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# Bis(4-nitrobenzoato)bis(trimethylsilylmethyl)tin(IV)

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**Key indicators**

Single-crystal X-ray study
*T* = 296 K
Mean σ(C–C) = 0.003 Å
*R* factor = 0.025
*wR* factor = 0.069
Data-to-parameter ratio = 19.3

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



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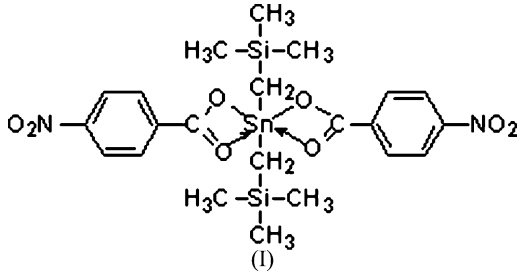
In the structure of the title compound, $[Sn(C_7H_4N_2O_3)_2(C_4H_{11}Si)_2]$, the geometry at the six-coordinate Sn atom is distorted octahedral with an approximately planar equatorial belt made up of the four O atoms of two carboxylate groups and the axial positions occupied by two trimethylsilylmethyl groups.

## Comment

Many methods have been developed to decrease the toxicity of organotin compounds, and organosilicon ligands have been shown to be effective (Xie & Liu, 1998). Research has shown that the biological activity of diorganotin compounds depends mainly on the alkyl groups and the ligands (Gielen, 1996; Yang *et al.*, 1996). The structure of the title compound, (I), is analogous to that of bis(4-methoxylbenzoato)phenyl-(trimethylsilylmethyl)tin(IV) which we have reported previously (Lin *et al.*, 2005).




(I)

The carboxylate groups act as asymmetric chelating groups. In each carboxylate group, one Sn—O bond is much longer then the other. The carboxylate O atoms coordinate strongly to the Sn atom [Sn—O = 2.0862 (14) and 2.1001 (13) Å] while the carbonyl O atoms are much more weakly bound [Sn—O = 2.6874 (16) and 2.5537 (17) Å]. All Sn—O distances are within expected ranges.

The angle between the two strongly bound *cis*-O atoms, O1—Sn1—O3, is 83.40 (5)°, while for the weakly bound O atoms O4—Sn1—O2 is 167.75 (5)°, leaving one side of the Sn atom open to bind the two axial ligands [C15—Sn1—C16 = 136.49 (8)°]. There are no classical hydrogen bonds in the crystal structure.

## Experimental

$[(CH_3)_3SiCH_2]_2SnCl_2$ (1.46 g), *p*-$N_2O_1C_6H_4COOH$ (1.33 g) and triethylamine (0.81 g) were mixed in 40 ml toluene and heated for several hours under reflux. The solvent was removed and the residue recrystallized from toluene. Single crystals suitable for X-ray diffraction analysis precipitated after several days (m.p. 411.5 K).

*Crystal data*

| | |
|---|---|
| $[Sn(C_7H_4N_2O_3)_2(C_4H_{11}Si)_2]$ | $D_x$ = 1.442 Mg m$^{-3}$ |
| $M_r$ = 625.35 | Mo $K\alpha$ radiation |
| Monoclinic, $P2_1/n$ | Cell parameters from 5648 reflections |
| $a$ = 12.2840 (6) Å | $\theta$ = 2.3–25.2° |
| $b$ = 13.2343 (7) Å | $\mu$ = 1.01 mm$^{-1}$ |
| $c$ = 18.0000 (9) Å | $T$ = 296 (2) K |
| $\beta$ = 100.056 (1)° | Block, colourless |
| $V$ = 2881.3 (3) Å$^3$ | 0.46 × 0.40 × 0.30 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 5138 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int}$ = 0.021 |
| Absorption correction: none | $\theta_{max}$ = 27.0° |
| 19783 measured reflections | $h = -15 \rightarrow 15$ |
| 6218 independent reflections | $k = -16 \rightarrow 16$ |
| | $l = -22 \rightarrow 21$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | $w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.3107P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.025 | $(\Delta/\sigma)_{max}$ = 0.001 |
| $wR(F^2)$ = 0.069 | $\Delta\rho_{max}$ = 0.34 e Å$^{-3}$ |
| $S$ = 1.02 | $\Delta\rho_{min}$ = −0.41 e Å$^{-3}$ |
| 6218 reflections | |
| 322 parameters | |
| H-atom parameters constrained | |

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C15—Sn1 | 2.099 (2) | O2—Sn1 | 2.6874 (16) |
| C16—Sn1 | 2.102 (2) | O3—Sn1 | 2.1001 (13) |
| O1—Sn1 | 2.0862 (14) | O4—Sn1 | 2.5537 (17) |
| | | | |
| Si1—C15—Sn1 | 123.96 (12) | O3—Sn1—C16 | 102.32 (7) |
| Si2—C16—Sn1 | 120.14 (10) | O1—Sn1—O4 | 138.39 (5) |
| C1—O1—Sn1 | 106.18 (13) | C15—Sn1—O4 | 92.79 (9) |
| C1—O2—Sn1 | 79.35 (12) | O3—Sn1—O4 | 55.06 (5) |
| C8—O3—Sn1 | 102.42 (12) | C16—Sn1—O4 | 88.59 (7) |
| C8—O4—Sn1 | 82.32 (12) | O1—Sn1—O2 | 53.14 (5) |
| O1—Sn1—C15 | 103.20 (9) | C15—Sn1—O2 | 86.92 (8) |
| O1—Sn1—O3 | 83.40 (5) | O3—Sn1—O2 | 135.75 (5) |
| C15—Sn1—O3 | 113.87 (7) | C16—Sn1—O2 | 83.26 (7) |
| O1—Sn1—C16 | 104.21 (7) | O4—Sn1—O2 | 167.76 (5) |
| C15—Sn1—C16 | 136.49 (8) | | |

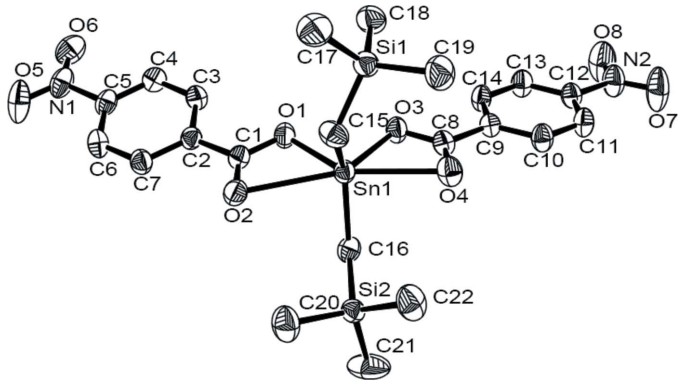



**Figure 1**
The molecular structure of title compound. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

H atoms were placed at calculated positions (C—H = 0.93–0.97 Å) and refined as riding, with $U_{iso}$(H) = 1.2 or 1.5 times $U_{eq}$(C).

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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