Writing Papers for Section C of Acta Crystallographica

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With the mandatory use of checkCIF, it is now rare for technically flawed CIFs to be submitted to *Section C* of *Acta Cryst*. However, the Comment section of the paper frequently lacks novel content, impact and quality. The following suggestions may help prospective authors prepare high-quality submissions.

The discussion of the presented crystal structure(s) must make a useful contribution to our knowledge of structural science and provide significant added value beyond the numerical data freely available in the CIF, which any interested reader can easily download. Crystal structure reports should be well crafted and have an informative discussion; it is not appropriate merely to quote some of the geometric parameters. In the case of structures that do not warrant significant discussion or have a more routine nature, it is better to submit the work to *Section E* of *Acta Cryst*.

The paper must be written in clear and grammatically correct prose. The journal editors are not available to rewrite or extensively correct text. Authors not fluent in English understandably have difficulty writing clear sentences and should seek local or professional assistance. Another option is to publish a briefer discussion in *Acta E*.

Present closely related structures in one paper for greater impact, rather than publishing them individually.

When using checkCIF, attempt to resolve ALL alerts, not just the "A" alerts. Addressing as many "B" and "C" alerts as possible will help speed your paper through the review process. Take care with methyl H atoms. With SHELXL, it is usually better to use HFIX 137 followed by difference map checks. Use of HFIX 33 often gives rise to incorrectly positioned H atoms, which, in turn, can generate "B" and "C" alerts.

The **Title** should be short:

- Use just the name of the compound or of a generic class of compound for multiple structures.
- Use a key feature of the structures if it is worth highlighting, e.g. "Hydrogen Bonded Sheets in..."
- Do not use "Structure of..." - Redundant information!

The **Abstract** should include:

- The full chemical names of the reported compounds, if not in the title.
- Any crystallographic symmetry in the moieties.
- A brief summary of all the salient points made in the Comment section.
- Do not include any crystal data, such as cell dimensions, *Z*, space group, or *R*-factors.
- Never start with "The structure of X has been determined". In a crystallographic journal, we know this implicitly!

Experimental details should include:

- Brief details of the preparation or isolation of the compound(s), or references thereto.
- Melting points, optical rotation (if enantiopure), solvents and method used for growing crystals.
- All non-routine refinement procedures, e.g. disorder treatment, twinning, H-atom treatment**.** Exclude standard procedures and software details.

Tables should include:

- Only interesting or unusual geometric parameters that are actually discussed. If there are none, omit the table.
- Details of classic hydrogen bonds. List C-H···X type interactions only if discussed.
- Non-standard tables may aid the comparison of several structures or the reporting of specific non-CIF parameters, e.g. puckering parameters.

The **Comment** section should be concise, yet informative:

- State why the presented crystal structures were determined and how a knowledge of the structures helps the understanding of the chemical or physical properties of the compounds. Avoid leaving hanging questions. If you start with: "In order to understand the reactivity of X, we investigated its crystal structure", you should return to this point later on and indicate how the new knowledge about the structure has helped you understand the reactivity. If you still don't know, or don't care, the introduction is pointless.
- State why the structures and the compounds themselves are novel and/or interesting, including the chemical, natural or biological background and significance of the compounds.
- Discuss only interesting, novel or unusual features and properties of the structures. Include worthwhile information that is not directly derivable from the CIF data. For example, one should comment on any crystallographic symmetry in the moieties, disorder or twinning. Then cover unusual geometry, coordination, conformations, or configurations, as well as intra- and intermolecular interactions, ring puckering, hydrogen bonding, packing arrangements, etc.
- Comment on conclusions that may be drawn concerning electronic properties, hybridization, etc.
- Compare the reported structures with related compounds. Avoid superficial comments and support the conclusions with numerical analyses of data taken from the literature.
- Hydrogen bonding details should include the type of networks formed and a graph set motif, if possible, not just a statement that the interactions exist. Include C-H···X type interactions only when their significance and influence are well understood.

Avoid:

- Redundant statements and throw-away statements of low, or no, relevance or scientific value.
- Making broad assertions without giving specific details and using literature data, where necessary, to support them.
- Duplicating parameters in the text that are in tables.
- Over-analysis of the structures. Do not describe a feature simply because PLATON lists it as a potential one, unless the feature is considered to be interesting, important, or unusual – and you understand it.
- Stating "this is a hot topic" and citing only your own work or one reference. If no-one else is doing it, it is not hot!

Examples of improvements:

"The molecule has a similar conformation to those of related compounds (ref.)". Expand to indicate specifically what these similar compounds are and highlight specific similarities and differences, e.g. calculate the r.m.s. fit of the atoms.

In an abstract, "The crystal structure of 1-chloro-2-nitrobenzene, $C_6H_4ClNO_2$, is reported" has little and redundant information. It is more compact and informative to write: "Molecules of 1-chloro-2-nitrobenzene, $C_6H_4ClNO_2$, are linked by NO···Cl interactions."

"The structure is stabilised by intermolecular C-H···O hydrogen bonds" tells us little. Give specific details of the type of interactions present and networks formed. The statement is incorrect, because calculations show that such interactions do not stabilise the lattice energy significantly. A better statement is: "Intermolecular C-H···O hydrogen bonds involving X and Y, link the molecules into extended chains which run parallel to the [1 0 0] direction and can be described by a graph set motif of C(12)".