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[4-(2-Hydroxybenzylamino)benzoato-κO]-triphenyltin(IV)

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In the title compound, $[Sn(C_6H_5)_3(C_{14}H_{12}NO_3)]$, the coordination geometry around the Sn atom is slightly distorted tetrahedral, comprising three C atoms from three phenyl groups and one O atom from a 4-(2-hydroxybenzylamino)benzoate anion. The crystal packing involves inversion-generated pairs of molecules linked by two O—H···O hydrogen bonds.

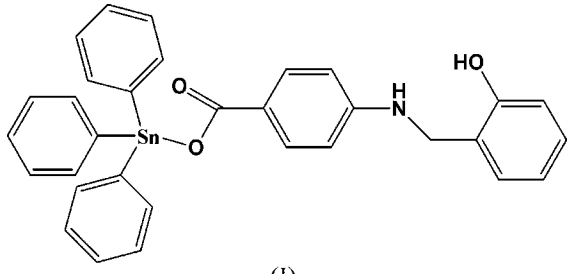
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.062
Data-to-parameter ratio = 20.3

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

Comment

Organotin(IV) carboxylates form an important class of compounds which find many applications in chemistry and biology, such as agricultural biocides, catalysts and stabilizers (Lockhart *et al.*, 1987; Teoh *et al.*, 1997; Basu *et al.*, 2005). To widen their scope of application there is a need to prepare further examples of these compounds. In this paper, the structure of the title compound, (I), is described.



(I)

As shown in Fig. 1, the coordination polyhedron around the Sn atom in (I) is a slightly distorted SnC_3O tetrahedron comprising three C atoms from three phenyl groups and one O atom from a 4-(2-hydroxybenzylamino)benzoate (L^-) anion. The Sn1—O1 distance in (I) is similar to those in related compounds (Rehman *et al.*, 2005). In addition, there is a weak Sn1···O2 interaction in (I) of 2.904 (3) Å, which is considerably shorter than the sum of the van derWaals radii of Sn and O atoms (3.68 Å; Bondi, 1964; Zhang *et al.*, 2006).

In the crystal structure, inversion-generated dimeric associations of molecules arise, bridged by two O—H···O hydrogen bonds (Fig. 1 and Table 2). However, the NH group does not participate in hydrogen bonding.

Experimental

A mixture of NaL (0.094 g, 0.4 mmol) and Ph_3SnCl (0.154 g, 0.4 mmol) in CH_2Cl_2 (25 ml) was stirred at room temperature for 12 h, and the resulting precipitated NaCl was removed by filtration. The solvent was removed *in vacuo*, and yellow plates of (I) were recrystallized from CH_2Cl_2–EtOH (3:1 *v*/*v*).

Crystal data

$[Sn(C_6H_5)_3(C_{14}H_{12}NO_3)]$
M_r = 592.24
Monoclinic, $P2_1/c$
a = 15.133 (5) Å
b = 10.119 (5) Å
c = 19.134 (5) Å
β = 111.889 (5)°
V = 2718.8 (18) Å^3
Z = 4
D_x = 1.447 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.97 mm^{-1}
T = 293 (2) K
Plate, yellow
0.40 × 0.31 × 0.09 mm

Data collection

Bruker APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.698, T_{max} = 0.918
16269 measured reflections
6405 independent reflections
4436 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.062
S = 0.91
6405 reflections
316 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0311P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.055 (2)	Sn1—C1	2.123 (2)
Sn1—C7	2.118 (2)	Sn1—C13	2.124 (2)
O1—Sn1—C7	109.35 (8)	O1—Sn1—C13	98.03 (8)
O1—Sn1—C1	113.42 (7)	C7—Sn1—C13	112.37 (9)
C7—Sn1—C1	110.87 (9)	C1—Sn1—C13	112.21 (9)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3*O*···O2^{i}	0.88 (2)	1.89 (2)	2.744 (2)	167 (3)

Symmetry code: (i) $-x, -y, -z+1$.

All C-bound H atoms were placed geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The imine and hydroxy H atoms were located in a difference map. Their positions were freely refined with U_{iso}(H) = 1.5U_{eq}(N,O); N—H = 0.85 (2) Å and O—H = 0.88 (2) Å.

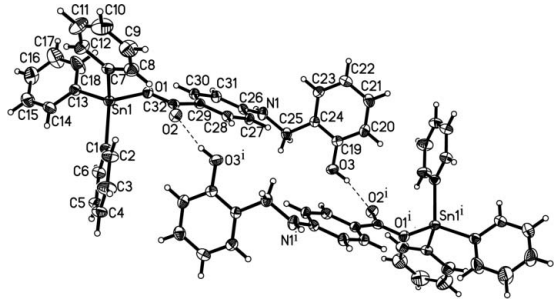


Figure 1
View of the dimeric association of molecules of (I). Displacement ellipsoids are drawn at the 30% probability level (arbitrary spheres for H atoms). Hydrogen bonds are indicated by dashed lines. [Symmetry code: (i) $-x, -y, 1-z$.]

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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References

Basu, B. T. S., Rynfah, W., Rivarola, E., Pettinari, C. & Linden, A. (2005). *J. Organomet. Chem.* **690**, 1413–1421.
Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.
Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
Lockhart, T. P., Calabrese, J. C. & Davidson, F. (1987). *Organometallics*, **6**, 2479–2483.
Rehman, S. U., Khadija, S., Saqib, A., Moazzam, H. B. & Masood, P. (2005). *J. Organomet. Chem.* **690**, 1396–1408.
Sheldrick, G. M. (1990). *SHELXTL-Plus.* Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Teoh, S. G., Ang, S. H., Looi, E. S., Leok, C. A., Teo, S. B. & Fun, H. K. (1997). *J. Organomet. Chem.* **527**, 15–19.
Zhang, W.-L., Ma, J.-F. & Jiang, H. (2006). *Acta Cryst.* E**62**, m460–m461.