

Editorial

One year and 12 issues have passed since *Section C* underwent a major revision to its format. Judging from the positive response received, these changes have gone some way towards satisfying the publication needs of the structural science community. We believe that the new *Contents* format, and the increased preparative chemistry information, have resulted in a wider readership among chemists. The simplified 1994 *Notes for Authors* resulted in improved adherence to the submission criteria. These are positive outcomes to significant journal changes - something that one takes on in publishing with a certain trepidation!

As with the introduction of electronic submissions, these changes are first steps in improving the overall communication of accurate structural information. *Section C* is moving ahead cautiously. Network facilities for the electronic delivery of text and data are evolving rapidly. A commitment to one of these will not be made until we are confident of an approach that will provide long-term benefits to structural scientists. Several delivery approaches will be examined and tested this year with the aim of providing additional electronic services at the start of 1996. In the meantime, readers may access the electronic archive of published CIF material at the *Acta Crystallographica* office by contacting the Managing Editor.

A revised version of the [Notes for Authors](#) is published in this issue. The *Section C* submission requirements remain basically unchanged from 1994. There are, however, important shifts in emphasis that are worth highlighting.

There will be an increased effort to improve publication times, which were reduced in 1994 but are still significantly longer than those which we believe our publication process is capable of. We cannot hope to emulate the speed of expensive journals with large staffs, nor of those with very low acceptance rates, but streamlining present procedures will improve our throughput significantly, employing the following strategies.

(a) Electronic CIF submission will be very strongly encouraged with the aim to have 100% CIF submission by January 1996. Hard-copy manuscripts require more editorial effort, are less reliable, and consequently have a much slower throughput than CIF submissions.

(b) Entry submission criteria will be strictly administered. The onus will be on authors to correct submission inadequacies rather than the editorial staff. This will enable them to concentrate on

processing complete submissions. Checks on entry submissions will include the completeness of published and supplementary data, and the need for publication-quality diagrams.

(c) To complement the above strategies, authors are now asked to validate CIF's remotely by e-mail before submission. A CIF may be e-mailed to **checkcif@iucr.ac.uk** and a check report returned automatically, usually within minutes. The checks applied are not exhaustive, but they will eliminate most delays that result from common CIF submission errors.

(d) There will be a general tightening of acceptance criteria. In the past there has been some flexibility with acceptance standards, particularly for new authors. The rising cost of publication, and the increasing number of submissions (with the prospect of future diffraction measurements in hours rather than days) now makes this impractical. Marginal submissions consume significantly more editorial resources than good ones and the onus will be on authors to meet the journal standards at the outset, or risk immediate rejection.

The new *Notes for Authors* contain a summary of the errors most commonly encountered with submitted experimental data (see §3.8). Authors should take particular note of these. Each represents a potential problem area which should be resolved before an analysis is started, and must certainly be addressed prior to submission to *Section C*. For example, too many structures are being submitted in a space-group symmetry lower than that permitted by the diffraction information. Checks must always be made for the correct space group by carefully examining the cell choice and the systematically absent intensities. Automatic alignment routines can get it wrong because they do not analyse the effects of multiple diffraction. Remember that a higher symmetry results in a more precise determination (because there are less refinable parameters) and avoids incorrect geometry and chemical conclusions!

Too often absorption corrections are being applied without regard to the magnitude of the absorption coefficient, the crystal shape, or the appropriateness of the correction methodology. Poor absorption practices arise for a variety of reasons: the tendency to take computational 'short cuts' rather than making additional measurements, general lack of understanding of the physical phenomena or calculations involved, and even the use of a rigid computational approach that does not take into account variations in the materials being studied. Delta F -refined absorption corrections are particularly problematic because they do not adequately use the crystal information and they depend critically on when they are applied in the analysis, and on other systematic errors in the data. In future submissions, absorption procedures will be reviewed very carefully for applicability and to see if the resulting transmission factors make physical sense.

Finally, authors are asked to take a closer look at the use of 'observed' thresholds in the partitioning of reflection data. This concept is a historical artefact which has little relevance to current structure analyses where the estimated errors for diffraction intensities should be used in the weights of the refinement process. Authors are encouraged to improve the precision of the refined parameters by lowering, or removing, this threshold, rather than raising it in order to reduce the R value.

I want to conclude with some news about an additional *Section C* service and a general realignment of Co-editorial duties. As announced earlier in the *IUCr Newsletter*, starting with this issue 25 free reprints of each *Section C* paper will be sent to the contact author. There has also been an important organizational change to the IUCr Commission on Journals in that members are now nominated for participation in the individual Co-editorial groups for each section. This is a level of specialization that was inevitable as the journals focus on the needs of their readership. The Co-editors listed at the front of a *Section C* issue are specialists in structural science; all are active in the review of *Section C* papers. This is a positive step for the journals, which depend heavily on the expert, efficient and dedicated efforts of their Co-editors.

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