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New Form of Bis(*p*-chlorophenyl) Ditelluride, $C_{12}H_8Cl_2Te_2$

By G. Van den Bossche, M. R. Spirlet, O. Dideberg and L. Dupont

Institut de Physique B5, Université de Liège au Sart Tilman, B-4000 Liège, Belgium

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Abstract. $M_r = 506 \cdot 36$, orthorhombic, $P2_12_12_1$, $a = 10 \cdot 602\,(3)$, $b = 14 \cdot 543\,(4)$, $c = 8 \cdot 713\,(3)$ Å, $V = 1343\,(1)$ Å^3, $Z = 4$, D_m (by flotation) $= 2 \cdot 49$, $D_x = 2 \cdot 50$ Mg m^{-3}, λ(Mo $K\alpha$) $= 0 \cdot 7107$ Å, μ(Mo $K\alpha$) $= 4 \cdot 68$ mm^{-1}, $F(000) = 872$, $T = 293$ K. $R = 0 \cdot 045$ for 1959 unique reflections. The Te—Te bond length of 2·680 (1) Å is shorter than the values reported for diphenyl ditellurides in earlier investigations. The value of the dihedral angle C—Te—Te/Te—Te—C is 88·8 (4)°. The molecular geometries observed in diphenyl ditellurides seem dependent on the packing modes alone.

Introduction. Within the framework of diamagnetic-anisotropy studies, single-crystal-growing experiments were undertaken on diphenyl ditelluride analogues and derivatives. For the title compound we obtained two different varieties of single crystals. One corresponds to the variety described by Kruse, Marsh & McCullough (1957), the other is a polymorphic form for which we have determined the structure.

Experimental. Solutions in dichloroethane give garnet-red needles identical with those of Kruse, Marsh & McCullough (1957), while solutions in benzene/petroleum ether (b.p. 333–353 K) give light-red prisms.

Crystal 0·28 × 0·20 × 0·50 mm. Space group from Weissenberg and precession photographs, cell dimensions by least squares from angle data for 10 reflections ($30 \cdot 56 < 2\theta < 42 \cdot 94°$). Hilger & Watts four-circle diffractometer, Zr-filtered Mo $K\alpha$ radiation, ω–2θ scan technique [$(\sin\theta/\lambda)_{\max} = 0 \cdot 7035$ Å^{-1}]. Intensities corrected for Lorentz and polarization effects and, semi-empirically, for absorption (North, Phillips & Mathews, 1968; limit values 0·697 and 0·997). h 0→14, k 0→20, l 0→12; standard reflections 402 and $\bar{6}00$ stable [$2157 < F_o(402) < 2231$; $1714 < F_o(\bar{6}00) < 1755$]. 2471 reflections measured [2351 with $I > 2\sigma(I)$ and 2165 unique with $R_{\rm int} = 0 \cdot 015$]. Structure solved by direct methods

Table 1. *Fractional atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *with e.s.d.'s in parentheses*

	x	y	z	U_{eq}*(Å^2)
Te(1)	0·2175 (1)	0·4655 (1)	0·9716 (1)	0·0381 (4)
Te(2)	0·2600 (1)	0·2839 (1)	0·9776 (1)	0·0374 (4)
Cl(1)	−0·2171 (4)	0·5138 (3)	1·5133 (5)	0·054 (2)
Cl(2)	0·6919 (4)	0·2390 (3)	1·5235 (6)	0·060 (2)
C(1)	0·069 (1)	0·474 (1)	1·138 (2)	0·035 (7)
C(2)	0·009 (1)	0·401 (1)	1·198 (2)	0·040 (8)
C(3)	−0·081 (1)	0·411 (1)	1·313 (2)	0·037 (7)
C(4)	−0·108 (1)	0·499 (1)	1·363 (2)	0·042 (8)
C(5)	−0·053 (1)	0·574 (1)	1·305 (2)	0·042 (8)
C(6)	0·040 (1)	0·563 (1)	1·187 (2)	0·041 (8)
C(7)	0·399 (1)	0·273 (1)	1·158 (2)	0·031 (6)
C(8)	0·460 (1)	0·352 (1)	1·214 (2)	0·042 (8)
C(9)	0·550 (1)	0·341 (1)	1·329 (2)	0·043 (8)
C(10)	0·578 (1)	0·253 (1)	1·380 (2)	0·036 (7)
C(11)	0·516 (1)	0·177 (1)	1·326 (2)	0·044 (8)
C(12)	0·424 (2)	0·188 (1)	1·213 (2)	0·044 (8)

* $U_{eq} = \frac{1}{3}$ trace $\tilde{\mathbf{U}}$.

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

Te(1)–Te(2)	2·680 (1)		
Te(1)–C(1)	2·14 (1)	C(6)–C(1)	1·40 (2)
Te(2)–C(7)	2·16 (1)	C(7)–C(8)	1·41 (2)
C(1)–C(2)	1·34 (2)	C(8)–C(9)	1·40 (2)
C(2)–C(3)	1·39 (2)	C(9)–C(10)	1·39 (2)
C(3)–C(4)	1·37 (2)	C(10)–Cl(2)	1·75 (1)
C(4)–Cl(1)	1·76 (1)	C(10)–C(11)	1·38 (2)
C(4)–C(5)	1·34 (2)	C(11)–C(12)	1·40 (2)
C(5)–C(6)	1·43 (2)	C(12)–C(7)	1·35 (2)

C(1)–Te(1)–Te(2)	99·5 (4)	C(4)–C(5)–C(6)	118·0 (1·)
C(7)–Te(2)–Te(1)	101·7 (4)	C(5)–C(6)–C(1)	119·0 (1·)
Te(1)–C(1)–C(2)	125·0 (1·)	C(6)–C(1)–C(2)	119·9 (1·)
Te(1)–C(1)–C(6)	115·0 (1·)	C(7)–C(8)–C(9)	118·4 (1·)
Te(2)–C(7)–C(8)	120·4 (1·)	C(8)–C(9)–C(10)	118·4 (1·)
Te(2)–C(7)–C(12)	117·3 (1·)	C(9)–C(10)–Cl(2)	118·8 (1·)
C(1)–C(2)–C(3)	121·9 (1·)	C(9)–C(10)–C(11)	122·4 (1·)
C(2)–C(3)–C(4)	117·8 (1·)	Cl(2)–C(10)–C(11)	118·8 (1·)
C(3)–C(4)–Cl(1)	118·9 (1·)	C(10)–C(11)–C(12)	118·9 (1·)
C(3)–C(4)–C(5)	123·3 (1·)	C(11)–C(12)–C(7)	119·5 (1·)
Cl(1)–C(4)–C(5)	117·8 (1·)	C(12)–C(7)–C(8)	122·3 (1·)

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Table 3. Te—Te *bond* (Å) *and characteristic angles* (°) *in diphenyl ditellurides*

	φ—Te—Te—φ	CH$_3$—φ—Te—Te—φ—CH$_3$	Cl—φ—Te—Te—φ—Cl	
	$P2_12_12_1$ (*a*)	$Pbc2_1$ (*b*)	$P2_1/n$ (*c*)	$P2_12_12_1$ (*d*)
Te—Te bond	2·712 (2)	2·697 (3)	2·702 (10)	2·680 (1)
Dihedral angle	91·5	85·7 (4)	72·4	88·8 (4)
Angle of relative rotation of benzene rings	20·1	73·4 (3)	128·4	88·9 (4)
Angle of rotation of benzene ring I relative to the C(1)—Te(1)—Te(2) plane	92·3	38·0 (4)	68·3	11·8 (4)
Angle of rotation of benzene ring II relative to the C(7)—Te(2)—Te(1) plane	84·9	37·0 (4)	50·9	12·6 (4)
Torsional angle C(1)—Te(1)—Te(2)—C(2)	91·5	85·8 (4)	77·4	88·8 (4)

References: (*a*) Llabrès, Dideberg & Dupont (1972); (*b*) Spirlet, Van den Bossche, Dideberg & Dupont (1979); (*c*) Kruse, Marsh & McCullough (1957); (*d*) this work.

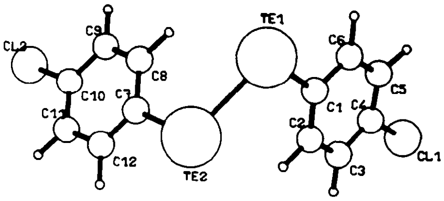

Fig. 1. Perspective view of the molecule showing the labelling scheme.

[*MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980)] and refined anisotropically, except for hydrogens, by least squares [*SHELX*76 (Sheldrick, 1976)] on 1959 unique reflections [$F \geq 3\sigma(F)$ and unit weights]. H atoms in calculated positions (assuming a C—H bond length of 1·08 Å). $R = 0{\cdot}045$, $wR = 0{\cdot}056$.* $(\Delta/\sigma)_{\max} = 0{\cdot}05$, $\Delta\rho$ in final difference Fourier map $\leq 0{\cdot}65$ e Å^{-3} (not due to residual peaks around Te atoms). Neutral-atom scattering factors for Te from *International Tables for X-ray Crystallography* (1974), for Cl, C and H as in *SHELX*. Drawing by *PLUTO* (Motherwell, 1972).

Discussion. Tables 1 and 2 give atomic parameters and molecular geometry, Fig. 1 shows a projection of the molecule.*

The Te—Te bond distance of 2·680 (1) Å is the shortest of the values reported for diphenyl ditellurides (Table 3). With respect to the value of 2·74 Å for a covalent single bond (Pauling, 1960), the shortening of the Te—Te bond corresponds to 19% double-bond character, probably arising from π overlap between filled p orbitals of one atom and empty d orbitals of the other; indeed π bonding is most pronounced when the dihedral angle is near 90° and when two $p\pi$–$d\pi$ overlaps, at right angles, are possible. Te—C and Cl—C bond distances correspond to the values expected for covalent single bonds (Pauling, 1960). The benzene rings are planar within the limits of the standard deviations and exhibit normal bond lengths and internal angles. While Cl(2) is in the plane of the benzene ring to which it is linked, Cl(1) is 0·08 Å out of the corresponding benzene plane. Both Te(1) and Te(2) are out of the benzene-ring planes. In the packing, one short intermolecular contact of 3·59 (1) Å is observed between Te(1) and C(6).

In Table 3, some characteristic angles describing the molecular conformation of diphenyl ditelluride compounds are compared. It appears that the overall conformation of bis(p-chlorophenyl) ditelluride, in the orthorhombic crystal, differs considerably from that previously reported for the monoclinic form. In fact, interplanar angles, as well as torsional angles, compare more favourably with those of the ditolyl derivative. Thus the molecular geometry in diphenyl ditelluride derivatives seems to be only dictated by steric hindrances arising from the different stackings.

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* Lists of structure factors, anisotropic thermal parameters, least-squares planes and hydrogen-atom coordinates have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39221 (13 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.