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Inorganic chemists, biochemists.

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In general, authors should not include a detailed text description of data collection, crystal structure solution and refinement, especially if these followed standard procedures and no difficulties were met. Reference to a previous paper containing a more detailed experimental description can be given if relevant. However, if any parts of the structure analysis were unusual, and affected the presentation and/or accuracy of the results, then these should be discussed. The following crystallographic data should be given, all contained in a paragraph (if one structure reported), or table (two or more structures).

(i) Colour, habit and size of crystals used, and behaviour of the compound under ambient conditions if not mentioned elsewhere in the paper.
(ii) Chemical Formula. This should correspond to the complete chemical unit encompassing crystallographic symmetry (e.g., a centrosymmetric dimer should be included in full form). The use of fractional coefficients (e.g. 0.5H2O), should be used, only, if the unit has partial occupancy of its site. Formulae should be presented in a way that molecules, ionic fragments, solvate molecules etc. are separately identified.

(iii) Unit cell parameters with esds and X-ray wavelength used.

(iv) Crystal system, space group and number of complete chemical units (see ii) per cell.

(v) Type of diffractometer used and method of data collection. Total number of data collected, excluding any intensity controls, number unique Rint value, number observed (with cut-off parameter), and completeness of data to suitable 2 or sin/limit, use or otherwise of absorption correction.

(vi) Final results. Give values of R, Rw (and their definitions) and number of parameters. Indicate form of refinement (F or F2) and treatment of hydrogens.

Note. Easily derived parameters should not be given unless required in discussion of other data (e.g. number of solvent molecules, etc).

Discussion of the Structure. This must include a clear, labelled diagram of the structure (molecule, complex ion or unit cell contents if the structure is polymeric), and a list of relevant geometry parameters - interatomic distances, interbond angles, torsion angles etc. Data for geometrically less important parts of the structure, such as ligand sub groups (phenyl rings, alkyl groups etc.), should not be given. Packing diagrams of crystal structures of "molecular" compounds should not be given unless there are chemically important intermolecular interactions.

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