CHECK LIST FOR AUTHORS AND REVIEWERS OF STRUCTURE REPORTS

Author:
Title:

ABSTRACT

The following crystallographic information should be included in the text of the abstract. Do not add additional crystallographic information. When the manuscript contains multiple structures and has a more general focus than the structures reported, the crystallographic information may be omitted from the abstract.

____ Chemical Formula
____ Lattice Constants with esd's
____ Crystal System
____ Space Group
____ Number of Molecules per Cell, Z

EXPERIMENTAL

Please minimize what you report in the Experimental Section of an Article or Note. A full presentation of the information below must be deposited as part of the Crystallographic Information Format (CIF) file. An *abbreviated* Table (see below) must be included in the text for an Article or Note or appear as running text in a footnote for a Communication. The abbreviated Table or footnote will appear in the printed version of your manuscript.

____ Source of material studied
____ Color of the crystals studied
____ Habit of the crystals
____ Lattice Constants
____ Wavelength of X-ray used
____ Temperature at which data were collected
____ Was a beam monochromator used?
____ Was space group determination unambiguous?
____ Were crystal dimensions measured?
____ Was absorption coefficient, μ, calculated?
____ Was range of transmission factors calculated?
____ Was program used for absorption correction stated?
____ Was type of diffractometer stated?
____ Was diffraction geometry specified?
____ Was 2 θ range for data collection stated?
____ Were octants $\pm h, \pm k, \pm l$ collected stated?
____ Was total number of reflections collected stated?
____ Was number of independent reflections used in refinement stated?
____ Was an estimate of agreement between equivalent reflections made?

STRUCTURE DETERMINATION AND REFINEMENT

____ Was an outline of method of structure solution given?
____ Were computer programs used stated?
____ Was the source for scattering factors, f_o, f', and f'' referenced?
____ Were final *R*-factor and weighted *R*-factor stated?
____ Were tests for chirality, polarity, etc. made if crystal was non-centrosymmetric?
____ Were corrections for presence of extinction made?

STRUCTURAL RESULTS

Information to be included in the abbreviated Table or as a footnote in a Communication is shown below:

Table I. Crystallographic Data for .... (This table will be published. Please do not add additional information.)

chemical formula	formula weight ....
a = ... (esd) Å	space group ... (No.)
b = ... (esd) Å	T = ...°C
c = ... (esd) Å	λ = ...Å
α, β, γ (esd's) (if appropriate)	D_{obsd} = ... g cm^{-3}. D_{calcd} = g cm^{-3}
	μ = ... cm^{-1}
V = ... Å^3	$R(F_o$ or $F_o^2) $ = ...
Z = ...	$R_w(F_o$ or $F_o^2) $ = ...

____ Definition of *R* factors should be provided in a footnote to Table I.

The printed version of the paper should also contain:

____ Table of *selected* bond lengths and angles with esd's. In a Communication, this information may be in a footnote or figure caption.

SUPPORTING INFORMATION

Items below are for deposit in the CIF file as Supporting Information. Other information enumerated under Experimental (see above) must also be included in the CIF file.

____ Final atomic coordinates with esd's (with definition of B_{eq} or U_{eq} provided in a footnote) for all non-hydrogen atoms. We no longer publish this table when a CIF has been deposited unless it is essential for the clarity of the publication.
____ Complete bond distances and angles including "non-essential" bond lengths and angles such as in peripheral phenyl rings.

____ Calculated coordinates of all atoms introduced at fixed positions
____ Anisotropic thermal parameters as U_{ij}'s or B_{ij}'s
____ Least Squares planes and deviations therefrom

____ Is a Supporting Information paragraph included in the manuscript?

____ Legible tables of h, k, l, F_o, F_c. Note that these tables are not required for submission and are *not* deposited in the Supporting Information or CIF file. However, structure factor tables should be available and may be requested for review purposes.

FIGURES

____ One figure; should show the labeling of atoms and the thermal vibrational (%) ellipsoids.
____ Stereoviews; should be deposited unless they contribute to the discussion. Only one full cell or packing diagram at the correct magnification (55-60 mm or 2 1/2 inches between image centers) should be included.