Editorial Announcement

Crystal structure studies

Crystallographic work will be assessed mainly for its chemical interest. Thus crystallographic work carried out as part of a wider chemical study should not normally be submitted for publication separately from the results of that study. However, papers reporting only the results of crystal structure determinations may be accepted for publication provided that these results are considered to possess specific chemical significance.

Crystal structure studies submitted as articles

Structure reports should include each of the measured and calculated quantities specified below. Although provided for review purposes, only a limited amount of this material will be included in the published text. *All refined parameters or quantities calculated from these parameters should be accompanied by their estimated standard deviations (e.s.d.s).*

1. Abstract

The abstract should contain the chemical formula, lattice constants with e.s.d.s, crystal system and space group (Hermann–Mauguin symbol), and number of formulas per unit cell (Z).

2. Experimental

The description of the data collection and structural analysis should be as brief as possible for routine structure determinations. A description of these aspects of the work can usually be accomplished in one short table and include the following information: (a) chemical formula, source of material and habit; (b) lattice constants, wavelength assumed in their calculation, temperature at which they were measured; radiation used in intensity measurement; type of filter or monochromator; (c) space group (method of distinguishing between groups with the same absences); (d) crystal dimensions, μ, range of absorption (or transmission) factors; method of correcting for absorption; (e) type of diffractometer, diffraction geometry, conditions for collecting reflections (i.e. 2θ range and sign(s) for *hkl* data collected); (f) number of reflections measured, number of independent reflections when multiple forms of the data have been collected; (g) final R factors (weighted and unweighted). A brief outline of the method used for the structure solution should be given. Computer programs and source of atomic scattering factors and anomalous dispersion ($\Delta f'$ and $\Delta f''$) should be appropriately referenced. Tests for the chirality of a non-centrosymmetric crystal (assuming that anomalous scattering is included) and corrections for extinction should be included when appropriate. Designation of atoms refined with anisotropic thermal parameters, treatment of hydrogen atoms, and geometrical constraints should be described.

3. Structural results

A clear distinction should be made between material to appear in print and material for the referees which will be deposited as 'Supplementary material'.

3.1. For publication in the Journal: in addition to the discussion of the structure the following should be provided: (a) a table of final *fractional atomic coordinates* (labelled x, y, z); (b) a table of selected *bond lengths and angles*, with e.s.d.s; (c) drawings of crystal or molecular structures, made with the non-crystallographer in mind. If the structure was refined anisotropically, the orientations and magnitudes of vibrational ellipsoids should be displayed.

3.2. For the referees and/or for deposition: (a) all calculated atomic coordinates; (b) all anisotropic thermal parameters, as either U_{ij} or B_{ij} values; (c) a complete list of bond lengths and angles; (d) least-squares planes and atomic deviations therefrom; (e) important intermolecular contacts; (f) unit cell and packing diagrams; (g) structure factor tables listing h, k, l, F_o, V_c, $\sigma|F_o|$.

Crystal structure studies submitted as letters and short communications

All of the material required for a full paper, including the structure factor table, should be submitted for examination by the reviewers and the editor. The manuscript itself should provide the following: chemical formula; lattice constants and standard deviations, crystal system, space group (Hermann–Mauguin symbol), and number of formulas per unit cell (Z); intensity measurement method used and temperature; refinement method and final R factor on F (if on F^2, state explicitly); description of the overall structure, including bond lengths and angles of major interest, in tabular form or on the figure. An ORTEP or equivalent projection of the molecular structure with thermal ellipsoids should be provided. All other information accompanying the structure determination should be submitted in a form suitable for deposition as 'Supplementary material'.

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Editor-in-Chief