Table 4. *Deviations* (Å) *of atoms from the least-squares planes for various parts of the molecule*

C(3)′ through N(9)′ are generated from the asymmetric unit by the molecular mirror symmetry. Atoms marked with an asterisk have been included in the calculation of the plane.

C(1)	−0·033*	0·004
N(2)	0·000*	0·009
C(3)	0·003*	0·000*
C(4)	0·025*	−0·006*
C(5)	0·042*	−0·003*
C(6)	0·052*	−0·021*
C(7)	−0·023*	−0·028*
C(8)	0·006*	0·016*
N(9)	−0·074*	−0·146
C(3)′	−0·110	
C(4)′	−0·211	
C(5)′	−0·317	
C(6)′	−0·308	
C(7)′	−0·269	
C(8)′	−0·114	
N(9)′	−0·549	

Barnes, 1960), although those observed here seem particularly marked. They are most probably due to intermolecular interactions; it may be significant that proflavine, like the hemisulphate, contrasts with most other aminoacridine crystal structures in not being highly stacked.

The crystal structure (Fig. 3) is shown in **c** projection. The molecules are held together by a network of hydrogen bonds between the proflavine N atoms and H_2O molecules, which are situated on crystallographic mirrors. N(2)–O(10) is 2·703 Å, with the H_2O acting as donor. Each H_2O is also hydrogen bonded (3·008 Å) to two symmetry-related N(9) atoms in adjacent molecules. The proflavine bases are notably unstacked in the lattice, with only minimal overlap between a molecule and its *C*-centred mate.

We are grateful to the Cancer Research Campaign and the Lawson Tait Trust for support.

References

JONES, A. & NEIDLE, S. (1975). *Acta Cryst.* **B31**, 1324–1333.

LERMAN, L. S. (1961). *J. Mol. Biol.* **3**, 18–30.

OBENDORF, S. K., CARRELL, H. L. & GLUSKER, J. P. (1974). *Acta Cryst.* **B30**, 1408–1411.

PHILLIPS, D. C. (1956). *Acta Cryst.* **9**, 237–250.

PHILLIPS, D. C., AHMED, F. R. & BARNES, W. H. (1960). *Acta Cryst.* **13**, 365–377.

Acta Cryst. (1976). B**32**, 2539

Indium Polytelluride In_2Te_5

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(*Received* 22 *March* 1976; *accepted* 9 *April* 1976)

Abstract. In_2Te_5, $M=867·64$, monoclinic, *Cc*; $a=4·39$ (1), $b=16·39$ (1), $c=13·52$ (1) Å, $\beta=91·65$ (5)°, $D_m=5·95$, $D_c=5·94$ g cm^{-3}; $U=969·5$ Å^3, $Z=4$, $F(000)=1432$. The structure was solved from Patterson syntheses with Mo $K\alpha$ X-ray data and refined by block-diagonal least squares to $R=8\%$ for 1223 structure factors. The material is composed of two sheets of atoms running perpendicular to **c***. These are constructed of chains of four-membered In–Te rings; each In is tetrahedrally coordinated indicating that it may be thought of as being sp^3 hybridized with an average In–Te bond of 2·832 (6) Å, alternating with, and cross-linked by, groups of three Te atoms which on an ionic description are $(Te_3)^{2-}$ polyanions. The average Te–Te bond in this anion is 2·837 Å with an included angle of 100·1 (2)°.

Introduction. Cell parameters for a phase, In_2Te_5, have been quoted (Schubert, Dorre & Gunzel, 1954; Gerasimov, Abbasov & Nikolskaya, 1962) and the existence of a phase with this formula was postulated as a result of a DTA and X-ray investigation of the In–Te system (Grochowski, Mason, Schmitt & Smith, 1964). Following the phase diagram produced by Grochowski *et al.*, an intimate mixture of In and Te in the correct stoichiometric proportions to produce In_2Te_5 was placed in a sealed evacuated pyrolysed tube and heated to 550 °C. This temperature was maintained for 24 h whilst the tube was shaken to ensure mixing. The sample was then directionally frozen at 2 mm h^{-1} to 400 °C and was held there for 48 h before being allowed to cool slowly. This process was repeated with starting compositions to either side of In_2Te_5. In all cases the resulting boules were inhomogeneous but did contain regions of shiny black lamellar material from which crystals were extracted which proved to be In_2Te_5. The density measured experimentally by toluene immersion was 5·95 g cm^{-3}. 1223 reflexions, of which 57 were recorded as zero were collected from Weissenberg photographs taken about **a** with multiple-film packs and Mo $K\alpha$

radiation. Intensities for 908 reflexions were measured with a Joyce–Loebl flying-spot densitometer. Very weak reflexions were measured visually. Data were corrected for Lorentz and polarization factors and, for visual data, for spot elongation on upper layers. No absorption correction was made since the crystal was fairly regular in cross-section with $\mu R < 0{\cdot}5$. Overall scale and temperature factors were obtained by Wilson's (1942) method. The structure was solved from minimum functions based on generalized Patterson syntheses. Block-diagonal least-squares refinement of positional, scale and anisotropic thermal parameters resulted in a final $R=0{\cdot}08$ where $R=\sum||F_o|-|F_c||/\sum|F_o|$. Scattering factors were from *International Tables for X-ray Crystallography* (1974). Table 1 gives the atomic coordinates and anisotropic thermal parameters; bond lengths and angles within the two sheets of atoms forming the structure are given in Table 2; other relevant interatomic distances including those between sheets are given in Table 3.*

Discussion. Due to their similar scattering powers it is difficult to distinguish the atom types from X-ray data; an analysis of interatomic distances leads to the atom designations and the system of bonding shown in Fig. 1. The material is composed of endless parallel chains of atoms running along **a** based on four-membered In–Te rings In(1), Te(1), In(2) and Te(2). These chains alternate with, and are cross-linked by, tightly bound Te(3)–Te(4)–Te(5) groups to form a continuous sheet of atoms perpendicular to **c***. The structure contains two such sheets; within each sheet there is a pseudo centre of symmetry midway between In(1) and In(2) and a pseudo twofold axis parallel to **a** through Te(4). These symmetry operations hold only within their particular sheet of atoms and do not extend to neighbouring sheets.

The existence of systems of tightly bound Te atoms in the structure was expected in that valence saturation could only be achieved by the formation of a Te polyanion. Since the two In atoms are not mutually bonded but occur in environments that are almost identical and which are typical of trivalent In, then on an ionic formulation the compound can only be $2(In^{3+})(Te_3^{2-})2(Te^{2-})$. This necessitates a triatomic anion which was identified as Te(3)–Te(4)–Te(5). In isolation

Table 1. *Fractional coordinates* ($\times 10^4$) *and thermal parameters* ($\times 10^3$ Å^2) *with e.s.d.'s in parentheses*

Thermal parameters are defined as $\exp[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{23}klb^*c^*+2U_{13}hla^*c^*)]$.

	X/a	Y/b	Z/c	U_{11}	U_{22}	U_{33}	$2U_{12}$	$2U_{13}$	$2U_{23}$
In(1)	44 (10)	−17 (2)	1398 (2)	25 (2)	16 (1)	29 (1)	−1 (2)	2 (2)	−9 (2)
In(2)	5238 (10)	1157 (2)	3132 (2)	24 (2)	21 (1)	34 (1)	3 (2)	4 (2)	−5 (2)
Te(1)	238 (9)	95 (1)	3535 (2)	25 (2)	16 (1)	26 (1)	4 (2)	0 (2)	2 (2)
Te(2)	4974 (9)	1041 (2)	1001 (2)	22 (2)	16 (1)	31 (1)	−4 (2)	−5 (2)	4 (2)
Te(3)	496 (9)	3075 (2)	2326 (2)	23 (2)	17 (1)	28 (1)	6 (2)	0 (2)	2 (2)
Te(4)	4810 (9)	2706 (1)	3870 (2)	25 (2)	17 (1)	23 (1)	−1 (2)	−1 (2)	−3 (2)
Te(5)	4479 (9)	3405 (2)	765 (2)	29 (2)	19 (1)	21 (1)	−4 (2)	2 (2)	−4 (2)

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

The subscript code is as follows:

(1) $x-1,y,z$; (2) $x+\frac{1}{2},y+\frac{1}{2},z$; (3) $x-\frac{1}{2},y-\frac{1}{2},z$; (4) $x+\frac{1}{2},\frac{1}{2}-y,z+\frac{1}{2}$; (5) $x-\frac{1}{2},y+\frac{1}{2},z$; (6) $x-\frac{1}{2},\frac{1}{2}-y,z+\frac{1}{2}$; (7) $1+x,y,z$; (8) $x,\bar{y},\frac{1}{2}+z$; (9) $x-1,\bar{y},\frac{1}{2}+z$.

In(1)–Te(1)	2·894 (6)	In(2)–Te(2)	2·886 (6)	Te(4)–Te(3)	2·843 (6)
In(1)–Te(2)	2·837 (7)	In(2)–Te(1_7)	2·842 (7)	Te(4)–Te(5)	2·831 (6)
In(1)–Te(2_1)	2·860 (7)	In(2)–Te(1)	2·866 (7)	Te(4)–Te(3_1)	3·355 (7)
In(1)–Te(5_3)	2·733 (6)	In(2)–Te(3)	2·736 (6)	Te(4)–Te(5_1)	3·377 (7)
Te(1)–In(1)–Te(2)	98·6 (2)	Te(2)–In(2)–Te(1_7)	99·2 (2)	Te(3)–Te(4)–Te(5)	100·1 (2)
Te(1)–In(1)–Te(2_1)	98·6 (2)	Te(2)–In(2)–Te(1)	98·1 (2)	Te(3)–Te(4)–Te(3_1)	89·8 (2)
Te(1)–In(1)–Te(5_3)	111·9 (2)	Te(2)–In(2)–Te(3)	115·1 (2)	Te(5)–Te(4)–Te(5_1)	89·6 (2)
Te(2)–In(1)–Te(2_1)	100·8 (2)	Te(1_7)–In(2)–Te(1)	100·6 (2)	Te(3_1)–Te(4)–Te(5_1)	80·5 (1)
Te(2)–In(1)–Te(5_3)	125·6 (2)	Te(1_7)–In(2)–Te(3)	124·0 (2)	Te(3)–Te(4)–Te(5_1)	170·2 (2)
Te(2_1)–In(1)–Te(5_3)	116·9 (2)	Te(1)–In(2)–Te(3)	115·7 (2)	Te(5)–Te(4)–Te(3_1)	170·0 (2)

Table 3. *Other relevant interatomic distances* (Å)

Te(4)–Te(2)	4·288	Te(3)–Te(2_6)	4·169	Te(1)–Te(5_6)	3·912
Te(4)–Te(2_1)	4·467	Te(3)–Te(2_4)	4·157	Te(1)–Te(2_8)	4·302
Te(4)–Te(1_2)	4·216	Te(3)–Te(5_4)	3·712	Te(1)–Te(2_9)	4·513
Te(4)–Te(1_5)	4·379	Te(3)–Te(5_6)	3·963	Te(1)–Te(2)	4·344
Te(4)–In(2)	3·908	Te(3)–Te(1_2)	3·947	Te(1)–Te(2_1)	4·362
Te(4)–In(2_1)	4·067			Te(1)–Te(3_3)	3·947
Te(4)–In(1_2)	3·935				
Te(4)–In(1_5)	4·112				

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31791 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

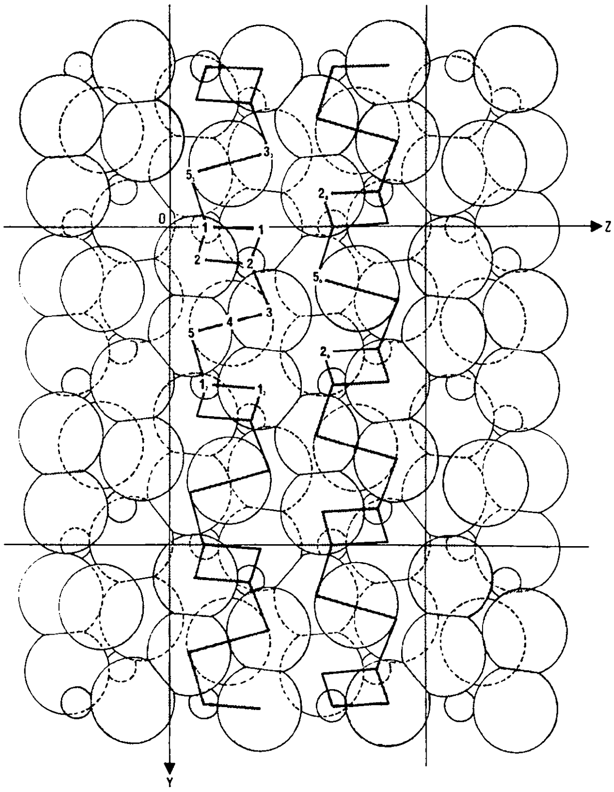

Fig. 1. In_2Te_5. A projection of the structure down a showing the method of bonding. The atoms are scaled to the respective ionic radii of In^{3+} (0·81 Å) and Te^{2-} (2·22 Å). Shaded and non-shaded atoms lie near $x=\frac{1}{2}$ and 0 respectively.

an analysis of bond lengths leads to an ambiguity in the designation of Te(4) which arises because the typical In–Te bond distance is 2·85 Å, whereas the average bond length in this group is 2·832 (6) Å with an included angle of 100·1 (2)°. This bond length, however, is similar to the Te–Te bond of 2·70 (1) Å found in *p,p'*-dichlorodiphenylditelluride (Kruse, Marsh & McCullough, 1957) and to the Te covalent single bond radius (2·74 Å), whilst the configuration is similar to that of the $(S_3)^{2-}$ polyanion in BaS_3 (Miller & King, 1936) which has an included angle of 103°. In elemental hexagonal Te, which contains endless spiral chains of atoms, the average Te–Te bond in the chain is 2·86 Å with a Te–Te–Te bond angle of 102°; the closest distance of approach of the chains is 3·47 Å (Wyckoff, 1963). Refinement of the structure with the central atom in the group as In resulted in significantly low thermal parameters for this atom. It was therefore concluded that the central atom in this group was a Te atom, Te(4); the group thus forms a triatomic anion. In In_2Te_5 the $(Te_3)^{2-}$ anions are arranged in chevron formation in the *xz* plane and the closest distances of approach between the anions are Te(4)–Te(3_1) = 3·355 (7) and Te(4)–Te(5_1) = 3·377 (7) Å.

The environment of Te(4), the central atom of the $(Te_3)^{2-}$ anion, indicates that this atom may be thought of as being in a state of sp^3 hybridization with two lone pair orbitals, the repulsion from which would account for the reduction of the Te(3)–Te(4)–Te(5) bond angle from the ideal tetrahedral value.

Bonds and contacts from Te(1) and Te(2) not involving the polyanion suggest that these two atoms have a diameter comparable with that of Te^{2-} (4·44 Å.) In this respect these two atoms are very similar to those existing in In_4Te_3. In both structures the short axial length is determined by this diameter. An analysis of the contacts and bonds around Te(3) and Te(5) show that these are on average significantly shorter by about 0·15 Å than other comparable distances in the structure. The shortest Te–Te distances in the structure, with the exception of those around Te(4), are those of 3·712 (1) Å between the end atoms of neighbouring $(3Te)^{2-}$ anions in adjacent sheets of atoms, Te(3)–Te(5_4). This distance is approximately 0·3 Å less than the usual value indicating a reduction in the radius of the end atoms of 0·15 Å. The bonds from Te(3) and Te(5) to In(2) and In(1_2) are also significantly shorter than other In–Te bonds in the structure, averaging 2·73 against 2·86 Å. Each In is surrounded by four Te atoms in approximately tetrahedral coordination indicating that on a covalent description they may be thought of as being sp^3 hybridized. The average In–Te bond lengths quoted above compare with that of 2·88 Å found in In_3Te_4 (Hogg & Sutherland, 1973).

The authors thank Mr G. Bucknell for the preparation of the samples, Dr P. G. Nelson for advice concerning the bonding, the SRC for the grant to purchase the densitometer and Drs C. Morgan, H. H. Sutherland and M. J. Mottram for the computer programs. One of us (P.D.W.) is indebted to Reckitt and Colman Ltd. for the funding of a research studentship.

References

Gerasimov, Y. I., Abbasov, A. S. & Nikolskaya, A. V. (1962). *Dokl. Akad. Nauk. SSSR*, **147**, 835–838.

Grochowski, E. G., Mason, D. R., Schmitt, G. A. & Smith, P. H. (1964). *J. Phys. Chem. Solids*, **25**, 551–558.

Hogg, J. H. C. & Sutherland, H. H. (1973). *Acta Cryst.* **B29**, 2483–2487.

International Tables for X-ray Crystallography (1974). Vol. IV. Birmingham: Kynoch Press.

Kruse, F. H., Marsh, R. E. & McCullough, J. D. (1957). *Acta Cryst.* **10**, 201–208.

Miller, W. S. & King, A. J. (1936). *Z. Kristallogr.* **94A**, 439–446.

Schubert, K., Dorre, E. & Gunzel, E. (1954). *Naturwissenschaften*, **41**, 448.

Wilson, A. J. C. (1942). *Nature, Lond.* **150**, 151–152.

Wyckoff, R. W. G. (1963). *Crystal Structures*, Vol. 1. New York: John Wiley.