutional and consortial circulation totals

|                       | 2003 | 2004 |
|-----------------------|------|------|
| Consortia site access |      | 1748 |
| 1. Europe             |      | 882  |
| 2. USA                |      | 210  |
| 3. Canada             |      | 32   |

|                             |     |     |
|-----------------------------|-----|-----|
| 4. Aus/NZ                   |     | 83  |
| 5. Japan                    |     | 86  |
| 6. Rest of World            |     | 455 |
| Institutional subscriptions | 581 | 576 |
| Online                      | 45  | 68  |
| Standard                    | 534 | 502 |
| Online Collection           | 2   | 6   |
| Personal subscriptions      | 131 | 120 |

### Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 13         | 17         |
|                               | Standard          | 180        | 173        |
|                               | Online Collection | 2          | 2          |
| <b>1. Europe Total</b>        |                   | <b>195</b> | <b>192</b> |
| 2. North America              | Online            | 23         | 38         |
|                               | Standard          | 208        | 186        |
|                               | Online Collection | 0          | 4          |
| <b>2. North America Total</b> |                   | <b>231</b> | <b>228</b> |
| 3. Aus/NZ                     | Online            | 1          | 1          |
|                               | Standard          | 11         | 11         |
| <b>3. Aus/NZ Total</b>        |                   | <b>12</b>  | <b>12</b>  |
| 4. Japan                      | Online            | 8          | 11         |
|                               | Standard          | 80         | 74         |
| <b>4. Japan Total</b>         |                   | <b>88</b>  | <b>85</b>  |
| 5. Rest of World              | Online            | 0          | 1          |
|                               | Standard          | 55         | 58         |
|                               | Online Collection | 0          | 0          |
| <b>5. Rest of World Total</b> |                   | <b>55</b>  | <b>59</b>  |
| <b>Grand Total</b>            |                   | <b>581</b> | <b>576</b> |

## APPENDIX - Background information on Section F

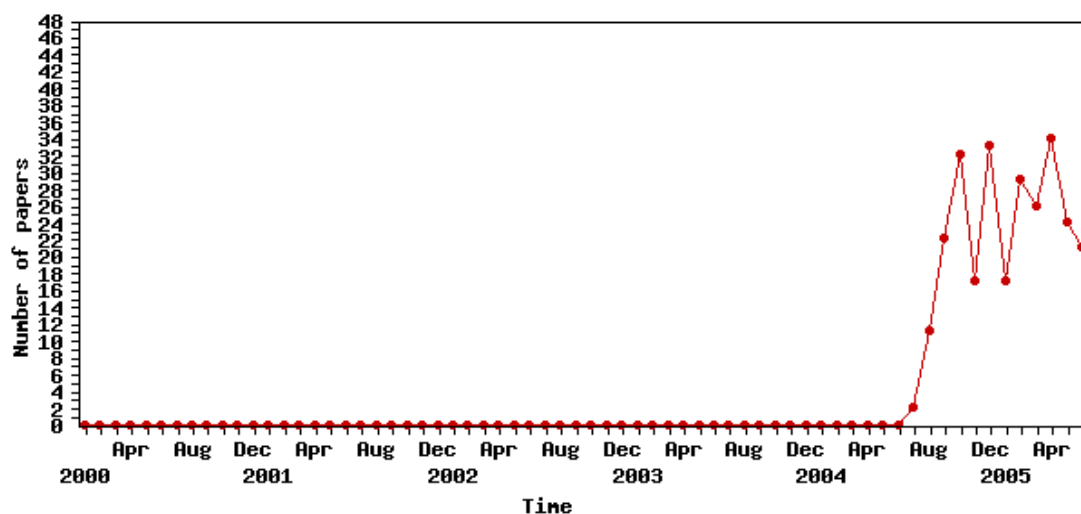
### Aims and scope

Acta Crystallographica Section F Structural Biology and Crystallization Communications aims to provide a home for communications on the crystallization and structure determination of biological macromolecules. It includes three categories of publication:

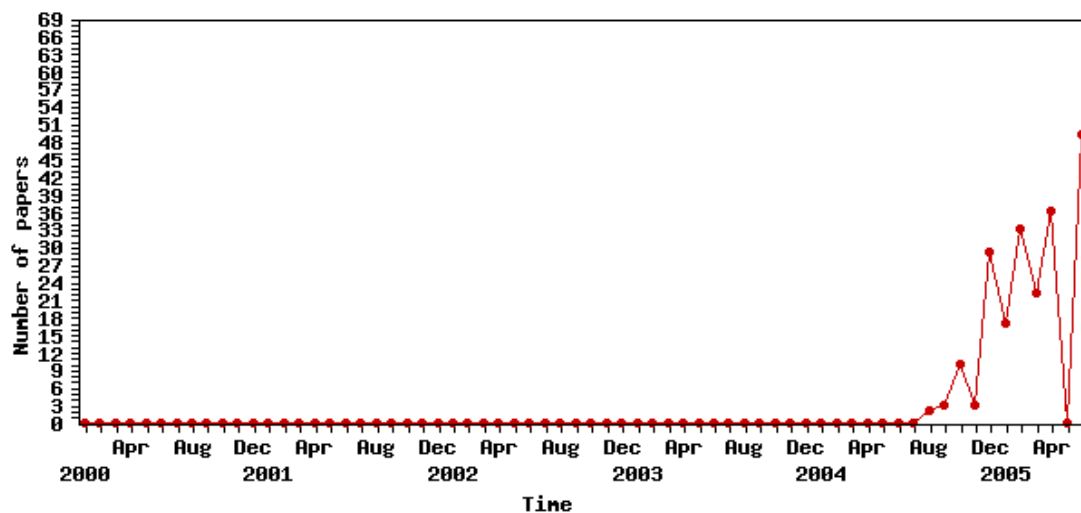
- Structural genomics communications
- Protein structure communications
- Crystallization communications

Articles are available online when ready, making publication as fast as possible, and include unlimited free colour illustrations, movies and other enhancements. The editorial process is completely electronic with respect to deposition, submission, refereeing and publication.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Summary of statistics for 1 January 2005-30 June 2005

Manuscripts submitted 151

Manuscripts accepted 154

Papers published 175

Pages published 620

Average paper length 3.5 pages

Average review time 1.6 months

Average technical editing time 0.5 months

Average total publication time 2.2 months

# JAC agenda

## Grand Hotel Panoramic, Montecatini Terme, Italy

22 August, 16:15-17:25 (Editors are encouraged to join a meeting for another journal before this meeting)

### CHAIR: Gernot Kostorz

Attendees: JAC Editors and Co-editors, and any other interested Editors

IUCr staff attending: Peter Strickland

### 1. GENERAL

This item is intended cover general matters and to give the Editor or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

### 2. JOURNAL DEVELOPMENT

#### 2.1. Scientific development

Are there any new related scientific areas that are developing that the journal should cover?

If yes, should an appointment be made to the Board to cover this area?

Would a special issue on such developments be worthwhile?

Are there other areas on which special issues should be commissioned?

Does the expertise on the Board cover the aims and scope of the journal well, or are new appointments needed?

#### 2.2. Submissions

How can we encourage more submissions to JAC?

Are there any ideas on how an increase in submissions might be achieved?

What sort of papers should we be trying to attract and how can we encourage their submission?

#### 2.3. Impact factor

Is there any way that the journal impact factor can be increased?

Are there particular categories of paper that should be encouraged/discouraged?

Are there particular topics that are more highly cited?

Are there particular authors that should be encouraged to write for the journal?

#### 2.4. Lead articles/topical reviews

What topics should be considered?

Who are potential candidate authors?

#### 2.5. Publication speed

Are there any ways in which we can increase publication speed or otherwise improve services to authors?

### 3. SUBMISSION AND REVIEW

Are the status pages useful?

What new submission system features would be useful for Co-editors?

How can the Notes for referees be improved?

How can the review form be improved before it is implemented online?

Are there any measures that would improve the consistency of the review process?

Are the documentation and help pages for authors, editors and referees clear?

Should JAC continue to allow hard-copy submission?

Above what number of authors would it be reasonable to ask for the roles of the authors?

### 4. JOURNAL PROMOTION AND SPONSORSHIP

#### 4.1. Promoting the journal using a marketing leaflet

The Journals Working Group would like comments on the leaflet promoting JAC. Ideas for future leaflets will be welcomed.

#### 4.2. In what other ways can JAC be promoted?

#### 4.3. How can advertising/sponsorship revenues be increased?

### 5. JOURNAL DESIGN

#### 5.1. PRINT:

Is the present design of the journal satisfactory?

Are there any items that can be removed from the print version of the journal?

## 5.2. ONLINE:

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

## 6. NOTES FOR AUTHORS

This is an opportunity to make suggestions for changes to the present Notes for Authors.

## 7. USE OF COLOUR

Should the Notes for Authors be made stricter on the use of colour?

Should the Notes for Reviewers be modified to emphasize restrictions in the use of colour to reviewers?

Should Main and Section Editors review all colour at the proof stage?

Should colour only be allowed online?

If so, can the caption in the printed journal refer to colour?

Should the journal charge for colour?

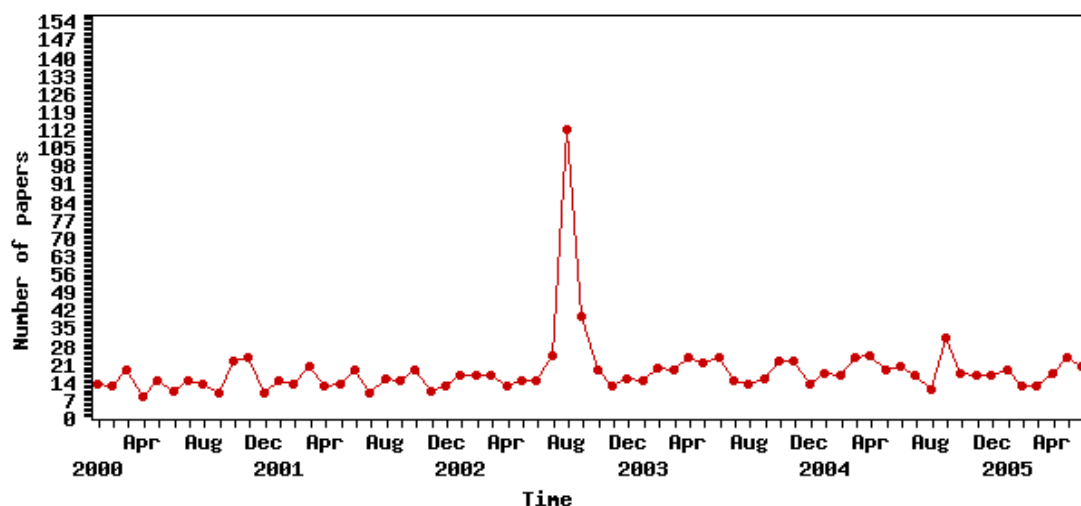
## 8. MATTERS ARISING FROM THE GENERAL AGENDA

## APPENDIX - Background information on Journal of Applied Crystallography

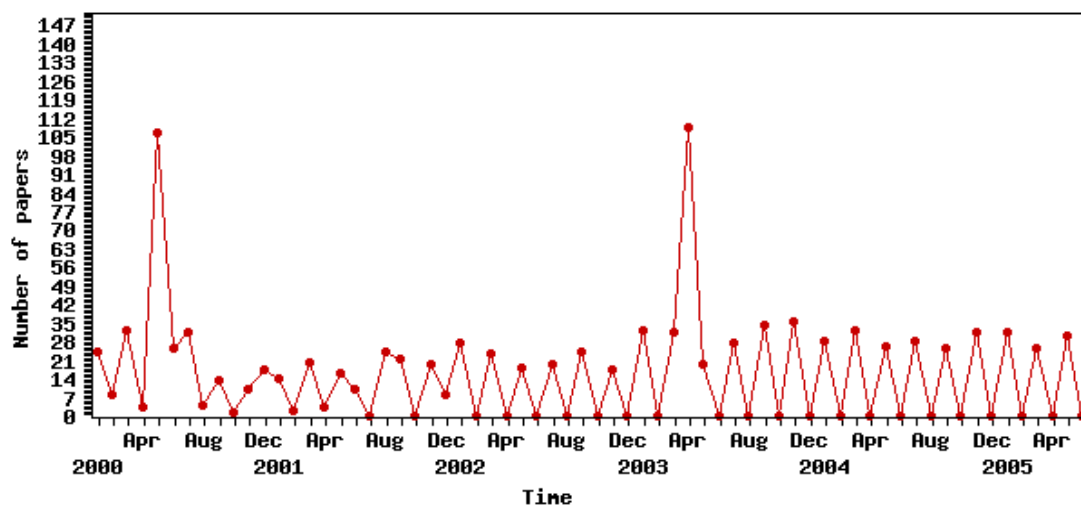
### Aims and scope

Journal of Applied Crystallography covers a wide range of crystallographic topics from the viewpoints of both techniques and theory. The journal presents papers on the application of crystallographic techniques and on the related apparatus and computer software. For many years, the Journal of Applied Crystallography has been the main vehicle for the publication of small-angle scattering papers and powder diffraction techniques. The journal is the primary place where crystallographic computer program information is published.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Journal of Applied Crystallography

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1891  |
| Institutional subscribers | 529   |
| Individual subscribers    | 98    |
| Impact factor (2004)      | 3.534 |
| Ranking                   | 2/24  |

### Journal of Applied Crystallography - competing journals based on citing

Number of times articles published in 2003 (in journals below) cited articles published in *Journal of Applied Crystallography*

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 11618   | 320  | 202  | 293  | 604  |                      |
| ACTA CRYSTALLOGR E | 1068    | 94   | 1    | 0    | 12   | 0.453                |
| J APPL CRYSTALLOGR | 641     | 33   | 41   | 66   | 118  | 2.324                |
| J BIOL CHEM        | 477     | 2    | 1    | 11   | 9    | 6.482                |
| ACTA CRYSTALLOGR C | 454     | 104  | 2    | 0    | 22   | 0.828                |
| ACTA CRYSTALLOGR D | 393     | 6    | 15   | 14   | 13   | 2.208                |
| J MOL BIOL         | 380     | 1    | 2    | 2    | 9    | 5.239                |
| INORG CHEM         | 268     | 3    | 1    | 0    | 2    | 3.389                |
| BIOCHEMISTRY-US    | 223     | 2    | 1    | 1    | 11   | 3.922                |
| DALTON T           | 203     | 2    | 0    | 0    | 4    | 2.908                |

### Journal of Applied Crystallography - list of cited journals

Number of times articles published in journals below (in years below) were cited in *Journal of Applied Crystallography* in 2003

| Citing Journal     | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|--------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS       | 5144    | 125  | 341  | 474  | 497  |                      |
| J APPL CRYSTALLOGR | 641     | 33   | 41   | 66   | 118  | 2.324                |
| ACTA CRYSTALLOGR A | 196     | 1    | 9    | 5    | 9    | 1.558                |
| MACROMOLECULES     | 118     | 1    | 7    | 7    | 7    | 3.621                |
| PHYS REV B         | 114     | 0    | 4    | 13   | 7    | 2.962                |
| PHYS REV LETT      | 114     | 2    | 10   | 6    | 9    | 7.035                |
| J CHEM PHYS        | 101     | 0    | 2    | 5    | 5    | 2.950                |
| J APPL PHYS        | 76      | 2    | 6    | 2    | 10   | 2.171                |
| ACTA CRYSTALLOGR B | 61      | 1    | 7    | 5    | 1    | 3.643                |
| PHYSICA B          | 60      | 0    | 1    | 7    | 18   | 0.908                |

### Journal of Applied Crystallography - citation report by issue

Special issues are shaded.

| 2001  |      |                                  |                        |                         | 2002  |      |                                  |                        |                         | 2003  |      |                                  |                        |                         |
|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|
| Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 17                               | 6.1                    | 0                       | 1     | 0    | 24                               | 3.1                    | 4                       | 1     | 0    | 28                               | 40.4                   | 3                       |
| 2     | 0    | 20                               | 6.7                    | 0                       | 2     | 0    | 22                               | 3.8                    | 4                       | 2     | 0    | 28                               | 5.8                    | 3                       |
| 3     | 0    | 25                               | 4.1                    | 0                       | 3     | 0    | 15                               | 3.0                    | 4                       | 3     | 1    | 96                               | 1.8                    | 3                       |
|       |      |                                  |                        |                         |       |      |                                  |                        |                         | 3     | 2    | 14                               | 4.9                    | 3                       |
| 4     | 0    | 19                               | 4.9                    | 0                       | 4     | 0    | 17                               | 1.8                    | 4                       | 4     | 0    | 24                               | 2.0                    | 3                       |
| 5     | 0    | 21                               | 3.5                    | 0                       | 5     | 0    | 23                               | 1.6                    | 4                       | 5     | 0    | 32                               | 2.0                    | 3                       |
| 6     | 0    | 19                               | 3.8                    | 0                       | 6     | 0    | 15                               | 1.3                    | 4                       | 6     | 0    | 30                               | 1.7                    | 3                       |

## Journal of Applied Crystallography - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| research papers                        | 85              | 85                              | 0                           | 4.7                    | 84              | 84                              | 0                           | 2.2                    | 224             | 214                             | 10                          | 7.4                    |
| short communications                   | 10              | 10                              | 0                           | 1.7                    | 11              | 11                              | 0                           | 3.3                    | 8               | 8                               | 0                           | 0.9                    |
| lead articles                          | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| topical reviews                        | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| teaching and education                 | 3               | 3                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| cryocrystallography papers             | 3               | 3                               | 0                           | 6.3                    | 2               | 2                               | 0                           | 2.0                    | 2               | 2                               | 0                           | 2.0                    |
| computer programs                      | 12              | 12                              | 0                           | 11.6                   | 12              | 12                              | 0                           | 4.8                    | 14              | 14                              | 0                           | 6.5                    |
| CIF applications                       | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 3               | 3                               | 0                           | 1.3                    |
| laboratory notes                       | 3               | 3                               | 0                           | 1.7                    | 3               | 3                               | 0                           | 2.3                    | 9               | 9                               | 0                           | 1.1                    |
| computer program abstracts             | 6               | 0                               | 6                           | 0.0                    | 8               | 0                               | 8                           | 0.0                    | 12              | 0                               | 12                          | 0.0                    |
| letters to the editor                  | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| addenda and errata                     | 3               | 3                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 1.0                    | 0               | 0                               | 0                           | 0.0                    |
| book reviews                           | 0               | 0                               | 0                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 4               | 0                               | 4                           | 0.0                    |
| books received                         | 2               | 0                               | 2                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 3               | 0                               | 3                           | 0.0                    |
| crystallographers                      | 6               | 2                               | 4                           | 0.0                    | 4               | 3                               | 1                           | 0.0                    | 4               | 2                               | 2                           | 0.0                    |
| editorial                              | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue preface                          | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| international union of crystallography | 2               | 0                               | 2                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| forthcoming meetings and short courses | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| meeting reports                        | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| notes and news                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| new commercial products                | 6               | 0                               | 6                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| obituaries                             | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| software reviews                       | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Journal of Applied Crystallography - 2001 |      |            |                   |              |                             |                                   |   |
|---|------|------------|-------------------|--------------|-----------------------------|-----------------------------------|---|
| Issue                                     | Part | First page | Paper category    | ISI citation | Total IUCr citation to date | Authors                           | Title   |
| 2   | 0    | 210        | computer programs | 35           | 13                          | <b>Toby, B.H.</b>                 | EXPGUI, a graphical user interface for GSAS   |
| 1   | 0    | 33         | research papers   | 33           | 2                           | <b>Kozin, M.B., Svergun, D.I.</b> | Automated matching of high- and low-resolution structural models                            |
| 1   | 0    | 82         | computer programs | 31           | 22                          | <b>Evans, G., Pettifer, R. F.</b> | CHOOCH: a program for deriving anomalous-scattering factors from X-ray fluorescence spectra |

|   |   |     |                   |    |    |   |  |
|---|---|-----|-------------------|----|----|---|--|
| 3 | 0 | 298 | research papers   | 31 | 9  | <b>Ungar, T.</b> , Gubicza, J., Ribarik, G., Borbely, A.  | Crystallite size distribution and dislocation structure determined by diffraction profile analysis: principles and practical application to cubic and hexagonal crystals |
| 2 | 0 | 130 | research papers   | 30 | 31 | <b>Weiss, M.S.</b>  | Global indicators of X-ray data quality  |
| 6 | 0 | 751 | research papers   | 27 | 6  | <b>Poulsen, H.F.</b> , Nielsen, S.F., Lauridsen, E.M., Schmidt, S., Suter, R.M., Lienert, U., Margulies, L., Lorentzen, T., Juul Jensen, D. | Three-dimensional maps of grain boundaries and the stress state of individual grains in polycrystals and powders   |
| 6 | 0 | 744 | research papers   | 21 | 6  | Lauridsen, E.M., Schmidt, S., Suter, R.M., <b>Poulsen, H.F.</b>   | Tracking: a method for structural characterization of grains in powders or polycrystals  |
| 4 | 0 | 496 | research papers   | 19 | 2  | <b>Striebeck, N.</b>  | Extraction of domain structure information from small-angle scattering patterns of bulk materials  |
| 2 | 0 | 97  | research papers   | 15 | 19 | <b>Brzozowski, A.M.</b> , Walton, J.  | Clear strategy screens for macromolecular crystallization  |
| 4 | 0 | 409 | research papers   | 15 | 6  | <b>Madsen, I.C.</b> , Scarlett, N.V.Y., Cranswick, L.M.D., Lwin, T.   | Outcomes of the International Union of Crystallography Commission on Powder Diffraction Round Robin on Quantitative Phase Analysis: samples 1a to 1h                     |
| 4 | 0 | 527 | computer programs | 15 | 2  | Konarev, P.V., Petoukhov, M.V., <b>Svergun, D.I.</b>  | MASSHA - a graphics system for rigid-body modelling of macromolecular complexes against solution scattering data   |
| 5 | 0 | 669 | computer programs | 15 | 3  | Ribarik, G., <b>Ungar, T.</b> , Gubicza, J.   | MWP-fit: a program for multiple whole-profile fitting of diffraction peak profiles by ab initio theoretical functions  |
| 3 | 0 | 398 | computer programs | 11 | 5  | Dusek, M., Petricek, V., Wunschel, M., Dinnebier, R.E., <b>Smaalen, S. van</b>  | Refinement of modulated structures against X-ray powder diffraction data with JANA2000   |
| 2 | 0 | 172 | research papers   | 11 | 3  | <b>Keen, D.A.</b>   | A comparison of various commonly used correlation functions for describing total scattering  |
| 2 | 0 | 214 | computer programs | 11 | 9  | Guillot, B., Viry, L., Guillot, R., Lecomte, C., <b>Jelsch, C.</b>  | Refinement of proteins at subatomic resolution with MOPRO  |
| 3 | 0 | 229 | research papers   | 11 | 4  | Kusz, J., <b>Spiering, H.</b> , Gutlich, P.   | X-ray structure study of the light-induced metastable states of the spin-crossover compound [Fe(mtz)6](BF4)2   |

#### Journal of Applied Crystallography - 2002

| Issue | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors   | Title   |
|-------|------|------------|----------------------|--------------|-----------------------------|---|---|
| 2     | 0    | 278        | short communications | 17           | 8                           | Santarsiero, B.D., Yegian, D.T., Lee, C.C., Spraggon, G., Gu, J., Scheibe, D., Uber, D.C., Cornell, E.W., Nordmeyer, R.A., Kolbe, W.F., Jin, J., Jones, A.L., Jaklevic, J.M., Schultz, P.G., <b>Stevens, R.C.</b> | An approach to rapid protein crystallization using nanodroplets   |
| 1     | 0    | 82         | research papers      | 14           | 4                           | Weislak, L., Klein, H., <b>Bunge, H.J.</b> , Garbe, U., Tschentscher, T., Schneider, J.R.   | Texture analysis with high-energy synchrotron radiation   |
| 2     | 0    | 168        | research papers      | 11           | 8                           | Cooper, R.I., Gould, R.O., <b>Parsons, S.</b> , Watkin, D.J.  | The derivation of non-merohedral twin laws during refinement by analysis of poorly fitting intensity data and the refinement of non-merohedrally twinned crystal structures in the program CRYSTALS |
| 6     | 0    | 734        | computer programs    | 10           | 10                          | <b>Favre-Nicolin, V.</b> , Cerny, R.  | FOX, 'free objects for crystallography': a modular approach to ab initio structure determination from powder diffraction  |
| 1     | 0    | 126        | computer programs    | 9            | 9                           | Grosse-Kunstleve, R.W., Sauter, N.K., Moriarty, N.W., <b>Adams, P.D.</b>  | The Computational Crystallography Toolbox: crystallographic algorithms in a reusable software framework   |

|   |   |     |                      |   |   |   |  |
|---|---|-----|----------------------|---|---|---|--|
| 2 | 0 | 282 | computer programs    | 9 | 1 | <b>Tanaka, H.</b> , Takata, M., Nishibori, E., Kato, K., Iishi, T., Sakata, M.                      | ENIGMA: maximum-entropy method program package for huge systems  |
| 1 | 0 | 34  | research papers      | 9 | 3 | Tanaka, I., Kurihara, K., Chatake, T., <b>Niimura, N.</b>   | A high-performance neutron diffractometer for biological crystallography (BIX-3)                                       |
| 3 | 0 | 319 | research papers      | 7 | 5 | <b>Bourgeois, D.</b> , Vernede, X., Adam, V., Fioravanti, E., Ursby, T.                             | A microspectrophotometer for UV-visible absorption and fluorescence studies of protein crystals                        |
| 1 | 0 | 137 | computer programs    | 7 | 0 | Madsen, D., <b>Kleywegt, G.J.</b>   | Interactive motif and fold recognition in protein structures   |
| 2 | 0 | 212 | research papers      | 7 | 0 | <b>Hernandez, O.</b> , Hedoux, A., Lefebvre, J., Guinet, Y., Descamps, M., Papoular, R., Masson, O. | Ab initio structure determination of triphenyl phosphite by powder synchrotron X-ray diffraction                       |
| 3 | 0 | 368 | computer programs    | 7 | 6 | <b>Smith, G.D.</b>  | Matching selenium-atom peak positions with a different hand or origin  |
| 3 | 0 | 371 | computer programs    | 7 | 4 | Stash, A., <b>Tsirelson, V.</b>   | WinXPRO: a program for calculating crystal and molecular properties using multipole parameters of the electron density |
| 3 | 0 | 338 | research papers      | 6 | 5 | Popa, N.C., <b>Balzar, D.</b>   | An analytical approximation for a size-broadened profile given by the lognormal and gamma distributions                |
| 2 | 0 | 274 | short communications | 6 | 0 | <b>Sitepu, H.</b>   | Assessment of preferred orientation with neutron powder diffraction data   |
| 2 | 0 | 163 | research papers      | 6 | 0 | Pfeiffer, F., Mennicke, U., <b>Salditt, T.</b>  | Waveguide-enhanced scattering from thin biomolecular films   |

#### Journal of Applied Crystallography - 2003

| Issue | Part | First page | Paper category    | ISI citation | Total IUCr citation to date | Authors  | Title   |
|-------|------|------------|-------------------|--------------|-----------------------------|--|---|
| 1     | 0    | 7          | research papers   | 1054         | 1010                        | <b>Spek, A.L.</b>  | Single-crystal structure validation with the program PLATON   |
| 2     | 0    | 220        | research papers   | 56           | 38                          | <b>Duisenberg, A.J.M.</b> , Kroon-Batenburg, L.M.J., Schreurs, A.M.M.                            | An intensity evaluation method: EVAL-14   |
| 3     | 2    | 944        | computer programs | 47           | 4                           | <b>Fenn, T.D.</b> , Ringe, D., Petsko, G.A.  | POVScript+: a program for model and data visualization using persistence of vision ray-tracing                      |
| 5     | 0    | 1277       | computer programs | 21           | 2                           | Konarev, P.V., Volkov, V.V., Sokolova, A.V., Koch, M.H.J., <b>Svergun, D.I.</b>                  | PRIMUS: a Windows PC-based system for small-angle scattering data analysis  |
| 3     | 1    | 860        | research papers   | 20           | 1                           | <b>Volkov, V.V.</b> , Svergun, D.I.  | Uniqueness of ab initio shape determination in small-angle scattering   |
| 2     | 0    | 308        | research papers   | 18           | 6                           | Walter, T.S., Diprose, J., Brown, J., Pickford, M., Owens, R.J., Stuart, D.I., <b>Harlos, K.</b> | A procedure for setting up high-throughput nanolitre crystallization experiments. I. Protocol design and validation |
| 4     | 0    | 1062       | research papers   | 13           | 2                           | <b>Poulsen, H.F.</b> , Fu, X.  | Generation of grain maps by an algebraic reconstruction technique   |
| 2     | 0    | 295        | research papers   | 12           | 1                           | <b>Angel, R.J.</b>   | Automated profile analysis for single-crystal diffraction data  |
| 1     | 0    | 117        | research papers   | 11           | 2                           | <b>Krøgløv, T.</b> , Schepper, I.M. de, Bouwman, W.G., Rekveldt, M.T.                            | Real-space interpretation of spin-echo small-angle neutron scattering   |

## Journal of Applied Crystallography - sales and circulation figures

### Institutional and consortial circulation totals

|                             | 2003 | 2004 |
|-----------------------------|------|------|
| Consortia site access       |      | 1891 |
| 1. Europe                   |      | 882  |
| 2. USA                      |      | 196  |
| 3. Canada                   |      | 32   |
| 4. Aus/NZ                   |      | 240  |
| 5. Japan                    |      | 86   |
| 6. Rest of World            |      | 455  |
| Institutional subscriptions | 544  | 529  |
| Online                      | 26   | 51   |
| Standard                    | 516  | 474  |
| Online Collection           | 2    | 4    |
| Personal subscriptions      | 92   | 98   |

### Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 7          | 15         |
|                               | Standard          | 223        | 207        |
|                               | Online Collection | 2          | 2          |
| <b>1. Europe Total</b>        |                   | <b>232</b> | <b>224</b> |
| 2. North America              | Online            | 7          | 18         |
|                               | Standard          | 156        | 140        |
|                               | Online Collection | 0          | 2          |
| <b>2. North America Total</b> |                   | <b>163</b> | <b>160</b> |
| 3. Aus/NZ                     | Online            | 2          | 5          |
|                               | Standard          | 9          | 8          |
| <b>3. Aus/NZ Total</b>        |                   | <b>11</b>  | <b>13</b>  |
| 4. Japan                      | Online            | 9          | 10         |
|                               | Standard          | 61         | 56         |
| <b>4. Japan Total</b>         |                   | <b>70</b>  | <b>66</b>  |
| 5. Rest of World              | Online            | 1          | 3          |
|                               | Standard          | 67         | 63         |
|                               | Online Collection | 0          | 0          |
| <b>5. Rest of World Total</b> |                   | <b>68</b>  | <b>66</b>  |
| <b>Grand Total</b>            |                   | <b>544</b> | <b>529</b> |

# JSR agenda

## Grand Hotel Panoramic, Montecatini Terme, Italy

22 August, 14:55-16:05 (Editors are encouraged to join a meeting for another journal before and after this meeting)

### CHAIR: Denny Mills/Ake Kvick

Attendees: JSR Editors and Co-editors, and any other interested Editors

IUCr staff attending: Tony Weight

#### 1. GENERAL

This item is intended cover general matters and to give the Editor or Co-editors the chance to raise important issues related to the journal that are not covered elsewhere in the agenda.

##### 1.1. Facility Information pages

A list of facilities taking part in these pages and a list of those contacted to do so is given in the APPENDIX.

Are there any ways in which we can make the design of the printed pages more unified (e.g. by positioning of logos and addresses, adopting common headings etc.)?

How can the online Facility Information pages be improved?

Should we develop these pages to provide additional information?

#### 2. JOURNAL DEVELOPMENT

##### 2.1. Scientific development

Are there any new related scientific areas that are developing that the journal should cover?

If yes, should an appointment be made to the Board to cover this area?

Would a special issue on such developments be worthwhile?

Are there other areas on which special issues should be commissioned?

Does the expertise on the Board cover the aims and scope of the journal well, or are new appointments needed?

##### 2.2. Submissions

How can we encourage more submissions to JAC?

Are there any ideas on how an increase in submissions might be achieved?

What sort of papers should we be trying to attract and how can we encourage their submission?

##### 2.3. Impact factor

Is there any way that the journal impact factor can be increased?

Are there particular categories of paper that should be encouraged/discouraged?

Are there particular topics that are more highly cited?

Are there particular authors that should be encouraged to write for the journal?

How successful have special issues been? Should the journal (or Acta D) cover the BIOXHIT meeting?

##### 2.4. Lead articles/topical reviews

What topics should be considered?

Who are potential candidate authors?

##### 2.5. Publication speed

Are there any ways in which we can increase publication speed or otherwise improve services to authors?

#### 3. SUBMISSION AND REVIEW

Are the status pages useful?

What new submission system features would be useful for Co-editors?

How can the Notes for referees be improved?

How can the review form be improved before it is implemented online?

Are there any measures that would improve the consistency of the review process?

Are the documentation and help pages for authors, editors and referees clear?

Above what number of authors would it be reasonable to ask for the roles of the authors?

#### 4. JOURNAL PROMOTION AND SPONSORSHIP

A list of facilities that subscribe to the journal is given in the APPENDIX.

##### 4.1. Promoting the journal using a marketing leaflet

The Journals Working Group would like comments on the leaflet promoting JSR. Ideas for future leaflets will be

welcomed.

4.2. In what other ways can JSR be promoted?

4.3. How can advertising/sponsorship revenues be increased?

## **5. JOURNAL DESIGN**

### **5.1. PRINT:**

Is the present design of the journal satisfactory?

Are there any items that can be removed from the print version of the journal?

### **5.2. ONLINE:**

Is the present design of the online journal satisfactory?

Are there any areas that can be improved on or any items that need to be included or made more prominent?

## **6. NOTES FOR AUTHORS**

This is an opportunity to make suggestions for changes to the present Notes for Authors.

## **7. USE OF COLOUR**

Should the Notes for Authors be made stricter on the use of colour?

Should the Notes for Reviewers be modified to emphasize restrictions in the use of colour to reviewers?

Should Main and Section Editors review all colour at the proof stage?

Should the running order of journal issues be relaxed to allow more economic use of colour?

Should colour only be allowed online?

If so, can the caption in the printed journal refer to colour?

Should the journal charge for colour?

## **8. MATTERS ARISING FROM THE GENERAL AGENDA**

## APPENDIX - Background information on JSR

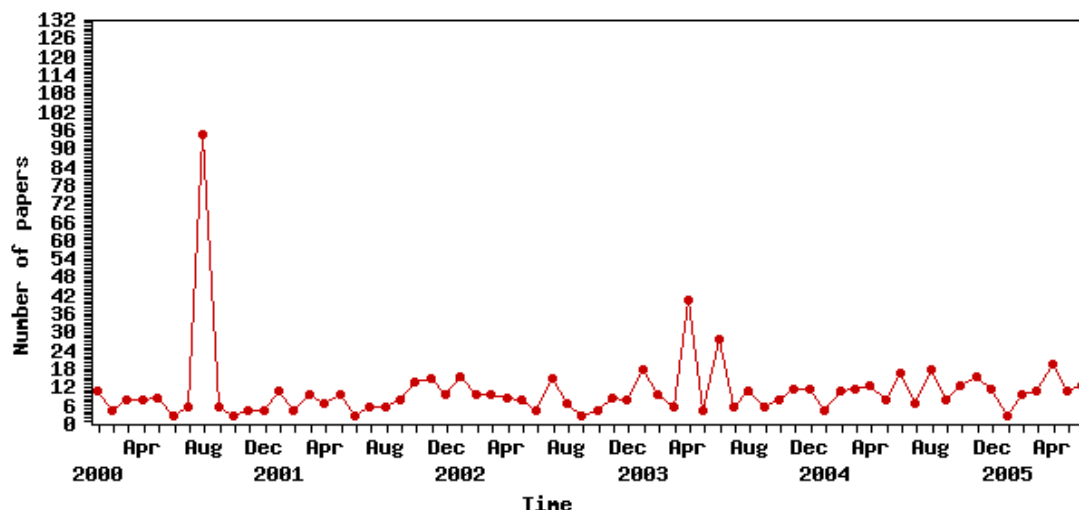
### Aims and scope

Synchrotron radiation sources and their associated technologies have expanded at an extremely rapid rate during the past 20 years. Through the 1990s, many new synchrotron radiation sources have been constructed and exploited worldwide.

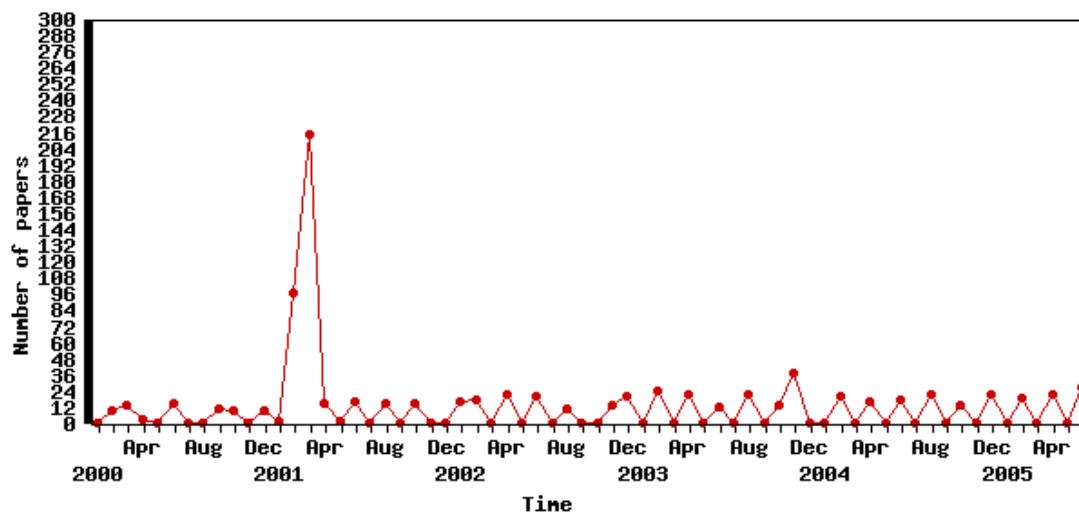
The Journal of Synchrotron Radiation aims to provide a focus in this rapidly expanding area. The topics covered by the journal include source technology, instrumentation and techniques over all the spectral ranges relevant to synchrotron radiation research. It thus draws together the full breadth of interests and skills of the synchrotron radiation community.

Contributions are invited within the general areas of instrumentation, methods and novel applications. The instrumentation topics include: synchrotron radiation sources and beamlines; optics; detectors; electronics and data acquisition; sample chambers and environment. The methods and applications topics are grouped within the following categories; diffraction; spectroscopy, imaging.

### Papers submitted (2000-2005)



### Papers published (2000-2005)



### Numbers at a glance Journal of Synchrotron Radiation

|                           |       |
|---------------------------|-------|
| Consortia deals           | 1891  |
| Institutional subscribers | 154   |
| Individual subscribers    | 67    |
| Impact Factor (2004)      | 1.919 |
| Ranking (2004)            | 4/25  |

### Journal of Synchrotron Radiation - competing journals based on citing

Number of times articles published in 2003 (in journals below) cited articles published in *Journal of Synchrotron Radiation*

| Citing Journal       | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|----------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS         | 1610    | 42   | 145  | 333  | 104  |                      |
| J SYNCHROTRON RADIAT | 162     | 15   | 19   | 44   | 7    | 1.144                |
| J PHYS IV            | 73      | 0    | 21   | 6    | 7    | 0.319                |
| PHYS REV B           | 71      | 1    | 4    | 20   | 1    | 2.962                |
| NUCL INSTRUM METH B  | 69      | 0    | 2    | 10   | 3    | 1.041                |
| REV MINERAL GEOCHEM  | 61      | 0    | 0    | 11   | 1    | 2.413                |
| ACTA CRYSTALLOGR D   | 43      | 0    | 12   | 3    | 3    | 2.208                |
| J APPL CRYSTALLOGR   | 41      | 1    | 7    | 2    | 4    | 2.324                |
| NUCL INSTRUM METH A  | 34      | 1    | 0    | 3    | 6    | 1.166                |
| J PHYS CHEM B        | 33      | 2    | 0    | 16   | 0    | 3.679                |

### Journal of Synchrotron Radiation - list of cited journals

Number of times articles published in journals below (in years below) was cited in *Journal of Synchrotron Radiation* in 2003

| Citing Journal       | All Yrs | 2003 | 2002 | 2001 | 2000 | Impact factor (2003) |
|----------------------|---------|------|------|------|------|----------------------|
| ALL JOURNALS         | 1951    | 59   | 108  | 220  | 164  |                      |
| J SYNCHROTRON RADIAT | 162     | 15   | 19   | 44   | 7    | 1.144                |
| PHYS REV B           | 151     | 0    | 8    | 12   | 13   | 2.962                |
| NUCL INSTRUM METH A  | 77      | 2    | 3    | 27   | 7    | 1.166                |
| PHYS REV LETT        | 62      | 2    | 2    | 11   | 10   | 7.035                |
| REV SCI INSTRUM      | 50      | 0    | 1    | 2    | 5    | 1.343                |
| BIOCHEMISTRY-US      | 45      | 0    | 1    | 3    | 4    | 3.922                |
| J AM CHEM SOC        | 41      | 0    | 0    | 1    | 1    | 6.516                |
| SCIENCE              | 40      | 2    | 2    | 3    | 2    | 29.781               |
| NATURE               | 38      | 0    | 0    | 3    | 5    | 30.979               |

### Journal of Synchrotron Radiation - citation report by issue

Special issues are shaded.

| 2001  |      |                                  |                        |                         | 2002  |      |                                  |                        |                         | 2003  |      |                                  |                        |                         |
|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|-------|------|----------------------------------|------------------------|-------------------------|
| Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations | Issue | Part | No . of articles in ISI database | Average citation count | Cover article citations |
| 1     | 0    | 7                                | 4.4                    | 0                       | 1     | 0    | 14                               | 1.5                    | 0                       | 1     | 0    | 16                               | 7.1                    | 0                       |
| 2     | 0    | 308                              | 1.6                    | 0                       | 2     | 0    | 14                               | 1.2                    | 0                       | 2     | 0    | 23                               | 1.7                    | 0                       |
| 3     | 0    | 11                               | 2.4                    | 0                       | 3     | 0    | 16                               | 2.6                    | 0                       | 3     | 0    | 21                               | 1.8                    | 0                       |
| 4     | 0    | 10                               | 3.9                    | 0                       | 4     | 0    | 16                               | 2.4                    | 0                       | 4     | 0    | 8                                | 1.2                    | 0                       |
| 5     | 0    | 8                                | 5.2                    | 0                       | 5     | 0    | 10                               | 2.5                    | 0                       | 5     | 0    | 18                               | 0.7                    | 0                       |
| 6     | 0    | 10                               | 4.3                    | 0                       | 6     | 0    | 12                               | 4.6                    | 0                       | 6     | 0    | 10                               | 2.3                    | 0                       |

## Journal of Synchrotron Radiation - citation report by category

| Category                               | 2001            |                                 |                             |                        | 2002            |                                 |                             |                        | 2003            |                                 |                             |                        |
|--|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|-----------------|---------------------------------|-----------------------------|------------------------|
|  | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count | No. of articles | No. of articles in ISI database | No. of articles not covered | Average citation count |
| research papers                        | 69              | 69                              | 0                           | 3.7                    | 66              | 66                              | 0                           | 2.8                    | 72              | 72                              | 0                           | 3.1                    |
| short communications                   | 279             | 278                             | 1                           | 1.5                    | 1               | 1                               | 0                           | 0.0                    | 6               | 6                               | 0                           | 1.3                    |
| lead articles                          | 0               | 0                               | 0                           | 0.0                    | 2               | 2                               | 0                           | 3.5                    | 1               | 1                               | 0                           | 3.0                    |
| computer programs                      | 0               | 0                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 5.0                    | 1               | 1                               | 0                           | 2.0                    |
| laboratory notes                       | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| computer program abstracts             | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| letters to the editor                  | 2               | 2                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 0.0                    | 3               | 3                               | 0                           | 0.0                    |
| teaching and education                 | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| addenda and errata                     | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 2               | 2                               | 0                           | 0.0                    |
| new commercial products                | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| book reviews                           | 2               | 0                               | 2                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 2               | 0                               | 2                           | 0.0                    |
| books received                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| editorial                              | 2               | 2                               | 0                           | 1.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue preface                          | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| issue foreword                         | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| international union of crystallography | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    | 1               | 0                               | 1                           | 0.0                    |
| forthcoming meetings and short courses | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| current events                         | 18              | 1                               | 17                          | 0.0                    | 20              | 10                              | 10                          | 0.0                    | 20              | 11                              | 9                           | 0.0                    |
| obituaries                             | 0               | 0                               | 0                           | 0.0                    | 1               | 1                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |
| abstract                               | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    | 0               | 0                               | 0                           | 0.0                    |

## Highly cited papers

| Journal of Synchrotron Radiation - 2001 |      |            |                      |              |                             |   |   |
|---|------|------------|----------------------|--------------|-----------------------------|---|---|
| Issue                                   | Part | First page | Paper category       | ISI citation | Total IUCr citation to date | Authors   | Title   |
| 2                                       | 0    | 322        | short communications | 26           | 3                           | <b>Newville, M.</b>   | IFEFFIT : interactive XAFS analysis and FEFF fitting  |
| 2                                       | 0    | 314        | short communications | 24           | 4                           | <b>Ravel, B.</b>  | ATOMS: crystallography for the X-ray absorption spectroscopist                                      |
| 5                                       | 0    | 1162       | research papers      | 17           | 3                           | <b>Meneghini, C.,</b> Artioli, G., Balerna, A., Gualtieri, A.F., Norby, P., Mobilio, S. | Multipurpose imaging-plate camera for in situ powder XRD at the GILDA beamline                      |
| 2                                       | 0    | 55         | research papers      | 13           | 1                           | <b>Thomas, J.M.,</b> Sankar, G.   | The role of XAFS in the in situ and ex situ elucidation of active sites in designed solid catalysts |

|   |   |      |                      |    |   |  |   |
|---|---|------|----------------------|----|---|--|---|
| 2 | 0 | 569  | short communications | 12 | 0 | <b>Yamashita, H.</b> , Harada, M., Misaka, J., Takeuchi, M., Ichihashi, Y., Goto, F., Ishida, M., Sasaki, T., Anpo, M.   | Application of ion beam techniques for preparation of metal ion-implanted <a href="#">TiO<sub>2</sub></a> thin film photocatalyst available under visible light irradiation: metal ion-implantation and ionized cluster beam method |
| 4 | 0 | 1087 | research papers      | 12 | 7 | <b>Benfatto, M.</b> , Della Longa, S.  | Geometrical fitting of experimental XANES spectra by a full multiple-scattering procedure   |
| 6 | 0 | 1172 | research papers      | 11 | 1 | Brown, S.D., Bouchenoire, L., Bowyer, D., Kervin, J., Laundy, D., Longfield, M.J., Mannix, D., Paul, D.F., Stunault, A., Thompson, P., <b>Cooper, M.J.</b> , Lucas, C.A., Stirling, W.G. | The XMaS beamline at ESRF: instrumental developments and high-resolution diffraction studies  |
| 3 | 0 | 1040 | research papers      | 11 | 0 | Tolentino, H.C.N., <b>Ramos, A.Y.</b> , Alves, M.C.M., Barrea, R.A., Tamura, E., Cezar, J.C., Watanabe, N.   | A 2.3 to 25 keV XAS beamline at LNLS  |
| 2 | 0 | 61   | research papers      | 10 | 0 | <b>Rehr, J.J.</b> , Ankudinov, A.L.  | Progress and challenges in the theory and interpretation of X-ray spectra   |
| 2 | 0 | 946  | short communications | 10 | 0 | <b>Kelly, S.D.</b> , Boyanov, M., Bunker, B., Fein, J.B., Fowle, D.A., Yee, N., Kemner, K.M.   | XAFS determination of the bacterial cell wall functional groups responsible for complexation of Cd and U as a function of pH  |
| 1 | 0 | 26   | research papers      | 9  | 1 | <b>Hiraoka, N.</b> , Itou, M., Ohata, T., Mizumaki, M., Sakurai, Y., Sakai, N.   | A new X-ray spectrometer for high-resolution Compton profile measurements at SPring-8   |
| 5 | 0 | 1149 | research papers      | 8  | 3 | <b>Fourme, R.</b> , Kahn, R., Mezouar, M., Girard, E., Hoerentrup, C., Prange, T., Ascone, I.  | High-pressure protein crystallography (HPPX): instrumentation, methodology and results on lysozyme crystals   |
| 5 | 0 | 1131 | research papers      | 8  | 5 | <b>Shastri, S.D.</b> , Zambianchi, P., Mills, D.M.   | Dynamical diffraction of ultrashort X-ray free-electron laser pulses  |
| 2 | 0 | 657  | short communications | 8  | 0 | <b>Sandstrom, M.</b> , Persson, I., Jalilehvand, F., Lindquist-Reis, P., Spangberg, D., Hermansson, K.   | Hydration of some large and highly charged metal ions   |
| 2 | 0 | 581  | short communications | 8  | 1 | <b>Bando, K.K.</b> , Saito, T., Sato, K., Tanaka, T., Dumeignil, F., Imamura, M., Matsubayashi, N., Shimada, H.  | In situ XAFS analysis system for high-pressure catalytic reactions and its application to CO <sub>2</sub> hydrogenation over a Rh/Y-zeolite catalyst  |

#### Journal of Synchrotron Radiation - 2002

| Issue | Part | First page | Paper category  | ISI citation | Total IUCr citation to date | Authors  | Title  |
|-------|------|------------|-----------------|--------------|-----------------------------|--|--|
| 6     | 0    | 355        | research papers | 10           | 14                          | <b>Ravelli, R.B.G.</b> , Theveneau, P., <a href="#">McSweeney</a> , S., Caffrey, M.  | Unit-cell volume change as a metric of radiation damage in crystals of macromolecules Presented at the 'Second International Workshop on Radiation Damage to Crystalline Biological Samples' held at Advanced Photon Source, Chicago, USA, in December 2001. |
| 6     | 0    | 361        | research papers | 8            | 6                           | <b>Snell, E.H.</b> , Judge, R.A., Larson, M., van der Woerd, M.J.  | Seeing the heat - preliminary studies of cryocrystallography using infrared imaging Presented at the 'Second International Workshop on Radiation Damage to Crystalline Biological Samples' held at Advanced Photon Source, Chicago, USA, in December 2001.   |
| 3     | 0    | 182        | research papers | 8            | 1                           | <b>Kamijo, N.</b> , Suzuki, Y., Awaji, M., Takeuchi, A., Takano, H., Ninomiya, T., Tamura, S., Yasumoto, M.                          | Hard X-ray microbeam experiments with a sputtered-sliced Fresnel zone plate and its applications   |
| 5     | 0    | 317        | research papers | 7            | 3                           | <b>Shastri, S.D.</b> , Fezzaa, K., Mashayekhi, A., Lee, W.-K., Fernandez, P.B., Lee, P.L.  | Cryogenically cooled bent double-Laue monochromator for high-energy undulator X-rays (50-200 keV)  |
| 5     | 0    | 313        | research papers | 7            | 1                           | <b>Yamauchi, K.</b> , Yamamura, K., Mimura, H., Sano, Y., Saito, A., Souvorov, A., Yabashi, M., Tamasaku, K., Ishikawa, T., Mori, Y. | Nearly diffraction-limited line focusing of a hard-X-ray beam with an elliptically figured mirror  |

|   |   |     |                   |   |    |  |  |
|---|---|-----|-------------------|---|----|--|--|
| 1 | 0 | 9   | research papers   | 6 | 0  | Di Matteo, S., <b>Natoli, C.R.</b>   | A multiple-scattering theory of circular and linear dichroism for photoemission and photoabsorption  |
| 6 | 0 | 347 | research papers   | 6 | 10 | Murray, J., <b>Garman, E.</b>  | Investigation of possible free-radical scavengers and metrics for radiation damage in protein cryocrystallography Presented at the 'Second International Workshop on Radiation Damage to Crystalline Biological Samples' held at Advanced Photon Source, Chicago, USA, in December 2001.                     |
| 4 | 0 | 202 | research papers   | 6 | 3  | <b>Hirai, M.</b> , Iwase, H., Hayakawa, T., Miura, K., Inoue, K.   | Structural hierarchy of several proteins observed by wide-angle solution scattering  |
| 4 | 0 | 246 | research papers   | 5 | 2  | <b>Kappen, P.</b> , Troger, L., Materlik, G., Reckleben, C., Hansen, K., Grunwaldt, J.-D., Clausen, B.S.   | Silicon drift detectors as a tool for time-resolved fluorescence XAFS on low-concentrated samples in catalysis   |
| 6 | 0 | 329 | research papers   | 5 | 8  | O'Neill, P., Stevens, D.L., <b>Garman, E.</b>  | Physical and chemical considerations of damage induced in protein crystals by synchrotron radiation: a radiation chemical perspective Presented at the 'Second International Workshop on X-ray Damage to Crystalline Biological Samples' held at the Advanced Photon Source, Chicago, USA, in December 2001. |
| 6 | 0 | 375 | research papers   | 5 | 3  | <b>Hanson, B.L.</b> , Harp, J.M., Kirschbaum, K., Schall, C.A., <a href="#">DeWitt</a> , K., Howard, A., Pinkerton, A.A., Bunick, G.J.   | Experiments testing the abatement of radiation damage in d-xylose isomerase crystals with cryogenic helium Presented at the 'Second International Workshop on Radiation Damage to Crystalline Biological Samples' held at Advanced Photon Source, Chicago, USA, in December 2001.                            |
| 6 | 0 | 342 | research papers   | 5 | 8  | <b>Weik, M.</b> , Berges, J., Raves, M.L., Gros, P., <a href="#">McSweeney</a> , S., Silman, I., Sussman, J.L., Houee-Levin, C., Ravelli, R.B.G.   | Evidence for the formation of disulfide radicals in protein crystals upon X-ray irradiation Presented at the 'Second International Workshop on Radiation Damage to Crystalline Biological Samples' held at Advanced Photon Source, Chicago, USA, in December 2001.   |
| 6 | 0 | 401 | computer programs | 5 | 9  | <a href="#">McPhillips</a> , T.M., <a href="#">McPhillips</a> , S.E., Chiu, H.-J., Cohen, A.E., Deacon, A.M., Ellis, P.J., Garman, E., Gonzalez, A., Sauter, N.K., Phizackerley, R.P., Soltis, S.M., <b>Kuhn, P.</b> | Blu-Ice and the Distributed Control System: software for data acquisition and instrument control at macromolecular crystallography beamlines   |
| 4 | 0 | 254 | research papers   | 5 | 1  | <b>Warwick, T.</b> , Ade, H., Kilcoyne, D., Kritscher, M., Tyliczszak, T., Fakra, S., Hitchcock, A., Hitchcock, P., Padmore, H.  | A new bend-magnet beamline for scanning transmission X-ray microscopy at the Advanced Light Source   |
| 1 | 0 | 17  | research papers   | 5 | 1  | <b>Shvyd'ko, Y.V.</b> , Lucht, M., Gerdau, E., Lerche, M., Alp, E.E., Sturhahn, W., Sutter, J., Toellner, T.S.   | Measuring wavelengths and lattice constants with the Mossbauer wavelength standard   |
| 4 | 0 | 206 | research papers   | 5 | 1  | Bodenthin, Y., Grenzer, J., Lauter, R., <b>Pietsch, U.</b> , Lehmann, P., Kurth, D.G., Mohwald, H.   | Temperature- and time-resolved X-ray scattering at thin organic films Presented at the 'ESF Exploratory Workshop on Time-Resolved Investigations with Neutrons and X-rays (TINX)' held in Berlin, Germany, in September 2001.  |
| 3 | 0 | 107 | research papers   | 5 | 1  | Baruchel, J., <b>Hartwig, J.</b> , Pernot-Rejmankova, P.   | Present state and perspectives of synchrotron radiation diffraction imaging  |
| 3 | 0 | 125 | research papers   | 5 | 0  | <b>Awaji, M.</b> , Suzuki, Y., Takeuchi, A., Takano, H., Kamijo, N., Tamura, S., Yasumoto, M.  | Zernike-type X-ray imaging microscopy at 25 keV with Fresnel zone plate optics   |

| Journal of Synchrotron Radiation - 2003 |      |            |                 |                 |                             |  |   |   |
|---|------|------------|-----------------|-----------------|-----------------------------|--|---|---|
| Issue                                   | Part | First page | Paper category  | ISI citation    | Total IUCr citation to date | Authors  | Title   |   |
| 1                                       | 0    | 51         | research papers | 19              | 6                           | <b>Benfatto, M.</b> , Della Longa, S., Natoli, C.R.  | The MXAN procedure: a new method for analysing the XANES spectra of metalloproteins to obtain structural quantitative information                               |   |
| 1                                       | 0    | 26         | research papers | 16              | 3                           | <b>Natoli, C.R.</b> , Benfatto, M., Della Longa, S., Hatada, K.  | X-ray absorption spectroscopy: state-of-the-art analysis  |   |
| 1                                       | 0    | 23         | research papers | 13              | 3                           | <b>Winn, M.D.</b>  | An overview of the CCP4 project in protein crystallography: an example of a collaborative project   |   |
| 1                                       | 0    | 16         | research papers | 13              | 3                           | <b>Ascone, I.</b> , Meyer-Klaucke, W., Murphy, L.  | Experimental aspects of biological X-ray absorption spectroscopy  |   |
| 1                                       | 0    | 9          | research papers | 12              | 5                           | <b>Hasnain, S.S.</b> , Strange, R.W.   | Marriage of XAFS and crystallography for structure-function studies of metalloproteins  |   |
| 2                                       | 0    | 125        | research papers | 9               | 0                           | Kilcoyne, A.L.D., Tyliczszak, T., Steele, W.F., Fakra, S., Hitchcock, P., Franck, K., Anderson, E., Harteneck, B., Rightor, E.G., Mitchell, G.E., Hitchcock, A.P., Yang, L., Warwick, T., <b>Ade, H.</b> | Interferometer-controlled scanning transmission X-ray microscopes at the Advanced Light Source  |   |
| 3                                       | 0    | 260        | research papers | 8               | 0                           | <b>D'Acapito, F.</b> , Davoli, I., Ghigna, P., Mobilio, S.   | The ReflEXAFS station at the GILDA beamline (BM08) of ESRF  |   |
| 5                                       | 0    | 398        | research papers | 7               | 3                           | Fischetti, R.F., Rodi, D.J., Mirza, A., Irving, T.C., Kondrashkina, E., <b>Makowski, L.</b>  | High-resolution wide-angle X-ray scattering of protein solutions: effect of beam dose on protein integrity  |   |
| 3                                       | 0    | 219        | research papers | 7               | 0                           | <b>Dix, W.-R.</b> , Kupper, W., Dill, T., Hamm, C.W., Job, H., Lohmann, M., Reime, B., Ventura, R.   | Comparison of intravenous coronary angiography using synchrotron radiation with selective coronary angiography  |   |
| 1                                       | 0    | 43         | research papers | 6               | 1                           | <b>Rehr, J.J.</b> , Ankudinov, A.L.  | New developments in the theory and interpretation of X-ray spectra based on fast parallel calculations  |   |
| 1                                       | 0    | 71         | research papers | 6               | 3                           | <b>Strange, R.W.</b> , Eady, R.R., Lawson, D., Hasnain, S.S.   | XAFS studies of nitrogenase: the <b>MoFe</b> and VFe proteins and the use of crystallographic coordinates in three-dimensional EXAFS data analysis              |   |
| 1                                       | 0    | 64         | research papers | 6               | 2                           | Mijovilovich, A., <b>Meyer-Klaucke, W.</b>   | Simulating the XANES of metalloenzymes - a case study   |   |
| 6                                       | 0    | 461        | research papers | 6               | 0                           | Quinn, F., <b>Poolton, N.</b> , Malins, A., Pantos, E., Andersen, C., Denby, P., Dhanak, V., Miller, G.  | The Mobile Luminescence End-Station, MoLES: a new public facility at Daresbury Synchrotron  |   |
|   | 2    | 0          | 137             | research papers | 6                           | 2  | <b>Tamura, N.</b> , <b>MacDowell, A.A.</b> , Spolenak, R., Valek, B.C., Bravman, J.C., Brown, W.L., Celestre, R.S., Padmore, H.A., Batterman, B.W., Patel, J.R. | Scanning X-ray microdiffraction with submicrometer white beam for strain/stress and orientation mapping in thin films |
| 4                                       | 0    | 332        | research papers | 5               | 0                           | <b>Berry, A.J.</b> , Shelley, J.M.G., Foran, G.J., O'Neill, H.S.C., Scott, D.R.  | A furnace design for XANES spectroscopy of silicate melts under controlled oxygen fugacities and temperatures to 1773 K   |   |
| 6                                       | 0    | 430        | research papers | 5               | 1                           | <b>Giles, C.</b> , Yokaichiya, F., Kycia, S.W., Sampaio, L.C., Ardiles-Saravia, D.C., Franco, M.K.K., Neuenschwander, R.T.   | High-resolution X-ray diffraction beamline at the LNLS for the study of charge, orbital and magnetic structures   |   |

|   |   |     |                 |   |   |   |  |
|---|---|-----|-----------------|---|---|---|--|
| 2 | 0 | 177 | research papers | 5 | 2 | <b>Martorana, A.</b> , Deganello, G., Longo, A., Deganello, F., Liotta, L., Macaluso, A., Pantaleo, G., Balerna, A., Meneghini, C., Mobilio, S.   | Time-resolved X-ray powder diffraction on a three-way catalyst at the GILDA beamline |
| 1 | 0 | 46  | research papers | 5 | 0 | <b>Di Cicco, A.</b>   | Local structure in molecular complexes probed by multiple-scattering XAS             |
| 1 | 0 | 4   | research papers | 5 | 1 | Quevillon-Cheruel, S., Collinet, B., Zhou, C.-Z., Minard, P., Blondeau, K., Henkes, G., Aufrere, R., Coutant, J., Guittet, E., Lewit-Bentley, A., Leulliot, N., Asccone, I., Sorel, I., Savarin, P., La Sierra Gallay, I.L. de, Torre, F. de la, Poupon, A., <b>Fourme, R.</b> , Janin, J., Tilbeurgh, H. van | A structural genomics initiative on yeast proteins                                   |

## Journal of Synchrotron Radiation - sales and circulation figures

### Institutional and consortial circulation totals

|                             | 2003 | 2004 |
|-----------------------------|------|------|
| Consortia site access       |      | 1891 |
| 1. Europe                   |      | 882  |
| 2. USA                      |      | 196  |
| 3. Canada                   |      | 32   |
| 4. Aus/NZ                   |      | 240  |
| 5. Japan                    |      | 86   |
| 6. Rest of World            |      | 455  |
| Institutional subscriptions | 150  | 154  |
| Online                      | 7    | 16   |
| Standard                    | 143  | 137  |
| Online Collection           | 0    | 1    |
| Personal subscriptions      | 72   | 67   |

### Institutional subscriptions by region

| Region                        | Sub Type          | 2003 Total | 2004 Total |
|-------------------------------|-------------------|------------|------------|
| 1. Europe                     | Online            | 3          | 6          |
|                               | Standard          | 60         | 57         |
|                               | Online Collection | 0          | 0          |
| <b>1. Europe Total</b>        |                   | <b>63</b>  | <b>63</b>  |
| 2. North America              | Online            | 5          | 4          |
|                               | Standard          | 28         | 34         |
|                               | Online Collection | 0          | 1          |
| <b>2. North America Total</b> |                   | <b>33</b>  | <b>39</b>  |
| 3. Aus/NZ                     | Online            | 1          | 3          |
|                               | Standard          | 5          | 4          |
| <b>3. Aus/NZ Total</b>        |                   | <b>6</b>   | <b>7</b>   |
| 4. Japan                      | Online            | 1          | 1          |
|                               | Standard          | 25         | 21         |
| <b>4. Japan Total</b>         |                   | <b>26</b>  | <b>22</b>  |
| 5. Rest of World              | Online            | 1          | 2          |
|                               | Standard          | 21         | 21         |
|                               | Online Collection | 0          | 0          |
| <b>5. Rest of World Total</b> |                   | <b>22</b>  | <b>23</b>  |
| <b>Grand Total</b>            |                   | <b>150</b> | <b>154</b> |

## Facility information pages

| Current  | Contacted |
|----------|-----------|
| APS      | BESSY     |
| ESRF     | DESY      |
| SPring-8 | Diamond   |
|          | LLS       |
|          | MAX-lab   |
|          | SLS       |
|          | SOLEIL    |
|          | SRS       |

## Facilities with subscriptions

|          |   |
|----------|---|
| Americas | Advanced Photon Source (APS), USA                                 |
|          | Cornell High Energy Synchrotron Source (CHESS), USA               |
|          | Canadian Light Source (CLS), Canada                               |
|          | Laboratorio Nacional de Luz Sincrotron (LNLS), Brazil             |
|          | Synchrotron Radiation Center (SRC), USA                           |
|          | Stanford Synchrotron Radiation Laboratory (SSRL), USA             |
| Europe   | DAFNE Light, Italy  |
|          | Diamond, UK   |
|          | Elettra Synchrotron Light Laboratory, Italy                       |
|          | European Synchrotron Radiation Facility (ESRF), France            |
|          | Hamburger Synchrotronstrahlungslabor (HASYLAB) at DESY, Germany   |
|          | Swiss Light Source (SLS), Switzerland                             |
|          | SOLEIL, France  |
|          | Synchrotron Radiation Source (SRS), UK                            |
| Asia     | INDUS 1/INDUS 2, India  |
|          | National Synchrotron Radiation Research Center (NSRRC), Taiwan    |
|          | Pohang Accelerator Laboratory (PAL), Korea                        |
|          | Photon Factory (PF), Japan  |
|          | Ultraviolet Synchrotron Orbital Radiation Facility (UVSOR), Japan |

## **Section Editors' Meeting**

**Grand Hotel Panoramic, Montecatini Terme, Italy**

22 August, 17:30-18:30

**CHAIR: John Helliwell**

Attendees: Main and Section Editors

IUCr staff attending: Peter Strickland, Tony Weight, Sean Conway, Gillian Holmes, Louise Jones, Jill Bradshaw, Sue Barnes

### **1. ELECTRONIC PROOFING ARRANGEMENTS FOR SECTION AND MAIN EDITORS**

Advance proofs, i.e. proofs sent out in advance of author proofs, are currently provided to the Editors of Sections B, C and E. Do any other Editors require this facility?

Are the proofing arrangements otherwise working satisfactorily?

### **2. STATISTICS**

The Chester Office has recently started to provide additional online statistics and graphs to show overall numbers of papers submitted, accepted, rejected, published and in various production stages. These are available from the link "Journal statistics" in the online status pages. Is there any particular additional information that it might be useful to include?

Currently, the Chester Office provides performance information for Co-editors.

Is this information adequate?

How can this information best be used?

Should statistics relating to appeals to Section Editors and the Editor-in-chief (number of appeals, number declined, number upheld) be published?

### **3. NEW CO-EDITOR APPOINTMENTS/EDITORIAL BOARDS**

Have Section and Main Editors encountered any problems in making new Co-editor appointments. Would it be useful to provide a summary of the procedures involved?

### **4. MATTERS ARISING FROM THE GENERAL AGENDA**

### **5. MATTERS FOR THE OPEN COMMISSION MEETINGS**

### **6. MATTERS TO BE RAISED WITH THE EXECUTIVE AND/OR FINANCE COMMITTEE IN FLORENCE**

### **7. JOURNALS' DEVELOPMENT SUMMARY**

John Helliwell has produced a report that summarises the development plans of the different IUCr Journals. It also makes a Strengths Weaknesses Opportunities and Threats (SWOT) analysis, a detailed risk analysis and a sensitivity analysis of outcomes and input parameters. The report has been circulated to Section and Main Editors, and to JComm meeting attendees; comments on the report are invited.