Important news for authors of articles containing X-ray crystallography

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New guidelines for the assessment and publication of X-ray crystallography in RSC Journals have been announced.

Pre-submission checks

Authors are required to provide both cifs and CheckCIF reports (as a pdf) for any crystallographic studies in their articles. The provision of CheckCIF reports will help expedite the assessment of the crystallographic aspects of articles. CheckCIF is a free-to-use cif checking web service provided by the International Union of Crystallography, and can be found *via*:

http://checkcif.iucr.org/

Presentation of data in the manuscript

The guidelines concerning the information appearing in journal articles have also been revised:

Full papers

Where appropriate, the description may be given in textual or tabular form, although the latter is more appropriate if several structure determinations are being reported in one paper. A table of selected bond lengths and angles, with estimated standard deviations should be restricted to significant dimensions only (for example it is rarely necessary to include data for phenyl rings). Average values may be given (with a range of e.s.d.s) for chemically equivalent groups or for similar bonds. Differences from expected norms should be noted.

Communications

Details of the data collection and CCDC number should be given in a footnote or in the References/Notes section. Selected bond lengths and angles, with estimated standard deviations, should be included in the figure caption and be restricted to significant dimensions only.

Data required for presentation in the manuscript

For both full papers and communications, the following information should be given in the manuscript if there is significant discussion of the crystallography:

- Chemical formula and formula weight (M)
- Crystal system
- Unit-cell dimensions (Å or pm, degrees) and volume, with estimated standard deviations, temperature
- Space group symbol (if non-standard setting give related standard setting)
- No. of formula units in unit cell (Z)
- Number of reflections measured and/or number of independent reflections, R_{int}
- Final R values (and whether quoted for all or observed data)

Authors are advised to read the full Author Guidelines for further information, available *via*:

http://www.rsc.org/Publishing/ReSourCe/AuthorGuidelines/Techniques/XRayCrystallography/index.asp

Jamie Humphrey
Editor, *Dalton Transactions* and *CrystEngComm*