Writing Papers for Section C of Acta Crystallographica

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With the mandatory use of checkCIF (derived from PLATON check.def [1]) it is now rare for technically incorrect CIFs to be submitted to Section C of Acta Crystallographica. Why then were almost half of the submissions to the journal in 2004 not accepted? Principally, either the Comment section of the paper did not provide the required significant added value to the numerical data freely available in the CIF, or the Comment section was poorly crafted and difficult to understand. It is a requirement that the paper be written in clear and grammatically correct prose. The discussion of the presented crystal structures should go well beyond merely quoting some of the geometrical parameters of the molecules being studied, which any interested reader can readily obtain by downloading the deposited CIF. The discussion should include: concise details of why the presented crystal structures were determined, why the structures and the compounds themselves are novel and/or interesting, the chemical, natural or biological background and significance of the compounds, interesting features of the structures that are not directly derivable from the CIF data, how a knowledge of the structures helps the understanding of the chemical or physical properties of the compounds, and a comparison with the structures of related compounds. Comparisons should be more than superficial comments and should detail similarities and differences based on numerical analyses of the literature data. Over-analysis of the structures and throw-away statements of low, or no, scientific value should be avoided.

[1] Spek A.L., J. Appl. Crystallogr., 2003, 36, 7.

Keywords: journal publication, publishing, technical writing