C7	0.1750 (6)	0.8793 (5)	0.1179 (2)	0.0308 (12)
C8	0.0069 (6)	0.9089 (5)	0.1053 (2)	0.0252 (11)
C9	−0.0812 (5)	0.9498 (5)	0.1506 (2)	0.0248 (11)
C10	−0.0053 (6)	1.0544 (5)	0.1840 (2)	0.0301 (12)
C11	−0.2490 (6)	0.9812 (5)	0.1388 (2)	0.0309 (12)
C12	−0.3273 (6)	0.8578 (5)	0.1187 (2)	0.0333 (13)
C13	−0.2407 (5)	0.7940 (5)	0.0776 (2)	0.0261 (11)
C14	−0.0684 (5)	0.7775 (5)	0.0876 (2)	0.0246 (11)
C15	0.0109 (6)	0.7183 (5)	0.0438 (2)	0.0288 (12)
C16	0.0120 (6)	0.5676 (5)	0.0398 (2)	0.0262 (12)
C17	−0.1457 (6)	0.5024 (5)	0.0430 (2)	0.0290 (12)
C18	−0.1622 (6)	0.3727 (5)	0.0166 (2)	0.0380 (14)
C19	−0.2802 (6)	0.2964 (6)	0.0425 (2)	0.0395 (14)
C20	0.3853 (7)	0.9742 (7)	0.2489 (2)	0.053 (2)
C21	0.3130 (7)	1.2041 (6)	0.2256 (2)	0.048 (2)
C22	−0.0071 (7)	1.1979 (5)	0.1633 (2)	0.0396 (14)
C23	0.0040 (6)	1.0152 (5)	0.0661 (2)	0.0339 (13)
C24	−0.3200 (6)	0.6620 (5)	0.0664 (2)	0.0275 (12)
C25	−0.2071 (6)	0.4677 (5)	0.0920 (2)	0.0317 (13)
C26	0.2547 (7)	0.5088 (6)	0.0724 (2)	0.0354 (13)
C27	0.3284 (7)	0.4391 (8)	0.1137 (2)	0.071 (2)

Table 2. *Selected geometric parameters (Å)*

O1—C24	1.422 (6)	C6—C7	1.527 (7)
O1—C17	1.438 (6)	C7—C8	1.544 (7)
O2—C25	1.387 (6)	C8—C23	1.541 (6)
O2—C24	1.431 (5)	C8—C14	1.556 (7)
O3—C19	1.369 (7)	C8—C9	1.558 (6)
O3—C25	1.445 (6)	C9—C11	1.541 (7)
O4—C19	1.199 (6)	C9—C10	1.563 (7)
O5—C26	1.362 (6)	C10—C22	1.552 (7)
O5—C16	1.456 (6)	C11—C12	1.524 (7)
O6—C26	1.194 (6)	C12—C13	1.533 (7)
C1—C2	1.529 (7)	C13—C24	1.526 (7)
C1—C10	1.545 (7)	C13—C14	1.545 (6)
C2—C3	1.515 (8)	C14—C15	1.546 (7)
C3—C4	1.534 (8)	C15—C16	1.512 (7)
C4—C21	1.536 (8)	C16—C17	1.530 (7)
C4—C20	1.540 (8)	C17—C18	1.507 (7)
C4—C5	1.551 (7)	C17—C25	1.537 (7)
C5—C6	1.528 (7)	C18—C19	1.481 (8)
C5—C10	1.567 (7)	C26—C27	1.512 (8)

Table 3. *Least-squares planes and deviations from planarity (Å)*

Plane	O1, O2, C17, C25	
Equation	6.05 (2)X + 6.76 (3)Y + 7.21 (6)Z = 2.70 (2)	
Deviations	O1	−0.081 (2)
	O2	0.086 (2)
	C17	0.122 (3)
	C25	−0.127 (3)
	C24	0.316 (7)
Plane	O3, C17, C19, C25	
Equation	−7.29 (1)X − 5.00 (2)Y + 6.83 (10)Z = 3.26 (1)	
Deviations	O3	−0.043 (3)
	C17	0.023 (2)
	C19	0.027
	C25	−0.039
	C18	0.327

During refinement a number of reflections with large negative values of F_o^2 were omitted. These have been flagged with negative standard deviations in the table of observed and calculated structure factors (deposited). The absolute configuration could not be determined [Flack (1983) x parameter = 3.9 (2.7)]. Each H atom was included in a calculated position and allowed to ride on the atom to which it is attached; each H-atom displacement parameter was taken as 20% greater than that of the parent atom.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Data reduction: local program. Program(s) used to solve structure: *SHELXS*86 (Sheldrick, 1985). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnston, 1976).

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: TA1034). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Bis(2-biphenyl) Telluride

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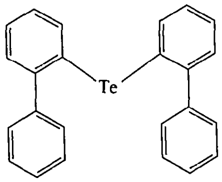
Abstract

The title compound, $C_{24}H_{18}Te$, consists of discrete molecules with the Te atom two-coordinate, Te—C 2.105 (5) and 2.125 (5) Å, and angle C—Te—C 96.2 (2)°. The biphenyl residues have their phenyl rings steeply inclined to each other, with dihedral angles of 66.5 (2) and 74.3 (3)°. The inter-ring bond lengths are 1.497 (7) and 1.480 (8) Å.

Comment

The crystal structure of the title compound, (I), has been determined as part of an ongoing study of organotellurium complexes. It was obtained as a by-product of a reaction involving dibenzotellurophene. We consider it probable that it was formed as an impurity in the preparation of dibenzotellurophene by the method of McCullough (1975).



(I)

The Te atom is bonded to two C atoms; the distances Te—C6 2.105 (5) and Te—C6′ 2.125 (5) Å (see Fig. 1) are in good agreement with the sum of the corresponding covalent radii (2.11 Å; Pauling, 1960) and with the mean value for Te—C(aromatic) bonds of 2.116 Å given by Allen, Watson, Brammer, Orpen & Taylor (1987). The valence angle at the Te atom is 96.2 (2)°. In the crystal structures of the analogous Te^{II} complexes *p*-ethoxyphenyl 2-(2-pyridyl)phenyl telluride (Al-Salim, West, McWhinnie & Hamor, 1988) and bis{2-[(4-methoxyphenyl)iminomethyl]phenyl} telluride (Sadekov *et al.*, 1989), the Te—C distances are slightly longer (range 2.128–2.162 Å) but the angles at the Te atom are quite similar (94.8 and 96.2°, respectively). An early analysis of bis(*p*-tolyl) telluride (Blackmore & Abrahams, 1955) based on only a partial data set yielded Te—C 2.04 and 2.06 Å, and C—Te—C 102°. The phenyl rings of the biphenyl residues are accurately planar (maximum atomic deviation of 0.012 Å). The interplanar angles are 66.5 (2) and 74.3 (3)° for the unprimed and primed residues, respectively (see Fig. 1), with corresponding inter-ring bond lengths of 1.497 (7) and 1.480 (8) Å. These values are typical of the inter-ring lengths in biphenyls, which appear to be insensitive to the inter-ring angle (Hamor & Hamor, 1980, and references therein).

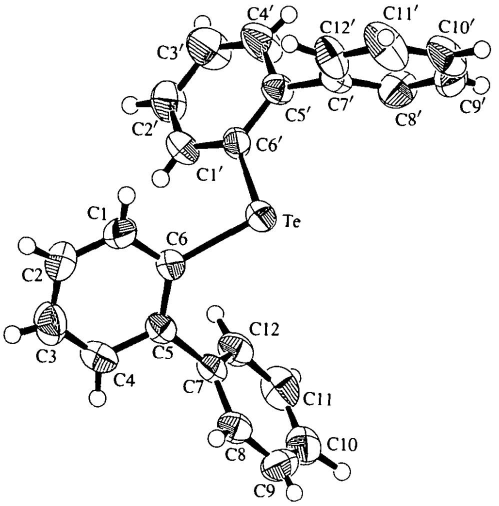


Fig. 1. The molecular structure showing 50% probability displacement ellipsoids.

Experimental

The compound arose as a by-product of the synthesis of dibenzotellurophene (McCullogh, 1975) and was crystallized from *n*-pentane.

Crystal data

$C_{24}H_{18}Te$
$M_r = 434.0$
Monoclinic
$P2_1/c$
$a = 7.784\ (3)$ Å
$b = 20.606\ (5)$ Å
$c = 11.705\ (3)$ Å
$\beta = 93.92\ (4)°$
$V = 1873.1$ Å^3
$Z = 4$
$D_x = 1.539$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9–15°$
$\mu = 1.642$ mm^{-1}
$T = 293$ K
Irregular
0.4 × 0.25 × 0.20 mm
Yellow

Data collection

CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: none
5671 measured reflections
2715 independent reflections
1828 observed reflections $[F > 4\sigma(F)]$

$R_{\text{int}} = 0.053$
$\theta_{\max} = 25°$
$h = 0 \rightarrow 9$
$k = -24 \rightarrow 24$
$l = -13 \rightarrow 13$
3 standard reflections
frequency: 120 min
intensity decay: 1.3%

Refinement

Refinement on F^2
$R(F) = 0.035$
$wR(F^2) = 0.090$
$S = 1.045$
2715 reflections
298 parameters
H atoms refined isotropically
$w = 1/[\sigma^2(F^2) + (0.0276P)^2 + 1.61P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.02$
$\Delta\rho_{\max} = 0.51$ e Å^{-3}
$\Delta\rho_{\min} = -0.71$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from *International Tables for Crystallography* (1992, Vol. C)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$$U_{\text{eq}} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Te	0.20407 (5)	0.02136 (2)	0.17617 (4)	0.054 (1)
C1′	0.4115 (8)	0.1265 (3)	0.3154 (6)	0.054 (2)
C1	0.5780 (8)	−0.0100 (3)	0.1621 (7)	0.058 (2)
C2′	0.4489 (9)	0.1867 (3)	0.3574 (6)	0.063 (2)
C2	0.7326 (8)	−0.0387 (3)	0.1850 (6)	0.059 (2)

C3′	0.3459 (11)	0.2374 (4)	0.3239 (8)	0.084 (3)
C3	0.7526 (9)	−0.0830 (3)	0.2699 (7)	0.065 (2)
C4′	0.2078 (11)	0.2280 (4)	0.2495 (8)	0.076 (2)
C4	0.6209 (8)	−0.0979 (3)	0.3351 (6)	0.054 (2)
C5′	0.1640 (7)	0.1669 (3)	0.2047 (5)	0.045 (2)
C5	0.4607 (6)	−0.0685 (2)	0.3150 (5)	0.039 (1)
C6′	0.2708 (6)	0.1152 (2)	0.2402 (5)	0.041 (1)
C6	0.4404 (6)	−0.0231 (3)	0.2272 (5)	0.044 (1)
C7′	0.0123 (8)	0.1593 (2)	0.1224 (6)	0.044 (2)
C7	0.3197 (7)	−0.0882 (2)	0.3885 (5)	0.041 (1)
C8′	−0.1531 (10)	0.1624 (3)	0.1569 (7)	0.064 (2)
C8	0.2566 (8)	−0.1505 (3)	0.3854 (5)	0.046 (2)
C9′	−0.2904 (11)	0.1586 (4)	0.0799 (9)	0.070 (2)
C9	0.1301 (9)	−0.1695 (4)	0.4542 (6)	0.059 (2)
C10′	−0.2728 (11)	0.1505 (3)	−0.0328 (8)	0.065 (2)
C10	0.0653 (9)	−0.1264 (4)	0.5289 (6)	0.062 (2)
C11′	−0.1116 (11)	0.1471 (4)	−0.0689 (8)	0.073 (2)
C11	0.1288 (10)	−0.0653 (4)	0.5341 (6)	0.066 (2)
C12′	0.0294 (9)	0.1513 (3)	0.0084 (6)	0.060 (2)
C12	0.2545 (8)	−0.0451 (3)	0.4660 (5)	0.050 (2)

Table 2. *Selected geometric parameters (Å, °)*

Te—C6	2.105 (5)	C5—C6	1.390 (7)
Te—C6′	2.125 (5)	C5—C7	1.497 (7)
C1′—C2′	1.359 (9)	C7′—C12′	1.360 (8)
C1′—C6′	1.377 (8)	C7′—C8′	1.377 (9)
C1—C2	1.352 (9)	C7—C8	1.374 (7)
C1—C6	1.383 (8)	C7—C12	1.391 (7)
C2′—C3′	1.358 (10)	C8′—C9′	1.352 (11)
C2—C3	1.350 (10)	C8—C9	1.370 (9)
C3′—C4′	1.351 (11)	C9′—C10′	1.347 (11)
C3—C4	1.355 (9)	C9—C10	1.367 (10)
C4′—C5′	1.397 (9)	C10′—C11′	1.353 (11)
C4—C5	1.392 (8)	C10—C11	1.352 (10)
C5′—C6′	1.397 (7)	C11′—C12′	1.376 (10)
C5′—C7′	1.480 (8)	C11—C12	1.368 (9)
C6—Te—C6′	96.2 (2)	C1—C6—Te	117.0 (5)
C2′—C1′—C6′	121.7 (6)	C5—C6—Te	123.7 (4)
C2—C1—C6	121.2 (7)	C12′—C7′—C8′	116.7 (6)
C3′—C2′—C1′	119.4 (7)	C12′—C7′—C5′	121.6 (5)
C3—C2—C1	119.9 (7)	C8′—C7′—C5′	121.6 (6)
C4′—C3′—C2′	120.3 (7)	C8—C7—C12	118.0 (5)
C2—C3—C4	121.0 (7)	C8—C7—C5	120.9 (5)
C3′—C4′—C5′	122.3 (7)	C12—C7—C5	121.0 (5)
C3—C4—C5	120.6 (6)	C9′—C8′—C7′	120.9 (7)
C4′—C5′—C6′	116.8 (6)	C9—C8—C7	121.3 (6)
C4′—C5′—C7′	120.2 (5)	C10′—C9′—C8′	122.1 (9)
C6′—C5′—C7′	123.0 (5)	C10—C9—C8	120.2 (7)
C6—C5—C4	118.3 (5)	C9′—C10′—C11′	118.1 (8)
C6—C5—C7	123.8 (4)	C11—C10—C9	119.0 (6)
C4—C5—C7	117.9 (5)	C10′—C11′—C12′	120.4 (8)
C1′—C6′—C5′	119.5 (5)	C10—C11—C12	122.1 (6)
C1′—C6′—Te	122.9 (4)	C7′—C12′—C11′	121.7 (7)
C5′—C6′—Te	117.6 (4)	C11—C12—C7	119.5 (6)
C1—C6—C5	119.0 (5)		

The structure was determined by direct methods and refined by least squares with anisotropic displacement parameters for the non-H atoms. All H atoms were located from difference Fourier syntheses and were refined isotropically.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989). Cell refinement: *CAD*-4 *Software*. Program(s) used to solve structure: *TEXSAN* (Molecular Structure Corporation, 1993). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CF1026). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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7-(2′-Deoxy-α-D-ribofuranosyl)hypoxanthine

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Abstract

The α-configured N7 analogue of 2′-deoxyinosine [7-(2′-deoxy-α-D-ribofuranosyl)hypoxanthine, $C_{10}H_{12}N_4O_4$] shows the following structural characteristics: (i) the furanose part of the molecule adopts the 2′-*endo* conformation [pseudorotation phase angle 166.4 (2)°]; (ii) the torsion angle χ (O4′—C1′—N7—C5) is *syn* [70.9 (1)°] with the base substituent pointing away from the sugar unit; (iii) the nucleobases are not hydrogen bonded to each other; only sugar-base hydrogen bonds between adjacent molecules were detected.