

Lists of atomic coordinates, displacement parameters, structure factors and complete geometry have been deposited with the IUCr (Reference: SK1062). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Acta Cryst. (1997). **C53**, 342–343

Bis(*p*-methoxyphenyl) Telluride

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(Received 26 July 1996; accepted 21 October 1996)

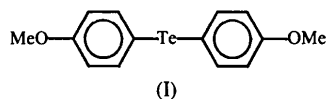
Abstract

The title compound, C₁₄H₁₄O₂Te, displays an angular geometry at tellurium, with a C—Te—C angle of 99.5(1)° and Te—C distances of 2.110(3) and 2.112(3) Å. The Te atom is displaced by 0.1963(3) and 0.0044(3) Å out of the planes of the aromatic rings. These rings are approximately perpendicular to one another [dihedral angle 70.4(1)°], while each methoxy group is almost coplanar with the phenyl ring to which it is bonded [dihedral angles 3.3(2) and 1.5(3)°].

Comment

Aside from the pioneering work of Blackmore & Abrahams (1955) on (*p*-MeC₆H₄)₂Te, based on a partial data set, only three other diaryl tellurides, Ar—Te—Ar', have been structurally characterized, viz. (*p*-EtOC₆H₄)Te[*o*-C₆H₄(*o*-C₅NH₄)] (Al-Salim, West & McWhinnie, 1988), [*o*-(*p*-MeOC₆H₄N:CH)C₆H₄]₂Te (Sadekov *et al.*, 1989) and (*o*-PhC₆H₄)₂Te (Chen, Hamor, Singh & McWhin-

nie, 1996). As part of our synthetic and structural studies on organotellurium compounds (Farran, Alvarez-Larena, Piniella, Germain & Torres-Castellanos, 1995*a,b*; Matheus, Torres, Piniella, Briansó & Miravittles, 1991; Matheus, Torres, Cabiativa, Fuertes & Miravittles, 1991; Matheus, Torres, Piniella & Miravittles, 1991; Torres, 1990), we report here the structure of bis(*p*-methoxyphenyl) telluride, (I).



The crystals of (I) contain discrete (*p*-MeOC₆H₄)₂Te molecules (Fig. 1) which display an angular geometry at tellurium, as predicted by the valence-shell electron-pair repulsion (VSEPR) model for an AX₂E₂ molecule (Gillespie & Hargittai, 1991, and references therein). The Te—C distances are equal within experimental error and their values are comparable with that of 2.116(20) Å tabulated by Allen *et al.* (1987) for Te—C(aryl) bonds, and with those of 2.105(5) and 2.125(5) Å observed in (*o*-PhC₆H₄)₂Te (Chen *et al.*, 1996). As expected, the C—Te—C angle is substantially smaller than the tetrahedral value (109.5°) due to the repulsion of bonded electron pairs by lone pairs. This angle, however, is somewhat larger than those observed in the above-mentioned diaryl tellurides; 94.8(2) in (*p*-EtOC₆H₄)Te[*o*-C₆H₄(*o*-C₅NH₄)] (Al-Salim *et al.*, 1988), 96.3(2) in [*o*-(*p*-MeOC₆H₄N:CH)C₆H₄]₂Te (Sadekov *et al.*, 1989) and 96.2(2)° in (*o*-PhC₆H₄)₂Te (Chen *et al.*, 1996).

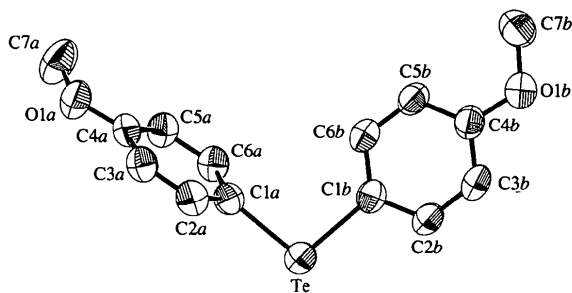


Fig. 1. The molecular structure of the title compound showing the displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity.

Each aromatic ring is planar [to within 0.007(3) Å]. The Te atom lies 0.1963(3) and 0.0044(3) Å from the planes of rings *a* and *b*, respectively. The angles between the C—Te—C plane and those of the phenyl rings differ [70.8(1) and 2.0(1)° for rings *a* and *b*] and the phenyl rings are approximately perpendicular to one another [inter-ring dihedral angle 70.4(1)°].

The methoxy groups are almost coplanar with their associated phenyl rings [dihedral angles 3.3 (2) and 1.5 (3)° for molecules *a* and *b*].

The crystal packing involves only van der Waals interactions.

Experimental

The title compound was synthesized according to the method of Morgan & Kellett (1926). Crystals suitable for X-ray analysis were obtained by slow evaporation of a dimethyl-sulfoxide (DMSO) solution.

Crystal data

$C_{14}H_{14}O_2Te$	Mo $K\alpha$ radiation
$M_r = 341.85$	$\lambda = 0.71069 \text{ \AA}$
Monoclinic	Cell parameters from 25 reflections
$P2_1/n$	$\theta = 11.6\text{--}14.0^\circ$
$a = 6.283 (1) \text{ \AA}$	$\mu = 2.190 \text{ mm}^{-1}$
$b = 26.437 (2) \text{ \AA}$	$T = 295 (2) \text{ K}$
$c = 8.1851 (9) \text{ \AA}$	Plate
$\beta = 96.54 (1)^\circ$	$0.41 \times 0.33 \times 0.11 \text{ mm}$
$V = 1350.7 (3) \text{ \AA}^3$	Colourless
$Z = 4$	
$D_x = 1.681 \text{ Mg m}^{-3}$	
D_m not measured	

Data collection

Enraf–Nonius CAD-4 diffractometer	1940 reflections with $I > 2\sigma(I)$
ω - 2θ scans	$\theta_{\max} = 25^\circ$
Absorption correction: empirical from ψ scans (North, Phillips & Mathews, 1968)	$h = -7 \rightarrow 7$
$T_{\min} = 0.547$, $T_{\max} = 0.786$	$k = 0 \rightarrow 31$
2373 measured reflections	$l = 0 \rightarrow 9$
2373 independent reflections	3 standard reflections frequency: 60 min intensity decay: none

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\max} = 0.001$
$R(F) = 0.0250$	$\Delta\rho_{\max} = 0.45 \text{ e \AA}^{-3}$
$wR(F^2) = 0.0688$	$\Delta\rho_{\min} = -0.58 \text{ e \AA}^{-3}$
$S = 1.084$	Extinction correction: none
2373 reflections	Scattering factors from <i>International Tables for Crystallography</i> (Vol. C)
156 parameters	
H atoms: see below	
$w = 1/[\sigma^2(F_o^2) + (0.0364P)^2 + 0.472P]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Table 1. Selected geometric parameters (\AA , $^\circ$)

Te—C1a	2.110 (3)	O1a—C7a	1.425 (5)
Te—C1b	2.112 (3)	C4b—O1b	1.369 (4)
C4a—O1a	1.364 (4)	O1b—C7b	1.398 (5)
C1a—Te—C1b	99.5 (1)	C2b—C1b—Te	117.1 (2)
C6a—C1a—Te	121.6 (2)	C6b—C1b—Te	124.8 (2)
C2a—C1a—Te	119.7 (2)	O1b—C4b—C5b	125.3 (3)
O1a—C4a—C5a	125.1 (3)	O1b—C4b—C3b	115.8 (3)
O1a—C4a—C3a	115.4 (3)	C4b—O1b—C7b	119.0 (3)
C4a—O1a—C7a	118.0 (3)		

The title structure was solved by direct methods. H atoms were placed in calculated positions using a riding model, with fixed C—H distances (0.93 \AA for C_{sp^2} , 0.96 \AA for C_{sp^3} and $U_{\text{iso}} = pU_{\text{eq}}(\text{parent atom})$ (where $p = 1.2$ for C_{sp^2} and 1.5 for C_{sp^3}). A single orientation parameter was refined for each methyl group. Geometrical calculations were carried out using the PARST95 program (Nardelli, 1995).

Data collection: CAD-4 Software (Enraf–Nonius, 1989). Cell refinement: CAD-4 Software. Program(s) used to solve structure: SHELXS86 (Sheldrick, 1990). Program(s) used to refine structure: SHELXL93 (Sheldrick, 1993). Molecular graphics: ZORTEP (Zsolnai & Pritzkow, 1994). Software used to prepare material for publication: SHELXL93.

The authors acknowledge the financial support of the EEC (project CI1*0574). MVC thanks the Ministerio de Educación y Ciencia of Spain for a sabbatical grant (project SAB95-0281). JF thanks the Generalitat de Catalunya for an FI grant. The X-ray measurements were carried out at the Servei de Difracció de Raigs-X of the Universitat Autònoma de Barcelona.

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