

BRIEF COMMUNICATIONS

The Space Group of AgTaS_3

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The crystal structure of AgTaS_3 , recently described in space group $Cmc2_1$, is properly described in $Cmcm$. The revised space group evidences the centrosymmetric nature of the structure. © 1993 Academic Press, Inc.

The crystal structure and some electrical properties of the ternary compound AgTaS_3 have recently been reported (1). The structure was described and refined, from powder diffraction data, in the noncentrosymmetric, polar space group $Cmc2_1$ (orthorhombic; $a = 3.3755(2) \text{ \AA}$, $b = 14.0608(11) \text{ \AA}$, $c = 7.7486(7) \text{ \AA}$, $Z = 4$). There seems to be no reason why it should not be described in the centrosymmetric space group $Cmcm$. The $Cmcm$ coordinates are given in Table I; they are obtained from those in Table II, Ref. (1), by incrementing the z 's by 0.25 and, for the S(2)–S(3) pair, averaging. No atom needs to be shifted by more than 3 esd's to conform to the higher symmetry.

The revised description evidences the centrosymmetry of the atom arrangement;

TABLE I
COORDINATES,^a SPACE GROUP $Cmcm$

Atom	Site	x	y	z
Ag	4(a)	0.0	0.0	0.5
Ta	4(c)	0.0	0.2621(3)	0.25
S(1)	4(c)	0.0	0.893(1)	0.25
S(2)	8(f)	0.0	0.672(6)	0.425(11)

^a Esd's are from Table II, Ref. (1).

indeed, the Ag atom lies on a crystallographic symmetry center. No other revision of the structure description is needed.

References

1. H. WADA, M. ONODA AND H. NOZAKI, *J. Solid State Chem.* **97**, 29–35 (1992).