

Editorial

The principle guiding the publication of *Section C* papers continues to be that the diffraction measurements and calculations must be appropriate to a high-quality structure determination of the compound under study. Our aim is to publish the best possible studies involving the most interesting structural science and materials. This goal may run counter to the 'pop another crystal on the automatic diffractometer' approach still prevalent in some laboratories, but we maintain that high standards are important for the future. The IUCr is committed through *Acta Crystallographica* to providing such long-term benefits for the discipline and for science as a whole.

This month's cover has special significance. Apart from being in colour, it is the first occasion that a CIF-access structure has been featured. The cover is also unusual in that this structure is from a 1997 issue, whereas all previous cover structures have been current. This is not because of a lack of suitable structures in this issue, but because the *speed* with which a CIF-access paper is published does not allow enough time to prepare the cover illustration for the issue in which it appears. As with every issue, the cover structure is selected because of its interest and quality, although on this occasion it also serves to emphasize that all papers published in *Acta Crystallographica* meet these requirements.

The 1998 *Notes for Authors* are included in this issue. The submission requirements are essentially unchanged from last year, except that authors will be required to pre-check their submissions using the e-mail CHECKCIF facility from June 1998 onwards. This requirement coincides with an increased use of automatic checking software, both in CHECKCIF and at the Chester office, to validate the submitted data. The checking software applies an extensive suite of data-validation tests, the algorithms for which are described at <http://www.iucr.org/journals/acta/dv.html>. These tests culminate in an assessment report containing 'alert' messages for any data problems detected. The severity of the alert varies according to the deviation of the data from the expected values.

Because CHECKCIF incorporates these tests, authors can now receive a detailed error assessment of their data prior to submitting the CIF for publication. The CHECKCIF report is the same as that used by the referees, so authors can circumvent delays in the review process by taking early corrective action. This will speed up publication times.

Alert messages generated by CHECKCIF will require a response from the author. Usually this will be to

eliminate the cause of the problem. However, if it is believed that the nature of the study warrants deviation from the *Section C* requirements, authors can insert an explanation into the CIF using an electronic form supplied with the CHECKCIF output. This provides a simple mechanism by which authors can respond to a potential review query. Without this, alerts detected by the data-validation tests at Chester may result in the submission being returned, and perhaps even rejected, before being sent for review. It must be emphasized, however, that responses such as 'the compound has a low melting point' without an attempt to collect low-temperature data, 'we lost the crystal' when inappropriate absorption corrections were applied, or 'the structure was determined in 1982' when the number of measured data is insufficient are unlikely to be accepted.

If authors show clearly that strenuous efforts were made to meet the data standards, but for reasons beyond their control they could not be met, due consideration will be given. However, such circumstances are rare and, if the paper is accepted, an explanation will need to be given within the text.

I return now to the increasing importance of CIF-access publications. This mode provides for the rapid publication of structure studies at the expense of a place in the printed journal. The data standards for these publications are identical to those for papers printed in full. The CIF-access mode is attractive not only because it saves time (for the authors and the journal) but also because it provides a complete yet condensed format for studies which may not be central to an author's main interests. With the increased throughput of area-detector diffractometers, this is certain to be a preferred publication route for many structures. Clearly, a CIF-access publication offers greater benefits to the author than direct database deposition, both in terms of the level of data validation applied and the extent of the archived data. The latter include all aspects of the diffraction study from the author's comments to the structure factors.

Readers who wish to access *Section C* publications via the web can obtain CIF browser software from <http://www.iucr.org/cif/home.html>. This enables the reader to retrieve the CIF for a paper from IUCr web servers within seconds and display and manipulate the molecule and cell on the screen with a few clicks of the mouse. This is the first step towards more versatile web tools for accessing CIF-based structural papers.

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