

Editorial

Improved crystallographic techniques are often closely linked to advances in technology. This relationship exists because of the computational and data intensive nature of our discipline. In recent times these advances have been nothing short of breathtaking, with desk-top computers rivalling the performance of yesterday's supercomputers and diffraction data being measured at rates faster than older machines took to align a crystal! For most of us these are exhilarating times which show no sign of abating. However, such advances are not without cost. Rapid improvements in data acquisition and processing must be matched by more effective methods of disseminating information, or bottlenecks will soon develop. This is one of the reasons why many scientific disciplines are pooling their data-handling knowledge and experience to cope with the so-called 'information explosion'. The proceedings of the recent UNESCO/ICSU conference on Electronic Publishing in Science provide interesting background to this topic (<http://www.lmcp.jussieu.fr/icsu/Information/Meetings/Summaries/>).

The need to improve the dissemination of crystal structure information has led to some important changes to the *Section C* submission requirements and publication options. These are summarized in the 1997 *Notes for Authors* on pages 147–162. Some of these changes are an extension to the electronic publication policies being applied to all IUCr journals, while others are in direct response to the rapid growth of *Section C* last year.

In 1996 *Section C* published 1285 papers (1511 structures and 3130 pages) as compared to 854 papers in 1994. This growth does, however, pose something of a paradox and is probably a good example of 'technology bite-back'! Journals depend on an active author interest, and if their submission format becomes the community standard this is an added bonus. However, significant increases in journal size are sustainable only when supported by increased income. Currently, subscriptions to all IUCr journals are on a slight decline. Although this is an industry-wide trend due to diminishing library and education budgets, it is simply not possible to expand a publication, with all of the editorial and printing costs that this entails, when the subscription base is diminishing.

It should be emphasized that the growth of *Section C* last year was not due to the publication of structures determined from area-detector data. This means that the expected surge of papers from these instruments is yet to come. If area detectors increase productivity at the rate that some predict then this must be allowed for in future publication policies. These were the major issues discussed at the Commission on Journals meetings in Seattle in August last year. A number of important policy recommendations were made at these meetings, which have now been approved by the IUCr Executive Committee.

The most important change in policy is that there are now two avenues for publishing structure studies. Authors must choose between full and CIF-access modes of publication. Details of these modes are given in the new *Notes for Authors*. Full papers are handled editorially in a way similar to 1996 submissions. CIF-access papers are not printed but are listed, within two months of acceptance, in the Table of Contents of the journal and on the *Section C* web page. This is a fast mode of disseminating complete, stringently tested structural data, albeit with reduced submission requirements for text items.

An integral part of both publication approaches is stricter data standards. The data checking has been automated where possible in order to reduce the time spent on submissions which are incomplete or contain identifiable data problems. The latest tests cover most aspects of the submitted data, and are intended to promote higher standards for published and archived structural data. An overview of the data requirements is provided in the 1997 *Notes for Authors*. More detailed information on the validation tests will be published in an IUCr booklet *A Guide for Section C Authors*, and will also appear on the web site <http://www.iucr.ac.uk/journals/acta/actac.html>. These standards are also intended as benchmarks for future software packages, with the long-term objective of making them part of the structure determination and refinement calculations.

Preparing and implementing the new data checking facilities has been, and continues to be, a major effort. Authors will have access to these tests *via* the 'checkcif' facility as quickly as possible. As in the past, the use of this service will avoid delays that can occur after the CIF has been submitted. When a submitted CIF has passed these checks it will be assigned a data-validation number (*e.g.* IUC97-A0856). This number is primarily the certification that a CIF contains structural data which meet the current IUCr standards for a reliable study. It will also be used to retrieve the archived CIF and as a reference code in publications.

There will also be changes to *Section C* layout. Starting next month (February 1997) coordinate tables will not be printed unless sites of special symmetry are present. The complete set of atomic parameters is, of course, available as CIF data. There will also be some style changes to the *Experimental* section and several new data items for area-detector data have been added. Additional space will be saved by stricter enforcement of the 'one diagram per structure' and the 'listing of novel geometry' guidelines.

Several important handling changes are to be instituted to speed up the publication times. Authors will now be required to respond to an editorial request within three months or the submission will be withdrawn. Because of delays associated with major revisions, editors now

reserve the right to reset the date of receipt if there are excessive delays. The fast-track option of previous years has been replaced by a more flexible approach which permits Co-editors to request the preferred handling of papers delayed during review through no fault of the authors.

The 1997 *Notes for Authors* have been reorganized to contain a section on data-validation criteria and a complete list of items required for submission. The electronic deposition of structure factors is now mandatory. This is consistent with the overall thrust of the recent policy decisions to raise the quality of published structural data, and to strengthen the usefulness of the CIF archives as a complete and reliable data resource. The CIF-access publication option is part of the effort to make complete structural data quickly available over the Internet. Software is already freely available for reading and displaying CIF data accessed *via* the Internet, and CIF browsers and visualization software are expected to be commonplace in the near future.

Changes to submission procedures can be disruptive not only for authors but also for editorial staff, and are made only when there are compelling reasons for doing so. Balancing the dichotomy of stability and innovation is always difficult. At a time of rapid change the *Section*

C Board has opted to provide both printed and electronic modes of dissemination, with a particular emphasis on the quality of structure determinations needed for future comparative studies. These initiatives are consistent with the responsibility of the IUCr to maintain the highest possible standards for our discipline. For most authors, and particularly those wanting to keep pace with an increasing rate of structure determinations, this choice will be welcomed.

To close on a light note, readers will have noticed this month's cover, the first for *Section C* in colour. It serves several purposes. As usual, it was selected to highlight a good crystallographic study of an interesting compound. More than that though, this structure's molecular 'garland of atoms' reminds us that, despite the helter-skelter pace of today's science, we are fortunate to be part of a profession which reveals such beautiful insights into nature. These discoveries provide us with moments of contemplation and wonder. As a Utopian, I believe that each new initiative, be it in science or publishing, provides additional opportunities for discovery, and is therefore to be explored with optimism.

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