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Structure of 3-Iodo-2,5-diphenyltellurophene, $C_{16}H_{11}ITe$

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Abstract. $C_{16}H_{11}ITe$, $M_r = 457.74$, orthorhombic, $Pbca$, $a = 8.588\,(1)$, $b = 24.280\,(3)$, $c = 13.992\,(2)$ Å, $V = 2918\,(1)$ Å^3, $Z = 8$, $D_x = 2.084$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 41.18$ mm^{-1}, $F(000) = 1696$, $T = 298$ K, $R = 0.043$ for 1617 observed reflections. The heterocyclic ring is essentially planar making dihedral angles of 126.0 (2) and 29.2 (5)° with the phenyl rings. Distances and angle around the Te atom are: Te—C 2.077 (9), 2.070 (9) Å and C—Te—C 82.7 (4)°.

Experimental. The data collection and refinement parameters are summarized in Table 1. The structure was solved using standard direct methods and difference Fourier techniques. In the final cycles of full-matrix least-squares refinement on F all non-H atoms were treated anisotropically; the H atoms were included, as fixed contributors, at positions found in a difference Fourier synthesis, all with a common isotropic temperature factor that refined to $U = 0.07\,(1)$ Å^2. Data were corrected for Lp and absorption, with maximum and minimum transmission factors of 1.59 and 0.84 (Walker & Stuart, 1983). Scattering factors for non-H atoms were taken from Cromer & Mann (1968) with corrections for anomalous dispersion taken from Cromer & Liberman (1970); for H atoms from Stewart, Davidson & Simpson (1965). Programs used: *SHELX*76 (Sheldrick, 1976) and *ORTEP* (Johnson, 1965). Most of the calculations were performed on a VAX 4620 computer of the Instituto de Física e Química de São Carlos.

Atomic coordinates are listed in Table 2,* bond lengths and bond angles are listed in Table 3. Fig. 1

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* Lists of H-atom positions, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54698 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0110]

Table 1. *Crystallographic summary*

Data collection[i,ii]	
Mode	ω–2θ
Scan rate (° min^{-1})	2.8–10.0
θ range (°)	0–28
Range of *hkl*	$-2\le h\le 11$, $0\le k\le 31$, $0\le l\le 18$
Total reflections measured	3611
Unique reflections	2919
$R_{\rm int}$	0.030
Approximate crystal dimensions (mm)	0.18 × 0.13 × 0.03
Structure determination[iii]	
Reflections used $[I > 3\sigma(I)]$[iv]	1617
No. of variables	164
R, *wR*	0.043, 0.041
Maximum shift/e.s.d.	0.001
Maximum, minimum density in final difference map (e Å^{-3})	0.98[v], −0.91
S	1.39

Notes: (i) Unit-cell parameters by least-squares refinement of the setting angles of 24 reflections with $10 < \theta < 21°$. (ii) Enraf–Nonius CAD-4 diffractometer with graphite monochromator. One standard reflection measured every hour showed no significant variation. (iii) Function minimized $\sum w(|F_o| - |F_c|)^2$, where $w^{-1} = [\sigma^2(F_o) + 0.0003F_o^2]$. (iv) Two reflections were excluded: $1,\bar{29},1$ and $\bar{3},25,\bar{2}$. (v) Less than 1 Å from the Te atom.

Table 2. *Final atomic coordinates and equivalent isotropic temperature factors* (Å^2)

$$B_{\rm eq} = (4/3)\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
Te	0.1525 (1)	0.4397 (1)	0.5401 (1)	3.64 (3)
I	0.4354 (1)	0.4245 (1)	0.2345 (1)	4.12 (3)
C(2)	0.260 (1)	0.4648 (4)	0.4145 (6)	2.6 (3)
C(3)	0.305 (1)	0.4203 (4)	0.3656 (6)	2.5 (3)
C(4)	0.284 (1)	0.3655 (4)	0.4050 (7)	2.8 (4)
C(5)	0.213 (1)	0.3622 (4)	0.4908 (6)	2.4 (3)
C(6)	0.281 (1)	0.5239 (4)	0.3946 (6)	2.4 (3)
C(7)	0.349 (2)	0.5575 (5)	0.4636 (8)	4.5 (4)
C(8)	0.371 (2)	0.6136 (5)	0.4466 (9)	4.5 (5)
C(9)	0.321 (2)	0.6353 (4)	0.361 (1)	4.9 (5)
C(10)	0.252 (2)	0.6033 (5)	0.2934 (8)	4.6 (5)
C(11)	0.232 (1)	0.5478 (4)	0.3098 (7)	3.2 (4)
C(12)	0.194 (1)	0.3115 (4)	0.5493 (7)	3.5 (4)
C(13)	0.294 (1)	0.2681 (5)	0.5410 (7)	3.9 (4)
C(14)	0.283 (2)	0.2225 (5)	0.5983 (9)	5.1 (5)
C(15)	0.161 (2)	0.2180 (5)	0.6641 (9)	5.3 (5)
C(16)	0.060 (2)	0.2609 (5)	0.6738 (8)	4.7 (5)
C(17)	0.075 (2)	0.3089 (4)	0.6173 (7)	4.1 (4)

is a projection of the molecule showing the atom numbering.

Related literature. The heterocyclic ring is essentially planar [$\sigma_{\rm av}$, defined as $(\sum_i d_i^2/N-3)^{1/2}$, is 0.03 Å], making dihedral angles of 126.0 (2) and 29.2 (5)° with the C(6)—C(11) and C(12)—C(17) phenyl rings, respectively. For an extensive review of the structural chemistry of compounds containing tellurophene rings see Hargittai & Rozsondai (1986).

Table 3. *Interatomic distances* (Å) *and angles* (°)

Te—C(2)	2.077 (9)	Te—C(5)	2.070 (9)
I—C(3)	2.108 (9)	C(2)—C(3)	1.34 (1)
C(2)—C(6)	1.47 (1)	C(3)—C(4)	1.45 (1)
C(4)—C(5)	1.35 (1)	C(5)—C(12)	1.49 (1)
C(6)—C(7)	1.39 (1)	C(6)—C(11)	1.39 (1)
C(7)—C(8)	1.40 (2)	C(8)—C(9)	1.38 (2)
C(9)—C(10)	1.36 (2)	C(10)—C(11)	1.38 (2)
C(12)—C(13)	1.36 (2)	C(12)—C(17)	1.40 (2)
C(13)—C(14)	1.37 (2)	C(14)—C(15)	1.40 (2)
C(15)—C(16)	1.36 (2)	C(16)—C(17)	1.41 (2)
C(2)—Te—C(5)	82.7 (4)	Te—C(2)—C(3)	108.9 (7)
Te—C(2)—C(6)	120.0 (7)	C(3)—C(2)—C(6)	131.0 (9)
I—C(3)—C(2)	123.3 (7)	I—C(3)—C(4)	115.8 (6)
C(2)—C(3)—C(4)	120.7 (9)	C(3)—C(4)—C(5)	116.7 (9)
Te—C(5)—C(4)	110.9 (7)	Te—C(5)—C(12)	122.8 (7)
C(4)—C(5)—C(12)	126.1 (9)	C(2)—C(6)—C(7)	119.4 (9)
C(2)—C(6)—C(11)	122.2 (9)	C(7)—C(6)—C(11)	118.4 (9)
C(6)—C(7)—C(8)	121 (1)	C(7)—C(8)—C(9)	119 (1)
C(8)—C(9)—C(10)	121 (1)	C(9)—C(10)—C(11)	120 (1)
C(6)—C(11)—C(10)	121 (1)	C(5)—C(12)—C(13)	122 (1)
C(5)—C(12)—C(17)	119.5 (9)	C(13)—C(12)—C(17)	119 (1)
C(12)—C(13)—C(14)	122 (1)	C(13)—C(14)—C(15)	120 (1)
C(14)—C(15)—C(16)	119 (1)	C(15)—C(16)—C(17)	121 (1)
C(12)—C(17)—C(16)	119 (1)		

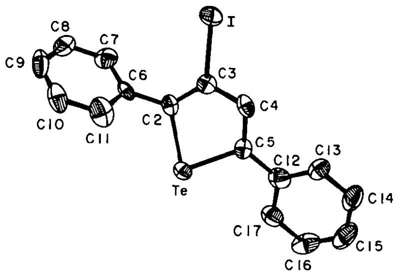

Fig. 1. Perspective view of the molecule showing the atom numbering. Thermal ellipsoids are drawn at the 50% probability level.

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