

CRYSTALLOGRAPHIC INSTRUCTIONS FOR AUTHORS

The recommendations of the Commission on Crystallographic Data of the International Union of Crystallography should be followed in reporting analyses (see Acta Cryst., 1967, 22, 445--449). Results should be presented as succinctly as possible. Tables of $\frac{1}{2}F_0$ and F_c should be submitted with the typescript for refereeing purposes. If the data were collected with counter techniques, a complete description of the type of instrument, type of scan, and method of handling background should be given. Drawings of crystal or molecular structures should be made with the non-crystallographer in mind. If the structure was refined anisotropically, the orientations and the magnitudes of vibrational ellipsoids should be displayed. A figure containing the fully labeled asymmetric unit, as a thermal ellipsoid plot, must be submitted (as supplementary material, if it is not otherwise used in the manuscript).

When reporting a crystal structure determination it is often appropriate to indicate this in the title. For papers containing multiple structures they should be referred to in the abstract. It is not necessary to report cell dimensions or other crystal data in the abstract.

Experimental Section

Routine crystal structure determinations should be reported concisely. When non-routine procedures have been employed a brief description of the methods used should be included. Crystal data, refinement details and data collection parameters may be given in textual or tabular form, although the latter may be more appropriate for multiple structure determinations. The following data should be reported in the manuscript:

1. Chemical formula and formula weight (M)
2. Crystal system
3. Unit-cell dimensions (\AA or pm, degrees) and volume, with estimated standard deviations, temperature
4. Space group symbol (if non-standard setting give related standard setting)
5. No. of formula units in unit cell (Z)
6. Linear absorption coefficient (μ)
7. Number of reflections measured and/or number of independent reflections, R_{int}
8. Final R values (and whether quoted for all or observed data)

Discussion Section

A concise description of the molecular and supramolecular structures should be included for each structure determination presented. Figures must be clearly and sensibly labeled. A thermal ellipsoid figure of the asymmetric unit may often be necessary to clearly show the numbering scheme. A figure of the supramolecular assembly is also required and may be submitted in color if necessary for clarification and understanding of the structure. Tables of selected bond lengths and angles (with standard uncertainties) should include significant values only. Averaged values (with standard uncertainties) for chemically equivalent or similar bonds may be included. Any differences from expected values should be noted.

Supplementary Material

A fully completed CIF (Crystallographic Information File) should be deposited with the CCDC (send files as attachments to deposit@ccdc.cam.ac.uk) and the returned deposition number quoted in the experimental section of the manuscript.