JOURNAL OF SOLID STATE CHEMISTRY 92, 594–595 (1991)

On the Space Groups of Tl_5Te_3 and Tl_2Te_3

RICHARD E. MARSH

The Beckmann Institute and The Division of Chemistry and Chemical Engineering, California Institute of Technology, Pasadena, California 91125*

Received October 1, 1990

Recently, Abba Toure *et al.* (*1*) reinvestigated the binary system Tl–Te by thermal analysis and X-ray diffraction, carrying out single-crystal studies of TlTe and of Tl_5Te_3 and a powder diffraction study of Tl_2Te_3. For TlTe they confirmed the structure, in space group *I*4/*mcm*, reported by earlier workers (*2, 3*); however, for Tl_5Te_3 they reported a space group, *I*4/*m*, different from either the $I\bar{4}$ (*4*) or the *I*4/*mcm* (*5*) that had been previously proposed. In fact, the structure derived by Abba Toure *et al.* (*1*) is properly described in *I*4/*mcm*, and is effectively the same as that reported in Ref. (*5*). The coordinates reported by Abba Toure *et al.* (*1*), symmetrized and averaged so as to conform to *I*4/*mcm*, are given in Table I; no coordinate (and no anisotropic coefficient U_{ij}) needed to be adjusted by more than one e.s.d. in order to satisfy the symmetry requirements of *I*4/*mcm*. Abba Toure *et al.* (*1*) reported the systematic absence only of reflections of the type $(h + k + l) = 2n + 1$, corresponding to the body-centered lattice; they do not mention the additional absences of the type $0kl, k(l) = 2n + 1$, which are required by the *c*-glide plane of space group *I*4/*mcm*. Bhan and Schubert (*5*) noted that these latter reflections are indeed absent.

TABLE I

Tl_5Te_3: COORDINATES, SPACE GROUP *P*4/*mcm*, WITH e.s.d's (IN PARENTHESES) AS ESTIMATED FROM THE VALUES IN TABLE VIII OF REF. (*1*); CELL DIMENSIONS: a = 8.917(3) Å, c = 12.613(3) Å

Atom	Site	x	y	z
Tl(1)	16(*l*)	0.3526(3)	0.1474	0.1590
Tl(2,3)	4(*c*)	0.0	0.0	0.0
Te(1)	4(*a*)	0.0	0.0	0.25
Te(2)	8(*h*)	0.3407(6)	0.1593	0.5

Since the coordinates are essentially unchanged, the interatomic distances reported by Abba Toure *et al.* (*1*) are also essentially unchanged. As noted earlier (*5*), the structure is isotypic with that of Cr_3B_5 (*6*).

In the case of Tl_2Te_3, Abba Toure *et al.* (*1*) reported the space group as *Cc*, with cell dimensions a = 13.31, b = 6.55, c = 7.91 Å, β = 107.42°. However, the powder

*Contribution No. 8089.

0022-4596/91 $3.00

diagram described in their Table II indicates systematic absences corresponding to a body-centered rather than to a *C*-centered lattice. For the space group to be the conventional *Cc*, the most convenient choice of axes is that reported by Bhan and Schubert (*5*): $a = 17.413$, $b = 6.552$, $c = 7.910$ Å, $\beta = 133.16°$.

References

1. A. Abba Toure, G. Kra, R. Eholie, J. Olivier-Fourcade, and J.-C. Jumas, *J. Solid State Chem.* **87,** 229 (1990).
2. K. Burkhardt and K. Schubert, *J. Less-Common Metals* **18,** 426 (1969).
3. J. Weis, H. Schäfer, B. Eisenmann, and G. Schön, *Z. Naturforsch. B (Anorg. Chem., Org. Chem.)* **29,** 585 (1974).
4. L. I. Man, R. M. Imamov, and Z. G. Pinsker, *Sov. Phys. Crystallogr. Engl. Transl.* **16,** 94 (1971).
5. S. Bhan and K. Schubert, *J. Less-Common Metals* **20,** 229 (1970).
6. F. Bertaut and P. Blum, *Compt. Rend.* **236,** 1055 (1953).