Guidelines for Publication of X-Ray Crystallography

Presentation of Crystallography in the Manuscript

For an article reporting a crystallographic structure determination it is often appropriate, although not essential to indicate this information in the title, *e.g.* by the words 'crystal structure of'. Whether or not the crystal structure determination is indicated in the title, reference should be made to it in the summary. The summary need not contain cell dimensions and other crystal data. Details of the data collection and structure analysis should be given in a footnote. Selected bond lengths and angles, with estimated standard deviations, should be included in the figure caption and be restricted to significant dimensions only. The following information should be given in the manuscript:

1. Chemical formula and formula weight (*M*)
2. Crystal system
3. Unit-cell dimensions (A 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)

Supplementary Data Required for Assessment and/or Deposition

Authors should submit all supplementary crystallographic data as a Crystallographic Information File (CIF) file (and the corresponding CCDC number, if available) *via* electronic mail. The submissions must be made to the journal e-mail account: **mc@ioc.ac.ru**.

Authors should combine multiple data sets for a given manuscript into a single file. This will minimise the chance that files will be misplaced or associated with the wrong manuscript. The individual structures in the combined file must be separated from each other by the sequence #===END at the beginning of a line.

Authors must identify which manuscript the electronic file is associated with when they send the file to the Editorial Office by entering the name of the manuscript at the top of the electronic file.

The information required for deposition includes:

- A table of final fractional atomic coordinates
- Any calculated coordinates (*e.g.* hydrogen)
- A full list of bond lengths and angles with estimated standard deviations.
- A full list of displacement parameters in the form B_{ij} or U_{ij} (in A^2 or pm^2)
- FULL details of the refinement, which should include the following data:
    1. Chemical formula and formula weight (*M*).
    2. Crystal system.
    3. Unit-cell dimensions (A 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, number of independent reflections, R_{int}, theta and index (*hkl*) range.
8. Final *R* value(s) and whether for all or observed data.
9. Method of determination of unit cell dimensions.
10. Type of filter or monochromator used.
11. Type and wavelength of radiation used.
12. Calculated density (D_c).
13. Method of structure solution (direct methods, heavy-atom method) and development (Fourier difference techniques).
14. Method of refinement, whether refinement carried out on *F* or F^2, treatment of hydrogen atoms.
15. Details of weighting scheme used.
16. No. parameters refined and any constraints or restraints applied.
17. Definition of *R* and *wR*, final value of *wR*, with a statement of whether unobserved data were included.
18. Goodness-of-fit (*S*) value, maximum/minimum residual electron densities, average and maximum shift/error.
19. Value of *F*(000).
20. Colour, shape and size of crystal used for data collection.
21. Range of absorption (or transmission) factors, method of correcting for absorption.
22. Type of diffractometer used, diffraction geometry, conditions for collecting data.
23. Programs or packages and computers used (with references).
24. Flack or Rogers parameter (if appropriate)

The CIF format has data names that correspond to these items.
For more information on the items that should be included in CIF submissions please visit **http://www.rsc.org/is/journals/authrefs/cif.htm**.
Tables of structure factors (F_o, F_c) should not be sent, but copies should be retained by the authors so that they may be made available *via* the Editorial Office if requested.
The Editorial Office will forward the deposited data to the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ once the paper has been accepted. Enquiries for data can be directed to **deposit@ccdc.cam.ac.uk** or Fax: +44 (0)1223 336033. Please include the CCDC numbers with your enquiries.