

BRIEF COMMUNICATION

The Crystal Structure of $\text{Cr}_2\text{Si}_2\text{Te}_6$: Corrigendum

RICHARD E. MARSH

Arthur Amos Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California 91125*

Received June 27, 1988

The structure of $\text{Cr}_2\text{Si}_2\text{Te}_6$, originally described in the noncentrosymmetric space group $R3$, is properly described in the centrosymmetric $R\bar{3}$. The structure of the related compound $\text{Fe}_2\text{P}_2\text{Se}_6$, which has also been described in $R3$, should probably be reinvestigated. © 1988 Academic Press, Inc.

The structure of $\text{Cr}_2\text{Si}_2\text{Te}_6$ has recently (*I*) been described in space group $R3$ (rhombohedral; hexagonal cell dimensions, $a = 6.7578(6)$, $c = 20.665(3)$ Å, $Z = 3$) and refined to an R of 0.033 for 456 reflections. It is properly described in the centrosymmetric space group $R\bar{3}$.

Starting coordinates in $R\bar{3}$ were obtained from the $R3$ coordinates (*I*) by decrementing the z 's by 0.64 and averaging over pairs of chemically equivalent atoms. Least-squares refinement was based on the 460 F values obtained from the supplementary material.¹ Convergence was quickly reached at the same R , 0.033, as reported earlier (*I*) but with 17 parameters rather

than 31. The final $R\bar{3}$ parameters are given in Table I.

The interatomic distances and angles are little changed. The two independent distances within the CrTe_6 octahedron are now statistically equal, at 2.775(4) and 2.779(4) Å; in the $R3$ description there were four independent distances, ranging from 2.751(14) to 2.803(12) Å. The Si-Te and Si-Si distances are effectively unchanged, at 2.505(6) and 2.268(9) Å. A more noticeable change is in the "temperature" coefficients $U(ij)$ for the Te atoms, which were highly anisotropic in the $R3$ description: the ratios of mean-square displacements along the major and minor axes were nearly 4:1 for Te(1) and nearly 10:1 for Te(2). On the other hand, the displacements are approximately isotropic for the $R\bar{3}$ description; indeed, refinement with all atoms isotropic led to nearly as low an $R(0.0335)$ as did the final anisotropic refinement (0.0328). The unrealistic anisotropies resulting from the $R3$ refinement undoubtedly were due to the near-singularities associated with refining

* Contribution No. 7807 from the Arthur Amos Noyes Laboratory of Chemical Physics.

¹ See NAPS Document No. 04514 for 3 pages of supplementary materials from ASIS/NAPS, Microfiche Publications, P.O. Box 3513, Grand Central Station, New York, NY 10163. Remit in advance \$4.00 for microfiche copy or for photocopy, \$7.75 up to 20 pages plus \$.30 for each additional page. All orders must be prepaid.

TABLE I
FINAL COORDINATES ($\times 10^5$) AND U_{ij} 's^a ($\times 10^4$), SPACE GROUP $R\bar{3}$

Atom	Position	x	y	z		
Te	18(f)	66902(15)	-2541(13)	24939(4)		
Cr	6(c)	0	0	33394(20)		
Si	6(c)	0	0	5488(31)		
Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te	126(4)	126(4)	111(4)	65(3)	0(3)	-5(3)
Cr	124(9)	U_{11}	108(14)	$\frac{1}{2}U_{11}$	0	0
Si	153(16)	U_{11}	111(27)	$\frac{1}{2}U_{11}$	0	0

Note. Scale factor (relative to supplemental F table), 3.014(6). Secondary extinction parameter, $1.55(12) \times 10^{-7}$. Estimated standard deviations are in parentheses.

^a The form of the "temperature" expression is $\exp(-2\pi^2)(U_{11}h^2a^{*2} \dots + 2U_{23}klb^*c^*)$.

an effectively centrosymmetric structure in a noncentrosymmetric space group (2, 3).

The earlier authors (1) chose the noncentrosymmetric $R\bar{3}$ on the presumption that the compound is isostructural with $\text{Fe}_2\text{P}_2\text{Se}_6$. In the description of the structure of this latter compound (4), coordinates are reported for refinements in both $R\bar{3}$ and $R3$; the $R3$ structure was preferred because it gave an $R(0.038)$ "smaller than the centric" space group. It was also noted that the $R3$ structure was preferred by the Hamilton test (5), but no details of the comparison are given. The differences between the $R3$ and the $R\bar{3}$ coordinates were very small, never more than 0.12 Å. In view of the great difficulties involved in attempting to find a correct and unambiguous noncentro-

symmetric description of a nearly centrosymmetric structure (6), a reinvestigation of the structure of $\text{Fe}_2\text{P}_2\text{Se}_6$ seems desirable.

References

1. G. OUVRARD, E. SANDRE, AND R. BREC, *J. Solid State Chem.* **73**, 27 (1988).
2. O. ERMER AND J. DUNITZ, *Acta Crystallogr. Sect. A* **26**, 163 (1970).
3. V. SCHOMAKER AND R. E. MARSH, *Acta Crystallogr. Sect. B* **35**, 1933 (1979).
4. W. KLINGEN, G. EULENBERGER, AND H. HAHN, *Z. Anorg. Allg. Chem.* **401**, 97 (1973).
5. W. C. HAMILTON, "Statistics in Physical Science," pp. 157, 216, Ronald Press Co., New York (1964).
6. R. E. MARSH, *Acta Crystallogr. Sect. B* **42**, 193 (1986).