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{4-[1-(4-Hydroxyphenyl)-1-methylethyl]-phenoxy}trimethyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 233 K
Mean σ(C–C) = 0.003 Å
R factor = 0.018
wR factor = 0.045
Data-to-parameter ratio = 18.5

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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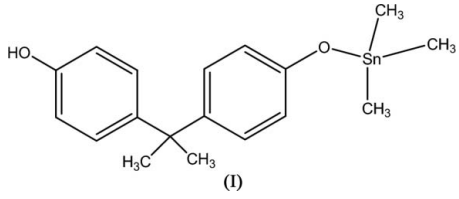
The crystal structure of the title compound, $[Sn(CH_3)_3(C_{15}H_{15}O_2)]$, is composed of polymeric chains of monomers, linked by secondary coordinating bonds from the O atoms of the hydroxyl group to the Sn atoms, with an Sn···O distance of 2.646 (2) Å. This additional bond leads to a distorted trigonal–bipyramidal geometry around the Sn atom, with three methyl C atoms in equatorial and two O atoms in axial positions.

Comment

Organotin compounds are of current interest due to the dramatic increase of their industrial, agricultural and biological applications (Xie *et al.*, 1996; Nath *et al.*, 2001). Numerous organotin compounds which exhibit a variety of biological properties have been synthesized and described in the literature (Magoś, 1986; Ronconi *et al.*, 2002). Several organotin compounds have been shown to exhibit important cytotoxic effects and are actively investigated as possible antitumour compounds (Penninks, 1990; Crowe, 1987).



(I)

Domingos & Sheldrick (1974) and Reuter & Schröder (1993) previously synthesized and characterized organotin alkoxides. We report here the structure of the title compound, (I). Fig. 1 shows the monomeric unit of the coordination polymer with four covalent bonds around the Sn atom (Table 1). By secondary coordination of the Sn atoms by the O atoms of neighbouring hydroxyl groups, a polymeric chain is generated with an Sn···O distance of 2.646 (2) Å. This is considerably shorter than the sum of the van der Waals radii of the two atoms (3.7 Å; Huheey *et al.*, 1993) and leads to a distorted trigonal–bipyramidal geometry around the Sn atom.

The polymeric chain is oriented along the [102] direction. These chains are crosslinked by chains along the $[\bar{1}02]$ direction *via* O—H···O intermolecular hydrogen bonds (Table 2 and Fig. 2).

Experimental

The title compound, (I), was prepared by the reaction of the monopotassium salt of bisphenol (1.0 g, 3.29 mmol) with trimethyltin chloride (0.65 g, 3.29 mmol) in dry methanol (60 ml). The reaction

mixture was refluxed for 6 h in a two-necked round-bottomed flask (250 ml), fitted with a magnetic stirrer and water condenser. It was allowed to stand overnight at room temperature. The resulting potassium chloride was removed by filtration and the solvent was evaporated at room temperature by slow evaporation, which resulted in plate-shaped colourless crystals (yield 1.31 g, 85%; m.p. 397 K).

Crystal data

$[Sn(CH_3)_3(C_{15}H_{15}O_2)]$
M_r = 391.06
Orthorhombic, $Pna2_1$
a = 12.6228 (3) Å
b = 13.0820 (3) Å
c = 10.7032 (2) Å
V = 1767.44 (7) Å^3
Z = 4
D_x = 1.470 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 12075 reflections
θ = 1.0–27.5°
μ = 1.45 mm^{-1}
T = 233 (2) K
Plate, colourless
0.35 × 0.35 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.663, T_{max} = 0.844
18702 measured reflections
3667 independent reflections
3566 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -16 \rightarrow 16$
$l = -11 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.045
S = 1.05
3667 reflections
198 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0225P)^2 + 0.5157P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.041
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0081 (4)
Absolute structure: Flack (1983), with 1537 Friedel pairs
Flack parameter: −0.042 (17)

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.094 (2)	Sn1—O2^{i}	2.646 (2)
Sn1—C1	2.117 (2)	O1—C10	1.366 (3)
Sn1—C2	2.120 (2)	O2—C16	1.380 (3)
Sn1—C3	2.115 (3)		
O1—Sn1—O2^{i}	174.6 (1)	C2—Sn1—O2^{i}	86.1 (1)
O1—Sn1—C1	92.6 (1)	C3—Sn1—O2^{i}	80.4 (1)
O1—Sn1—C2	99.2 (1)	C1—Sn1—C2	117.5 (1)
O1—Sn1—C3	97.6 (1)	C1—Sn1—C3	120.6 (1)
C1—Sn1—O2^{i}	84.1 (1)	C2—Sn1—C3	118.1 (1)

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+1$.

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2O···O1^{ii}	0.78 (2)	1.83 (3)	2.6234 (2)	174 (3)

Symmetry code: (ii) $\frac{1}{2}-x, -\frac{1}{2}+y, -\frac{1}{2}+z$.

The hydroxyl H atom was located in a difference map and refined isotropically with O—H restrained to 0.80 (2) Å. The remaining H atoms were positioned with C—H = 0.94 and 0.97 Å for methine and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

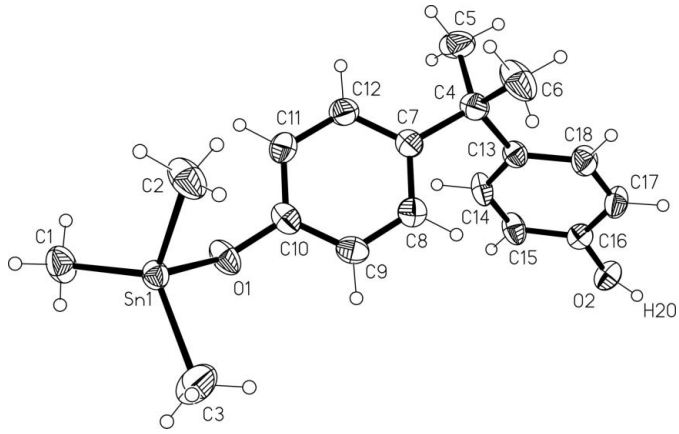


Figure 1
A view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

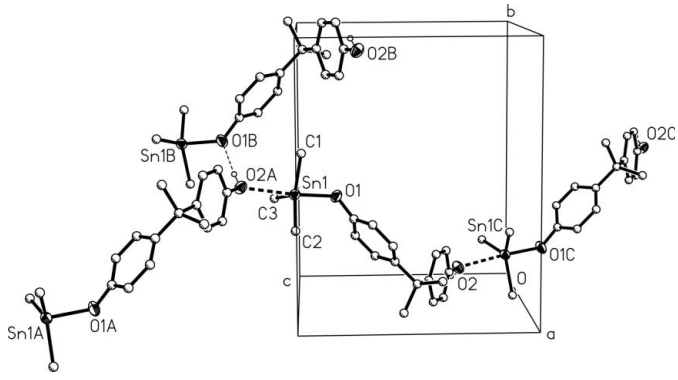


Figure 2
Packing diagram of (I). Hydrogen bonds and coordinating bonds are shown as dashed lines. H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry codes: (A) $\frac{1}{2}+x, \frac{1}{2}-y, 1+z$; (B) $1-x, 1-y, \frac{1}{2}+z$; (C) $-\frac{1}{2}+x, \frac{1}{2}-y, -1+z$.]

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997), *SCALEPACK* and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXL97*.

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