

hydrogen bonds. Within the pair the stacking distance is about 3.5 Å, the closest contact distances being C(5)*a*...C(5)*b* 3.507 (4), C(5)*a*...N(7)*b* 3.507 (3), C(6)*a*...C(8)*b* 3.433 (4), and C(8)*a*...C(6)*b* 3.453 (4) Å. The stacked bases are oriented so that N(1) and N(6) are near the ionized methylphosphonate group of the paired molecule. N(1)*a*—H...O(7)*b*, N(1)*b*—H...O(7)*a*, and N(6)*b*—H...O(6)*a* hydrogen bonds are present (Table 3), but N(6)*a* is further from O(6)*b* than from O(7)*b* [3.312 (4) versus 3.101 (3) Å], so that only a weak interaction with O(7)*b* is likely. The packing interactions are shown in Fig. 2.

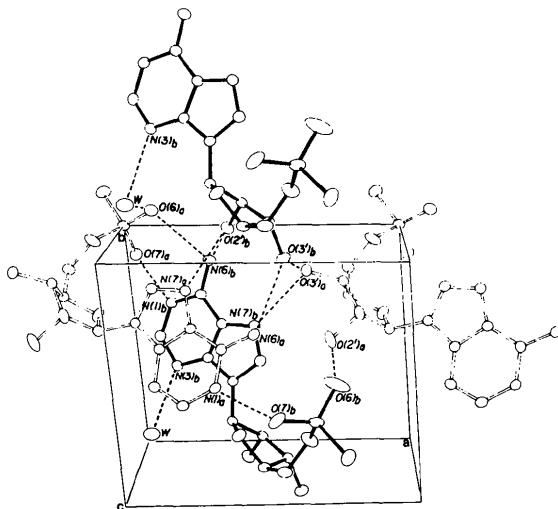


Fig. 2. Packing interactions. Molecule *A* is drawn with hollow bonds. Molecule *B* is drawn with solid bonds. The dashed lines represent hydrogen bonds. The thermal ellipsoids are drawn at the 30% probability level.

Adjacent *A*–*B* pairs are held together by stacking forces [stacking distances about 3.3 Å: N(1)*a*...C(2)*b* 3.458 (3), C(2)*a*...C(2)*b* 3.221 (4), C(2)*a*...N(3)*b* 3.360 (4), N(3)*a*...C(2)*b* 3.384 (4) Å, closest contacts] and an intricate network of hydrogen bonds, including interactions at position N(7) of both adenine rings. The water molecule participates as a donor in hydrogen bonds to N(3)*b* and O(6)*a*. Both C(8)–H groups are involved in close contacts: C(8)*a*...O(*w*) 3.134 (3), C(8)*b*...O(2')*a* 2.916 (3) Å.

Data collection at Oak Ridge National Laboratory was sponsored by the Division of Basic Energy Sciences of the Department of Energy under contract with Union Carbide Corporation.

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*Acta Cryst.* (1979). **B35**, 1727–1729

## Structure of *p,p'*-Ditolyl Ditelluride

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(Received 20 November 1978; accepted 27 March 1979)

**Abstract.** C<sub>14</sub>H<sub>14</sub>Te<sub>2</sub>, orthorhombic, *Pbc*2<sub>1</sub>, *a* = 8.305 (3), *b* = 26.329 (6), *c* = 6.439 (3) Å, *Z* = 4. The structure was determined by three-dimensional X-ray analysis. Positional and temperature-factor parameters for Te and C atoms have been refined by block-diagonal least-squares methods to a final *R* value of

0.057 for 1873 observed reflections. The Te–Te bond length of 2.697 (3) Å and the other observed intramolecular distances and angles are all consistent with the accepted values from earlier investigations. The value of the dihedral angle C–Te–Te/Te–Te–C is 85.7 (4)°.

0567-7408/79/071727-03\$01.00

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**Introduction.** The structure determination of the title compound was undertaken within the framework of magnetic-susceptibility studies on diphenyl ditelluride analogues and derivatives.

In this series of compounds the principal features describing molecular conformations are the dihedral angles  $C-X-X-X-C$  ( $X = \text{Te}, \text{Se}, \text{S}$ ) and the angles of relative rotation of the benzene rings.

Single crystals were obtained by slow evaporation of solutions in benzene and petroleum ether (313–333 K). The dark-red needles elongated along *c* tend to twin along the (010) plane. Preliminary Weissenberg and precession photographs displayed systematic absences consistent with space groups *Pbc*2<sub>1</sub> and *Pbcm*. The cell dimensions were established by the least-squares method from angle data recorded at  $293 \pm 1$  K for 12 reflections (Mo  $K\alpha$  radiation,  $\lambda = 0.7107$  Å). Integrated intensities of 2217 unique reflections were measured with a four-circle Hilger diffractometer. The intensities for all observed reflections were corrected for Lorentz and polarization effects. No corrections were made for absorption or extinction. The structure was solved by the direct method using the program *MULTAN* (Main, Lessinger, Woolfson, Germain & Declercq, 1977). The first stage of the procedure established that the space group is *Pbc*2<sub>1</sub>.

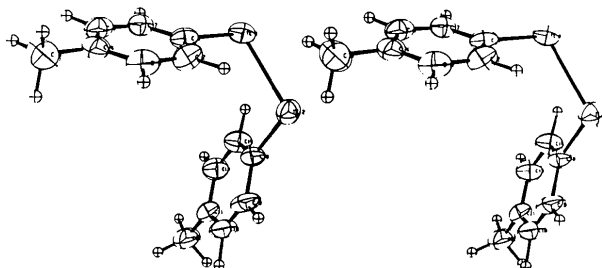


Fig. 1. Stereoscopic view of a molecule of the title compound. The viewing direction is along *c*; *b* runs horizontally from left to right.

Table 1. Atomic positional parameters with standard deviations for *p,p'*-ditolyl ditelluride

	<i>x</i>	<i>y</i>	<i>z</i>
Te(1)	-0.2972 (1)	0.1937 (1)	0.4652 (1)
Te(2)	-0.4547 (1)	0.1081 (1)	0.3577 (2)
C(1)	-0.093 (1)	0.1881 (4)	0.266 (2)
C(2)	-0.106 (2)	0.1691 (5)	0.068 (2)
C(3)	0.032 (2)	0.1639 (5)	-0.050 (3)
C(4)	0.183 (2)	0.1786 (5)	0.021 (3)
C(5)	0.333 (2)	0.1723 (7)	-0.119 (3)
C(6)	0.190 (1)	0.1985 (5)	0.226 (3)
C(7)	0.057 (2)	0.2018 (4)	0.343 (3)
C(8)	-0.343 (2)	0.0536 (4)	0.554 (2)
C(9)	-0.313 (2)	0.0045 (4)	0.472 (3)
C(10)	-0.239 (2)	-0.0313 (5)	0.598 (3)
C(11)	-0.186 (2)	-0.0205 (5)	0.796 (3)
C(12)	-0.103 (2)	-0.0595 (5)	0.930 (4)
C(13)	-0.214 (2)	0.0285 (5)	0.872 (3)
C(14)	-0.296 (2)	0.0648 (5)	0.757 (2)

Table 2. Bond lengths (Å) with standard deviations in parentheses

Te(1)—Te(2)	2.697 (3)	C(7)—C(1)	1.39 (2)
Te(1)—C(1)	2.13 (1)	C(8)—C(9)	1.42 (2)
Te(2)—C(8)	2.13 (1)	C(9)—C(10)	1.39 (2)
C(1)—C(2)	1.38 (2)	C(10)—C(11)	1.38 (3)
C(2)—C(3)	1.38 (2)	C(11)—C(12)	1.51 (3)
C(3)—C(4)	1.39 (2)	C(11)—C(13)	1.40 (2)
C(4)—C(5)	1.54 (2)	C(13)—C(14)	1.39 (2)
C(4)—C(6)	1.42 (2)	C(14)—C(8)	1.39 (2)
C(6)—C(7)	1.35 (2)		

Table 3. Bond angles (°) with standard deviations in parentheses

C(1)—Te(1)—Te(2)	100.0 (0.3)	C(4)—C(6)—C(7)	120.7 (1.3)
C(8)—Te(2)—Te(1)	101.5 (0.3)	C(6)—C(7)—C(1)	121.6 (1.3)
Te(1)—C(1)—C(2)	121.4 (1.0)	C(7)—C(1)—C(2)	119.7 (1.2)
Te(1)—C(1)—C(7)	118.8 (0.9)	C(8)—C(9)—C(10)	118.5 (1.4)
Te(2)—C(8)—C(9)	118.0 (1.0)	C(9)—C(10)—C(11)	122.8 (1.5)
Te(2)—C(8)—C(14)	122.4 (0.9)	C(10)—C(11)—C(12)	122.3 (1.4)
C(1)—C(2)—C(3)	118.7 (1.3)	C(10)—C(11)—C(13)	117.4 (1.4)
C(2)—C(3)—C(4)	122.8 (1.4)	C(12)—C(11)—C(13)	120.3 (1.4)
C(3)—C(4)—C(5)	120.5 (1.4)	C(11)—C(13)—C(14)	122.0 (1.4)
C(3)—C(4)—C(6)	116.3 (1.3)	C(13)—C(14)—C(8)	119.4 (1.3)
C(5)—C(4)—C(6)	123.2 (1.3)	C(14)—C(8)—C(9)	119.6 (1.2)

Table 4. Packing distances (Å): shortest intermolecular Te...Te, Te...C and C...C distances with standard deviations in parentheses

Key to symmetry operations relating designated atoms to reference atoms at (*x*, *y*, *z*)

(i)	<i>x</i> , 0.5 - <i>y</i> , 0.5 + <i>z</i>	(iv)	-1 - <i>x</i> , - <i>y</i> , -0.5 + <i>z</i>
(ii)	-1 + <i>x</i> , <i>y</i> , <i>z</i>	(v)	<i>x</i> , 0.5 - <i>y</i> , -0.5 + <i>z</i>
(iii)	<i>x</i> , <i>y</i> , -1 + <i>z</i>		

Te(1)...Te(1 <sup>i</sup> )	4.375 (1)	C(3)...C(7 <sup>v</sup> )	3.61 (2)
Te(2)...C(6 <sup>ii</sup> )	3.88 (1)	C(4)...C(6 <sup>v</sup> )	3.76 (2)
Te(2)...C(10 <sup>iv</sup> )	3.66 (2)	C(4)...C(7 <sup>v</sup> )	3.51 (2)
Te(2)...C(11 <sup>iv</sup> )	3.80 (1)	C(5)...C(6 <sup>v</sup> )	3.74 (2)
C(2)...C(14 <sup>iii</sup> )	3.75 (2)	C(6)...C(7 <sup>v</sup> )	3.77 (2)

Table 5. Best least-squares planes

Plane I: C(1), C(2), C(3), C(4), C(6), C(7)			
	$-0.1437x + 0.9236y - 0.3553z - 4.0704 = 0$ ( $\chi^2 = 4.50$ )		
Plane II: C(8), C(9), C(10), C(11), C(13), C(14)			
	$0.8816x + 0.3101y - 0.3558z + 3.3557 = 0$ ( $\chi^2 = 8.38$ )		
Plane III: C(1), C(2), C(3), C(4), C(5), C(6), C(7)			
	$-0.1425x + 0.9235y - 0.3562z - 4.0687 = 0$ ( $\chi^2 = 4.70$ )		
Plane IV: C(8), C(9), C(10), C(11), C(12), C(13), C(14)			
	$0.8829x + 0.3082y - 0.3542z + 3.3535 = 0$ ( $\chi^2 = 8.78$ )		
Distances (Å × 10 <sup>3</sup> ) of atoms from planes (e.s.d.'s in parentheses)			
	Plane I	Plane II	Plane III
C(1)	3 (12)	C(8)	14 (13)
C(2)	11 (14)	C(9)	10 (15)
C(3)	-13 (15)	C(10)	-21 (16)
C(4)	-0.2 (13)	C(11)	7 (13)
C(6)	15 (13)	C(13)	17 (15)
C(7)	-16 (12)	C(14)	-27 (15)
Te(1)	-69 (1)	Te(2)	90 (1)
		Te(1)	-73 (1)
		Te(2)	81 (1)
		C(1)	1 (12)
		C(2)	11 (14)
		C(3)	-11 (15)
		C(4)	2 (13)
		C(5)	-3 (17)
		C(6)	16 (13)
		C(7)	-17 (12)
		C(8)	11 (13)
		C(9)	9 (15)
		C(10)	-18 (16)
		C(11)	12 (13)
		C(12)	-6 (19)
		C(13)	20 (15)
		C(14)	-28 (15)

Table 6. Characteristic angles ( $^{\circ}$ ) compared with those for dichlorodiphenyl ditelluride and diphenyl ditelluride ( $^{\circ}$ ) (e.s.d.'s in parentheses)

	CH <sub>3</sub> - $\phi$ -Te-Te- $\phi$ -CH <sub>3</sub> (Pbc2 <sub>1</sub> ) (a)	Cl- $\phi$ -Te-Te- $\phi$ -Cl (P2 <sub>1</sub> /n) (b)	$\phi$ -Te-Te- $\phi$ (P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub> ) (c)
Dihedral angle	85.7 (4)	72.0	88.5
Angle of relative rotation of benzene rings	73.4 (3)	152.6	159.9
Angle of rotation of benzene ring I relative to the C(1)-Te(1)-Te(2) plane	38.0 (4)	50.7	87.7
Angle of rotation of benzene ring II relative to the C(8)-Te(2)-Te(1) plane	37.0 (4)	96.3	101.5

References: (a) this work; (b) Kruse, Marsh & McCullough (1957); (c) Llabrès, Dideberg & Dupont (1972).

The structure was refined by block-diagonal least-squares methods (Ahmed, Hall, Pippy & Huber, 1966) on 1873 reflections for which  $I > 2\sigma(I)$ . Refinement was completed varying coordinates and anisotropic temperature factor coefficients for Te and C atoms. H atoms were included at fixed positions, C-H bond lengths of 1.087 Å being assumed. A Cruickshank (1961) type of weighting scheme was used. The conventional discrepancy factor  $R$  for the observations used in the refinement was 0.057. The values of the final atomic coordinates are listed in Table 1.\*

**Discussion.** The molecular structure is shown in Fig. 1. Each atom is represented by its 50% probability ellipsoid (ORTEP-II, Johnson, 1971). Bond lengths, bond angles and packing distances are given in Tables 2, 3, and 4.

Using the method described by Schomaker, Waser, Marsh & Bergman (1959), we calculated the equations of the best least-squares planes through benzene rings I and II. These are reported in Table 5 together with the distances of atoms from the planes.

The bond lengths and angles in the benzene rings are all normal and the rings are planar to within the limits of the standard deviations. It can be clearly seen from Table 5 that C(5) and C(12) of the methyl groups are in the plane of the benzene rings to which they are linked while Te(1) and Te(2) are not.

The observed Te-Te bond length, 2.697 (3) Å, compares favorably with the values found in diphenyl ditelluride (Llabrès, Dideberg & Dupont, 1972) and p,p'-dichlorodiphenyl ditelluride (Kruse, Marsh & McCullough, 1957). It is significantly shorter than the single covalent Te-Te bond length (2.74 Å) of Pauling (1960). On the other hand, Te(1)-C(1) and Te(2)-C(8) distances correspond to single covalent bonds.

\* Lists of structure factors, anisotropic thermal parameters and H-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34337 (23 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

There is no intermolecular distance less than 3.5 Å between non-bonded atoms (Table 4) so that only van der Waals forces are present between molecules in the crystal.

In Table 6, some characteristic angles describing the molecular conformation of p,p'-ditolyl ditelluride are compared with the results of Llabrès *et al.* (1972) and Kruse *et al.* (1957) respectively for diphenyl ditelluride and p,p'-dichlorodiphenyl ditelluride. The great dissimilarity between the molecular orientation of the diphenyl ditelluride molecule in the three crystals seems likely to be due to steric hindrances arising from the different stackings.

The authors wish to thank Professor J. Toussaint for his interest in this work, Mr M. Vermeire for technical assistance and Dr J. L. Piette (Laboratoire de Chimie Organique de l'Université de Liège, Service du Professeur Renson) for providing the p,p'-ditolyl ditelluride.

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