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.

Keywords: IUCr journals, *Acta Cryst. D*, biological crystallography

OCM01.24.6

Acta Cryst. (2005). A**61**, C126

***Acta Crystallographica Section E: Structure Reports Online*: Rapid Growth 2001–2004**

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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.

Keywords: journal publishing, IUCr journals, crystallography journals online

OCM01.24.7

Acta Cryst. (2005). A**61**, C126

***Acta Crystallographica Section F*: Launch Year Report**

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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.

Keywords: *Acta Cryst. F*, crystallization, structural genomics

OCM01.24.8

Acta Cryst. (2005). A**61**, C126

Journal of Applied Crystallography

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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.

Keywords: journals commission, *Journal of Applied Crystallography*, IUCr publications

OCM01.24.9

Acta Cryst. (2005). A**61**, C126

***Journal of Synchrotron Radiation*: Current Status and Issues**

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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.

Keywords: IUCr journals, *Journal of Synchrotron Radiation*, current status

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OCM02 COMMISSION ON JOURNALS (II)

Coordinator: John R. Helliwell

OCM02.25.1

Acta Cryst. (2005). A**61**, C126-C127

Getting the best out of IUCr Journals (Practical Advice and Demonstrations)

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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.

Keywords: journal publishing, IUCr journals, Crystallography Journals Online

OCM03 THE CURRENT STATUS AND FUTURE PROSPECTS OF CIF

Coordinator: D. Brown

OCM03.26.1

Acta Cryst. (2005). A**61**, C127

mmCIF and Modern Macromolecular Structure Determination Software: Status and Perspectives

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As developers in the *Phenix* project [1], we are confronted with *mmCIF* in two ways. Firstly, our algorithms produce results that need to be archived. Secondly, access to information stored in databases, such as the PDB [2], is often invaluable in the development and testing of new methods. In contrast to most traditional, static file formats, *mmCIF* is highly flexible. Therefore we have the opportunity to export parameters and results of ever more complex algorithms in a uniform framework. However, it is non-trivial to import information from *mmCIF* files since their processing requires very sophisticated tools. Unfortunately, in many contexts adequate practical tools are not available. The limitations of traditional software development technology are probably the most important factors giving rise to this situation. Fortunately, many in the crystallographic methods development community have begun a transition to modern software technology. Database developers, most notably at the PDB, have already published comprehensive *mmCIF* libraries. Further development of such libraries in a collaborative effort with an open two-way exchange between the communities has the potential to stimulate a much wider use of *mmCIF* in the future.

[1] Adams P.D., Gopal K., Grosse-Kunstleve R.W., Hung L.-W., Ioerger T.R., McCoy A.J., Moriarty N.W., Pai R.K., Read R.J., Romo T.D., Sacchettini J.C., Sauter N.K., Storoni L.C., Terwilliger T.C., *J. Synchrotron Rad.*, 2004, **11**, 53-55. [2] Berman H.M., Westbrook J., Feng Z., Gilliland G., Bhat T.N., Weissig H., Shindyalov I.N., Bourne P.E., *Nucleic Acids Research*, 2000, **28**, 235-242.

Keywords: mmCIF, structure database, software development

OCM03.26.2

Acta Cryst. (2005). A**61**, C127

A Dictionary Approach to Translate Memory Variables from Crystallography Software to mmCIF Items

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A major obstacle in building CIF output from crystallography software is to address the relation between the information software can supply and the information mmCIF required. Generally the building process is time-consuming and even more effort is necessary to maintain the source code due to constant changes of the software. We present here, a dictionary-based approach, and the tool used to build such a dictionary. In this approach, the memory-to-mmCIF relation is classified as equivalence, conversion, constant, source conversion, comment, pending or unknown. Each mmCIF item is subject to classification by the developer's examination with the assistance from a domain expert. The CIF Translator Dictionary (CTD) builder is utilizing a dump of all global variables with its value in memory as source of information. This memory dump is in STAR format and allow the CTD developer to do realtime tracking of related variables in memory. Generally it is possible to fetch related variable names in 2 to 5 memory scan by a domain expert. Andfter addressing the relationship between these variables with mmCIF item, a CTD entry will be generated automatically for simple relation, or more infomation will be acquired for complicate relation.

To test the effectiveness of this approach, HKL2000 CTD is built in its initial stage. Automatic completion from HKL2000 memory is performed without human intervention. For more specific tuning toward publication quality CIF after autofill, HKL2000-CIF is also designed as a CIF editor featuring entities editing and providing an evolving amount of wizard procedures that assist further manual examination, and validation before final submission.

Keywords: CIF, CTD, mmCIF

OCM03.26.3

Acta Cryst. (2005). A**61**, C127

Analysis and Visualization of TLS Motion in Proteins using the mmLib Toolkit

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We have developed a programming library, mmLib [1], which provides a rich set of tools for the import, manipulation, and export of macromolecular structural models described in CIF and mmCIF. Using this toolkit, we are developing higher level tools for visualization and structural/functional analysis. We are in particular working to infer and model functionally important modes of protein flexibility directly from single crystal structures.

TLS (Translation/Libration/Screw) models describe rigid-body vibrational motions of arbitrary objects. A single-group TLS model can be used to approximate the vibration of an entire protein molecule within the crystal lattice. More complex TLS models are broadly applicable to describe inter-domain and other internal vibrational modes of proteins. We are developing a web-based analysis tool, **TLSMD**, that generates optimal multi-segment TLS models. These may be used to analyze the presence and physical significance of TLS motion in existing structures, to guide additional crystallographic refinement, or to generate target models of protein flexibility for use in computational protein-protein or protein-ligand docking.

The interactive graphics program **TLSVIEW** [2] allows visualization of these and other models for rigid-body motion in proteins, using animation and a variety of static representations.

Both tools are applicable to protein structures at any resolution.

[1] Painter J., Merritt E.A., *J. Appl. Cryst*.,2004, **37**, 174-178. [2] Painter J., Merritt E.A., *Acta Cryst*.,2005, **D61**, 465-471.

Keywords: graphics, dynamics, docking computation

OCM03.26.4

Acta Cryst. (2005). A**61**, C127-C128

CIF Operations and Applications at the CCDC

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Most major journals require CIF deposition to the CCDC, usually during the submission process, and more than 98% of raw input to the CSD now arrives in CIF form. The CCDC maintains a Supplementary Data Archive of deposited CIFs and, after publication, individual CIFs are made freely available via a simple Web-based request form. The CCDC program enCIFer is available for Web download to check, edit