Acta Cryst. (1976). **B32**, 2689

Indium Telluride

BY J. H. C. HOGG AND H. H. SUTHERLAND

Physics Department, The University of Hull, Hull, HU6 7RX, England

(*Received* 30 *March* 1976; *accepted* 16 *April* 1976)

Abstract. InTe, $M=242\cdot42$; tetragonal, $I4/mcm$; $a=b=8\cdot454$ (2), $c=7\cdot152$ (6) Å; $Z=8$, $D_c=6\cdot30$ g cm^{-3}; $U=511\cdot2$ Å^3; $F(000)=808$; $R=7$% for 399 reflexions. The cell contains two types of In atom site; one In is approximately tetrahedrally coordinated with four Te atoms with In–Te = 2·819 (1) Å, indicating that on a covalent description it exists in a state of sp^3 hybridization. The second In atom is surrounded by a cage-like system of eight Te atoms in a distorted square antiprismatic arrangement, all at distances of 3·576 (1) Å. The cage is completed by two further In atoms symmetrically disposed along **c** also at distances of 3·576 (1) Å. This environment is consistent with the extreme ionic formulation In^+ for this atom. The shortest Te–Te distance is 3·926 (1) Å.

Introduction. As part of a continuing investigation of phases existing in the In–Te system the structure of InTe (Schubert, Dorre & Kluge, 1955) has been refined to obtain accurate bond lengths. The original structure was deduced from 83 reflexions, the intensities of which were estimated on a strong, medium, weak scale.

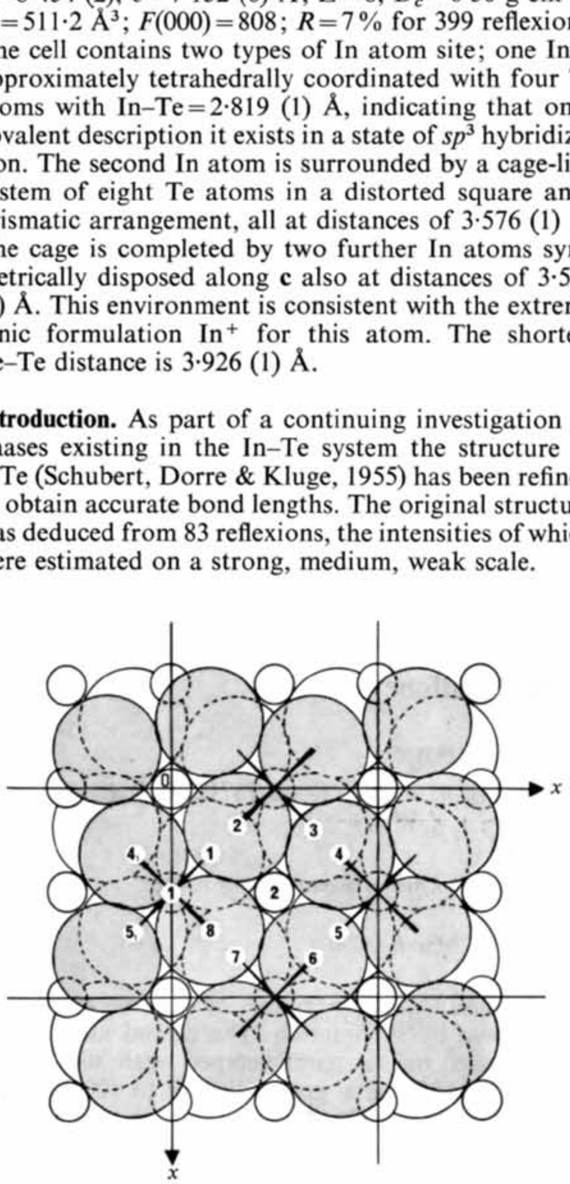

Fig. 1. InTe. A projection of the structure down **c** showing the method of bonding. The atoms are scaled for purposes of representation to the respective ionic radii of In^{3+} (0·81 Å) and Te^{2-} (2·22 Å). The In atoms lie at $z=\frac{1}{4},\frac{3}{4}$ and the Te atoms at $z=0,\frac{1}{2}$.

Small black needles of InTe were found in the inhomogeneous material obtained during the preparation and investigation of In_4Te_3 (Hogg & Sutherland, 1973).

444 unique reflexions, of which 49 were recorded as zero, were collected from Weissenberg photographs taken about **c** with multiple-film packs and Mo $K\alpha$ radiation. Intensities for 357 reflexions were measured with a Joyce–Loebl flying-spot integrating 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 had an approximately circular cross-section with $\mu R<0\cdot5$. Approximate values of absolute scale and temperature factors were determined by Wilson's (1942) method.

The coordinates of Schubert, Dorre & Kluge (1955) were used as the starting point for block-diagonal least-squares refinement of positional, scale and isotropic thermal parameters. This resulted in $R=0\cdot09$ where $R=\sum||F_o|-|F_c||/\sum|F_o|$. However, R for layer lines with l odd was on average some 3% lower than for l even. Analysis suggested that this could be accounted for by anisotropy of In(2). Anisotropic refinement of the In(2) thermal parameter showed this to be the case, giving a uniform distribution of R throughout the layers. The final R for 399 reflexions was 0·07.* Scattering factors were obtained from *International Tables for X-ray Crystallography* (1974). Table 1 gives the atomic coordinates and thermal parameters; bond lengths and angles are given in Table 2. Fig. 1 shows a projection of the structure down **c**.

---

* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31805 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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

	x	y	z	U_{iso}		
Te(1)	1823 (1)	1823 (1)	0	17 (1)		
In(1)	0	5000	2500	18 (1)		
				U_{11}	U_{22}	U_{33}
In(2)	0	0	2500	46 (5)	46 (5)	81 (3)

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

In(1)–Te(1)	2·819 (1)	Te(1)–In(1)–Te(8)	113·73 (2)
Te(1)–Te(4$_1$)	4·721 (1)	Te(1)–In(1)–Te(5$_1$)	101·26 (1)
Te(1)–Te(8)	4·721 (1)	Te(1)–In(2)–Te(2)	66·59 (2)
Te(1)–Te(5$_1$)	4·358 (1)	Te(2)–In(2)–Te(3)	82·61 (2)
Te(1)–In(2)	3·576 (1)	Te(1)–In(2)–Te(3)	75·52 (2)
Te(1)–Te(2)	3·926 (1)	Te(2)–In(2)–Te(4)	75·52 (2)
Te(2)–Te(3)	4·721 (1)	Te(1)–In(2)–Te(5)	120·00 (2)
Te(1)–Te(3)	4·379 (1)		
Te(1)–Te(4)	6·454 (1)		

Discussion. Since there is no evidence of polyionic formation in InTe, valence saturation rules give rise to an extreme ionic formulation $(In^{3+})(In^+)2(Te^{2-})$. The structure contains two different In atom sites as suggested by this formula. In(1) exists, on a covalent model, in a state of sp^3 hybridization, being surrounded by four Te atoms forming a tetrahedron slightly fore-shortened along **c**. The In–Te bond of 2·819 (1) Å compares favourably with that of 2·86 Å in In_4Te_3 where the tetrahedron has three Te and one In atom. In In_2Te_5 (Sutherland, Hogg & Walton, 1976) the tetrahedrally coordinated In has three In–Te bonds of 2·86 Å and one of 2·73 Å to the end member of a $(Te_3)^{2-}$ polyanion.

The environment of In(2) is consistent with the extreme ionic formulation In^+ for this atom. It is surrounded by a cage-like system of eight Te atoms in a distorted square anti-prismatic arrangement, again fore-shortened along **c**, with In–Te distances of 3·576 (1) Å. The cage is completed by two In atoms symmetrically disposed along **c**, also at distances of 3·576 (1) Å. These distances are comparable with those around In(4) in In_4Te_3 which is surrounded by seven Te atoms with an average In–Te distance of 3·49 Å and one In atom at 3·45 Å. The thermal parameters of In(2) were found to be significantly greater than those of In(1) and Te(1) and to be highly anisotropic with the maximum of the vibration ellipsoid occurring in the **c** direction towards the neighbouring In atoms.

The shortest Te–Te distance of 3·926 (1) Å [Te(1)–Te(2)] is comparable to that of 4·072 (2) Å found in In_4Te_3 and on average the Te atoms appear to have approximately the diameter of the Te^{2-} ion (4·44 Å) in both compounds.

The authors thank Mr G. Bucknell for the preparation of the samples; the S.R.C. for the grant to purchase the densitometer; and Drs C. Morgan, H. H. Sutherland and M. J. Mottram for the computer programs.

References

HOGG, J. H. C. & SUTHERLAND, H. H. (1973). *Acta Cryst.* B**29**, 2483–2487.

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

SCHUBERT, K., DORRE, E. & KLUGE, M. (1955). *Z. Metallkd.* **46**, 216–224.

SUTHERLAND, H. H., HOGG, J. H. C. & WALTON, P. D. (1976). *Acta Cryst.* B32, 2539–2541.

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

Acta Cryst. (1976). B**32**, 2690

8-Quinolyl Cyanomethyl Sulfone

BY R. L. HARLOW AND S. H. SIMONSEN

Department of Chemistry, The University of Texas at Austin, Austin, Texas 78712, *U.S.A.*

AND M. P. SAMMES

Department of Chemistry, University of Hong Kong, Pokfulam Road, Hong Kong

(*Received* 21 *February* 1976; *accepted* 23 *March* 1976)

Abstract. $C_{11}H_8N_2O_2S$, $M=232\cdot26$, monoclinic, $P2_1/c$ (No. 14), $Z=4$. At −40°C, $a=7\cdot419$ (1), $b=7\cdot968$ (1), $c=17\cdot636$ (2) Å, $\beta=100\cdot20$ (1)°, $V=1026\cdot1$ Å^3, $D_c=1\cdot503$ g cm^{-3}. Mo $K\alpha$ radiation, $\lambda=0\cdot71069$ Å, $\mu=1\cdot98$ cm^{-1}. Syntex diffractometer, 2066 reflections, 177 variables refined by full-matrix least squares, $R=0\cdot033$. NMR evidence for a possible C–H···N intramolecular interaction (between the methylene group and the N atom of the quinolyl moiety) is contradicted by the rather long H···N distance, 2·59 (2) Å, found in the crystal structure.

Introduction. Colorless crystals of the title compound were grown by sublimation. The crystal used in this investigation was a parallelepiped with dimensions 0·32 × 0·32 × 0·28 mm perpendicular to (001), (10$\bar{2}$), and (011) respectively. The space group and approximate unit-cell parameters were obtained from oscillation and Weissenberg photographs. The crystal was mounted on a Syntex $P2_1$ diffractometer (Mo $K\alpha$ radiation, monochromated with a graphite crystal) equipped with a low-temperature apparatus which kept the crystal cooled to −40°C. The unit-cell dimen-