CORRIGENDUM

Synthesis and Structure of Pr₃InSe₆: Corrigendum

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Received May 12, 1989

The monoclinic cell assigned previously to Pr_3InSe_6 (L. E. Aleandri and J. A. Ibers, J. Solid State Chem. **79**, 107 (1989)) is incorrect. The structure refines satisfactorily ($R(F^2) = 0.117$ and 1216 observations and 30 variables) in space group D_{2h}^{12} -Pnnm of the orthorhombic system in a cell of dimensions a = 17.413(2), b = 14.275(1), c = 4.109(1) Å. The structural details remain unchanged. © 1989 Academic Press, Inc.

We recently reported the structure of the new compound Pr_3InSe_6 in space group $P2_1/c$ of the monoclinic system (1). Long overdue perusal of the positional parameters (Table II of Ref. (1)) and a cell reduction suggest that the true cell is orthorhombic. This is confirmed by the satisfactory agreement (R = 0.069) obtained when the

TABLE I

Positional Parameters and Equivalent Isotropic Thermal Parameters for Pt_3InSe_6 in Space Group *Pnnm* of the Orthorhombic System

Atom	x	у	Z.	В
PR(1)	0.222068(60)	0.458373(63)	1/2	0.06(2)
PR(2)	0.394242(67)	0.247580(63)	$\frac{1}{2}$	0.13(2)
PR(3)	0.145322(63)	0.186783(60)	0	0.10(2)
1N(1)	0	0	$\frac{1}{2}$	0.18(3)
IN(2)	$\frac{1}{2}$	0	$\frac{1}{2}$	0.79(4)
SE(1)	0.41594(13)	0.09370(12)	0	0.19(3)
SE(2)	0.28538(13)	0.31820(12)	0	0.19(4)
SE(3)	0.24849(11)	0.11047(13)	12	0.21(4)
SE(4)	0.11228(13)	0.38673(13)	0	0.31(3)
SE(5)	0.01886(13)	0.18967(12)	$\frac{1}{2}$	0.17(3)
SE(6)	0.39716(12)	0.47730(12)	$\frac{1}{2}$	0.18(3)

indices are transformed and the absorptioncorrected F^2 values are averaged for *mmm* symmetry. A final refinement in space group *Pnnm* leads to a value of $R(F^2)$ of 0.117 for the 1216 unique, averaged reflections. The final parameters are given in Table I. The notation has been changed to correspond to the numbering scheme of Sm₃InS₆ (2), with which Pr₃InSe₆ is clearly isostructural. No metrical parameters change significantly as a result of this new refinement in the proper space group.

Acknowledgment

We are indebted to Dr. Richard E. Marsh for suggesting that we had erred in the cell assignment.

References

- 1. L. E. ALEANDRI AND J. A. IBERS, J. Solid State Chem. 79, 107 (1989).
- 2. D. MESSAIN, D. CARRÉ, AND P. A. LARUELLE, Acta Crystallogr. Sect. B 33, 2540 (1977).

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