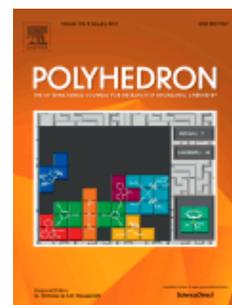




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Crystallographic data

Validation of Deposition of Crystallographic Data Information and Instructions to Authors of Papers Containing or Comprising Crystal Structure Determinations

1. Policy

The Journal will accept for publication, papers containing, or comprising the results of crystal structure determinations which will be of interest to inorganic chemists. Papers reporting only crystallographic results must relate to work of novelty or special significance to inorganic and organometallic chemistry which must be emphasised.

2. Submission of Papers

The following procedures should be followed:

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Data for **inorganic** compounds should be sent to: Fachinformationszentrum Karlsruhe (FIZ), by e-mail (address: crysdta@FIZ-Karlsruhe.de), by FTP (please contact FIZ if you choose this option), or on disk. No hard copy submissions will be accepted.

Within a day or two of submission the Data Centres will provide deposition codes for each data set. This should be noted in the Supplementary Material section at the end of the text file before the reference list in the manuscript submitted to the journal. The deposited data will be accessed by the journal and checked as part of the refereeing process.

b) When the paper is submitted to the Journal, the following guidelines should be adhered to: The **Title** should contain reference to the presence in the paper of X-ray crystallographic results. The **Abstract** should **not** contain crystal data, but should include a concise statement of the main features of the structural results.

The **Experimental** results must be presented in a concise format.

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. $0.5\text{H}_2\text{O}$), 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 R_{int} value, number observed (with cut-off parameter), and completeness of data to suitable 2θ or \sin/λ limit, use or otherwise of absorption correction.

(vi) Final results. Give values of R , R_w (and their definitions) and number of parameters. Indicate form of refinement (F or F_2) 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).

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