

Editorial note

DEPOSITION OF CRYSTAL STRUCTURE DATA

Authors of PRELIMINARY COMMUNICATIONS published in this Journal which contain details of crystal structures are expected to send a table of atomic coordinates and a full list of bond lengths and angles to the Cambridge Crystallographic Data Centre (CCDC). Notes for the guidance of authors issued by the CCDC are reproduced below.

Authors may if they wish send the material for deposition to the appropriate Regional Editor when submitting their Preliminary Communications for consideration. The material will then be sent on to the CCDC at the appropriate time.

Data deposition with the Cambridge Crystallographic Data Centre Notes for Authors

Data Deposition by Journal Editors

1. The CCDC accepts deposited data for all published crystal structures containing organic carbon except for proteins and other macromolecules.
2. The data must be submitted to the Journal Editor with the manuscript of the publication.
3. The following data are accepted for deposition :
Crystal Data : Unit cell, space group, Z, density, R factor.
Atomic coordinates.
Bond lengths and bond angles. [These are used for checking atomic positions and are not stored explicitly.]
Standard deviations should be given for all numeric data.
4. The following are not accepted for deposition :
Thermal parameters.
Structure factors.
Derived parameters eg. torsion angles, non-bonded distances.
5. In the table of coordinates disordered atoms and atoms refined as part of a rigid body should be clearly labelled, with details given in footnotes.
6. If the printed publication does not carry a chemical structural diagram indicating the atomic labelling scheme which has been used, then such a diagram should be included with the deposited data.
7. Data presented for deposition should be in the form of legible, concise, non-redundant tables. The interpretation of the tables should be immediately obvious.
8. The paper should carry the following note referring to deposited data.

"Atomic coordinates for this structure have been deposited with the Cambridge Crystallographic Data Centre and can be obtained on request from Dr. Olga Kennard, University Chemical Laboratory, Lensfield Road, Cambridge CB2 1EW, UK".