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Bis(4-methoxylbenzoato)phenyl(trimethylsilylmethyl)tin(IV)

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Key indicators

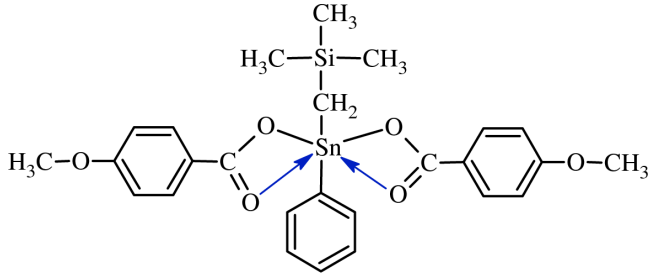
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.030
wR factor = 0.091
Data-to-parameter ratio = 17.0

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

The title compound, $[Sn(C_6H_5)(C_8H_7O_3)_2(C_4H_{11}Si)]$, was prepared by the reaction of $[(CH_3)_3SiCH_2]SnPhBr_2$ with $CH_3OC_6H_5COOH$ and spasmolytol in refluxing toluene, and characterized by IR, ^1H NMR and elemental analyses. The geometry at the six-coordinate Sn^{IV} atom is distorted octahedral with the equatorial plane made up of four O atoms of two carboxylate groups and the axial positions occupied by a phenyl substituent and a trimethylsilylmethyl group.

Comment

There is considerable interest in organotin complexes as a result of their striking antitumour activities and their structural variety (Zhou *et al.*, 2000). It has been shown that the biological activity of diorganotin compounds depends mainly on the alkyl groups and the ligands (Gielen, 1996; Yang *et al.*, 1996; Fang *et al.*, 2001). Trimethylsilylmethyl compounds also show a wide range of biological activities (Xie & Liu, 1998). To link the biological activities of organotin and organosilicon compounds, the title compound, (I), was synthesized and its crystal structure is reported here.



(I)

The molecular structure of (I) is shown in Fig. 1, while selected geometric parameters are given in Table 1. The geometry at the six-coordinate Sn^{IV} atom is distorted octahedral, with a roughly planar equatorial belt made up of atoms O1, O2, O4 and O5, and with atoms C17 of the phenyl ring and C23 of the trimethylsilylmethyl group in the axial positions. The bidentate carboxylate coordination is quite common for organotin complexes (Baul *et al.*, 2004, 2005). The two carboxylate groups act as *cis*-bidentate chelating agents, giving an equatorial plane around the Sn^{IV} atom formed by four asymmetrically coordinated O atoms.

The two chelate four-membered rings are coplanar, the maximum deviation from the least-squares plane through atoms Sn1, O1, O2, O4, O5, C1 and C9 being 0.025 (2) Å for atom C1. In each carboxylate group, the two chelate Sn—O

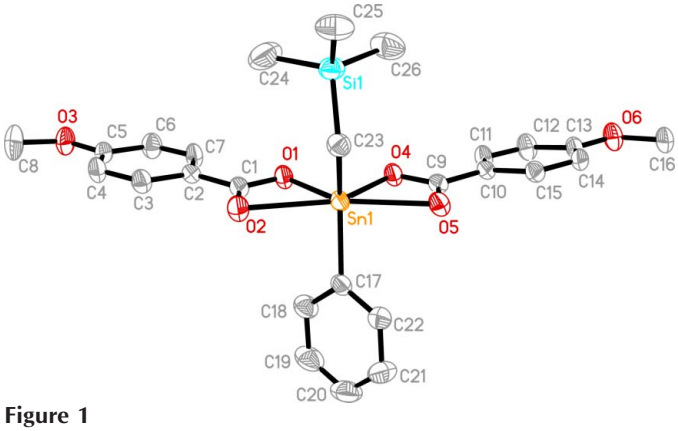


Figure 1
The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

bonds are different; one is much longer then the other. The carboxylate O atoms coordinate strongly to the Sn^{IV} atom [Sn—O = 2.1021 (18) Å and 2.1109 (18) Å], while the carbonyl O atoms are much more weakly bound to the Sn^{IV} atom [Sn—O = 2.5328 (19) Å and 2.473 (2) Å]. These values are in excellent agreement with those reported for dibutyltin(IV) complexes by Baul *et al.* (2004).

The O1—Sn1—O4 angle is 83.88 (7)° while the O5—Sn1—O2 angle is 164.03 (6)°, thereby leaving one side of the Sn atom quite open to combine with the two axial ligands, with a C23—Sn1—C17 angle of 136.08 (12).

The two carboxylate ligands are almost coplanar, the dihedral angle between the two benzene planes being 11.4 (2)°. The dihedral angles between the plane of the axial phenyl ring and the two equatorial benzene rings are 84.60 (11) and 85.79 (10)°.

No significant hydrogen-bonding interaction is observed in the crystal packing, except for a weak C16—H16*B*···O1^{i} [symmetry code: (i) $-x, \frac{1}{2}+y, \frac{3}{2}-z$] interaction, with a C16···O1^{i} distance of 3.492 (4) Å.

Experimental

$[(CH_3)_3SiCH_2]SnPhBr_2$ (1.77 g), *p*-$CH_3OC_6H_4COOH$ (1.22 g) and spasmolytol (0.81 g) were mixed in toluene (40 ml) and refluxed for several hours. The solvent was then removed, and the residue was recrystallized from toluene (yield 85%, m.p. 410.5 K). Analysis calculated for $C_{26}H_{30}O_6SnSi$: C 53.35, H 5.17%; found: C 53.67, H 5.31%. IR (cm^{-1}, group): 1601, 1352 (C═O carboxylate form), 1257 (SiC—H), 839, 731 (Si—C), 609, 517 (Sn—C), 445 (Sn—O); ^{1}H NMR ($CDCl_3$, p.p.m.): δ 0.152 (*s*, CH_3Si), 0.997 (*s*, $SiCH_2Sn$), 7.407∼7.770 (*m*, Ph), 3.898 (*s*, OCH_3), 6.967 and 8.157 (*d*, Ar).

Crystal data

$[Sn(C_6H_5)(C_8H_7O_3)_2(C_4H_{11}Si)]$	D_x = 1.426 Mg m^{-3}
M_r = 585.28	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6030 reflections
a = 20.1618 (4) Å	θ = 2.5–25.2°
b = 11.9426 (3) Å	μ = 1.02 mm^{-1}
c = 11.3334 (2) Å	T = 273 (2) K
β = 92.080 (1)°	Block, colourless
V = 2727.11 (10) Å^3	0.28 × 0.28 × 0.27 mm
Z = 4	

Data collection

Bruker APEX-II CCD area-detector diffractometer	4235 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.041
Absorption correction: none	θ_{max} = 26.0°
26 340 measured reflections	$h = -24 \rightarrow 24$
5315 independent reflections	$k = -14 \rightarrow 14$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.030	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.091	$(\Delta/\sigma)_{max}$ = 0.003
S = 1.01	$\Delta\rho_{max}$ = 0.95 e Å^{-3}
5315 reflections	$\Delta\rho_{min}$ = −0.60 e Å^{-3}
312 parameters	

Table 1
Selected geometric parameters (Å, °).

C17—Sn1	2.114 (3)	O2—Sn1	2.5328 (19)
C23—Sn1	2.103 (3)	O4—Sn1	2.1109 (18)
O1—Sn1	2.1021 (18)	O5—Sn1	2.473 (2)
C1—O1—Sn1	101.19 (16)	O1—Sn1—O5	140.36 (7)
C1—O2—Sn1	83.27 (16)	C23—Sn1—O5	86.29 (10)
C9—O4—Sn1	99.83 (16)	O4—Sn1—O5	56.49 (7)
C9—O5—Sn1	84.55 (16)	C17—Sn1—O5	88.09 (9)
O1—Sn1—C23	109.23 (10)	O1—Sn1—O2	55.60 (6)
O1—Sn1—O4	83.88 (7)	C23—Sn1—O2	86.07 (10)
C23—Sn1—O4	109.98 (10)	O4—Sn1—O2	139.47 (7)
O1—Sn1—C17	102.57 (10)	C17—Sn1—O2	87.71 (9)
C23—Sn1—C17	136.08 (12)	O5—Sn1—O2	164.03 (6)
O4—Sn1—C17	102.69 (9)		

The H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.93 (aromatic), 0.97 (methylene) and 0.96 Å (methyl), and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C) for other H atoms.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *APEX2*; program(s) used to refine structure: *APEX2*; molecular graphics: *APEX2*; software used to prepare material for publication: *APEX2*.

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