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Americium Ditelluride

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Abstract. $AmTe_{1.73(2)}$, tetragonal, $P4/nmm$, $a = 4.358$ (1), $c = 9.027$ (3) Å at 296 K, $Z = 2$, $D_c = 8.99$ Mg m^{-3}. Crystals were synthesized from elemental Te and ^{243}Am. The structure is of the anti-Fe_2As type and isomorphous with $NdTe_{1.8}$. Layers of Te atoms are interleaved with puckered double layers of composition AmTe. The amount of substoichiometry from $AmTe_2$ was determined, and it was found to result from random vacancies in the pure Te layers. Interatomic distances suggest that the nature of the Am–Te bonds is intermediate between ionic and covalent.

Introduction. Americium ditelluride was first prepared by Damien (1972) using the shorter-lived isotope ^{241}Am; he examined the compound by powder X-ray diffraction and found it to be isostructural with the lanthanide ditellurides (anti-Fe_2As type). Further, it was deduced that the compound exhibits a range of stoichiometry, $AmTe_{2-x}$, although the value of x was not determined. Similar ranges of composition have been found for $NdTe_{2-x}$ (Wang, Steinfink & Bradley, 1966), $NpTe_{2-x}$ (Damien, 1974), $PuTe_{2-x}$ (Allbutt, Dell & Junkison, 1970) and $CmTe_{2-x}$ (Damien, Wojakowski & Müller, 1976). A complete structural analysis was made for $NdTe_{1.8}$, but none of the transuranic tellurides were so analyzed; hence the determination of the structure of $AmTe_{2-x}$ by X-ray diffraction was undertaken.

Crystals were made by reacting ^{243}Am metal in an excess of Te, both sealed in a quartz tube under vacuum. The entire tube was heated at 823 K for 20 h; the excess Te was distilled away by heating one part of the tube at 733 K while the other part was kept cold.

For intensity measurements we used a black platelet of $AmTe_{2-x}$ (0·027 × 0·115 × 0·185 mm) sealed in a thin-walled glass tube for containment of the radioactivity. Data were collected by use of an automated Picker four-circle diffractometer and Zr-filtered Mo $K\alpha$ radiation ($\lambda = 0.70926$ Å). Unit-cell dimensions at 296 K were refined by a least-squares procedure from the angles of 12 centered reflections with 2θ near 48°. Intensities of all reflections in one octant of the reciprocal sphere up to $2\theta = 100°$ were measured by 2θ scans. These were corrected for absorption ($\mu = 34.5$ mm^{-1}) and Lp factors; then equivalent reflections were averaged to yield a set of F_o^2 values.

A least-squares refinement of the structure including anisotropic thermal parameters was carried out starting with the parameters of the $NdTe_{1.8}$ structure. Observations used were values of F_o^2, and the weights, $w = 1/\sigma^2(F_o^2)$, were derived from counting statistics. Both f' and f'' (Cromer & Liberman, 1970) were included in the calculated F's. Occupancy factors were varied for the Te(1) and Te(2) sites, and it was clear from the refinement that the vacancies are limited to the Te(1) sites. At convergence, the $R(F)$ was 0·049 based on the 349 values of $F_o^2 > 3\sigma(F_o^2)$.† The refined positional and thermal parameters are listed in Table 1. The occupancy factor for the Te(1) sites is 0·73 (1).

Discussion. The atomic arrangement in $AmTe_{1.73}$ is illustrated in Fig. 1, and interatomic distances and angles are given in Table 2. The structure is of the anti-Fe_2As type and has double, puckered layers of AmTe composition interleaved with planar layers containing only Te. The variable stoichiometry of $AmTe_{2-x}$ is correlated with random vacancies at sites within the pure Te layers. In the crystal studied here 27% of the sites in these layers are vacant, but Damien (1972) showed varying c/a ratios as evidence that the composition of each sample depends on the tem-

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† A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 33932 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Refined positional and thermal* (Å^2) *parameters and their e.s.d.'s*

	x	y	z (×10^4)	U_{11} (×10^4)	U_{33} (×10^4)
Am	¼	¼	7301 (1)	90 (2)	216 (4)
Te(1)	¼	¾	0	603 (20)	80 (11)
Te(2)	¼	¼	3691 (2)	85 (3)	159 (6)

$U_{22} = U_{11}$; $U_{12} = U_{13} = U_{23} = 0$

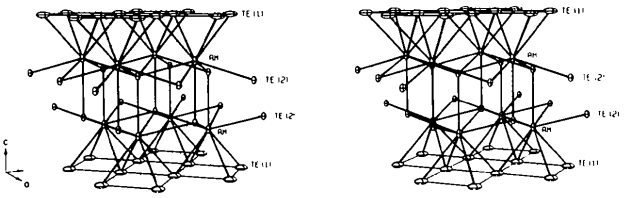

Fig. 1. Stereoscopic drawing of the structure. Atoms are represented by their thermal ellipsoids of 50% probability.

Table 3. *Comparison of distances* (Å) *in three tellurides,* MTe_{2-x}

	$LaTe_{2.0}$	$NdTe_{1.80}$	$AmTe_{1.73}$
M–Te(1)	3·38	3·29	3·27
M–Te(2)	3·29	3·27	3·26
M–Te(3)	3·26	3·22	3·21
Te(1)–Te(1)	3·19	3·10	3·08
Te(1)–Te(2)	4·04	3·99	3·98
Te(2)–Te(2)	4·01	3·91	3·88
c/*a*	2·03	2·07	2·07

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s*

Am–Te(1^{i})	3·269 (1)	Te(2)–Am–Te(2^{i})	73·83 (4)
Am–Te(2)	3·258 (2)	Te(2^{i})–Am–Te(2^{ii})	85·55 (2)
Am–Te(2^{i})	3·208 (1)	Te(2^{ii})–Am–Te(2^{iii})	147·66 (7)
Te(1)–Te(1^{v})	3·081 (1)	Te(2^{i})–Am–Te(1^{ii})	75·81 (3)
Te(1)–Te(2)	3·980 (2)	Te(2^{i})–Am–Te(1^{iii})	131·32 (3)
Te(2)–Te(2^{i})	3·884 (2)	Te(1^{i})–Am–Te(1^{iv})	56·23 (2)
		Te(1^{i})–Am–Te(1^{iii})	83·59 (4)

Symmetry code: (i) $1-x, 1-y, 1-z$; (ii) $1-x, -y, 1-z$; (iii) $-x, 1-y, 1-z$; (iv) $x, y, 1+z$; (v) $-x, 1-y, -z$.

perature of its preparation. From examination of the structure it seems reasonable that changes in stoichiometry limited to Te layers should affect the *c*/*a* ratio in this manner; namely that *a* decreases with increasing Te vacancies while *c* is little affected. In Table 3 can be seen some instances of the effect on *c*/*a* and on bond lengths of changing both the stoichiometry and the radius of the metallic element, *M*, in MTe_{2-x}.

Interatomic distances between Te(1) atoms are considerably less than van der Waals (4·4 Å) or Te^{2-} interionic distances (4·4 Å) and nearer to the Te–Te covalent bond length (2·8 Å); thus, there is probably some covalent bonding within the pure Te layer. The Te(2)–Te(2) distances are much longer than the Te(1)–Te(1) distances, and therefore can have much less, if any, electron interchange. The Am–Te(1) and Am–Te(2) bond lengths are not very different from each other in spite of the different structural role played by Te(1) and Te(2). These bonds are likely to have both ionic and covalent character.

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Structure of Potassium Hexabromostannate(IV) at Room Temperature

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Abstract. K_2SnBr_6 at room temperature, monoclinic, $P2_1/n$, $a = 10{\cdot}621\ (2)$, $b = 7{\cdot}427\ (2)$, $c = 7{\cdot}442\ (2)$ Å, $\beta = 90{\cdot}18\ (2)°$, $D_x = 3{\cdot}825$ Mg m^{-3} for $Z = 2$. The crystal structure is a distorted K_2PtCl_6 structure. The final R was 0·093 for 743 photographic data. The distortion from the ideal structure is described in terms of a rotation of the regular $SnBr_6^{2-}$ octahedron and a shift of the K^+ ion mostly in the *b* direction. The transition point at 399·8 (4) K was confirmed by thermal measurement.

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