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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.010$ Å
 R factor = 0.047
 wR factor = 0.105
Data-to-parameter ratio = 19.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

(4-Aminobenzoato)tris(2-methyl-2-phenylpropyl)tin(IV)

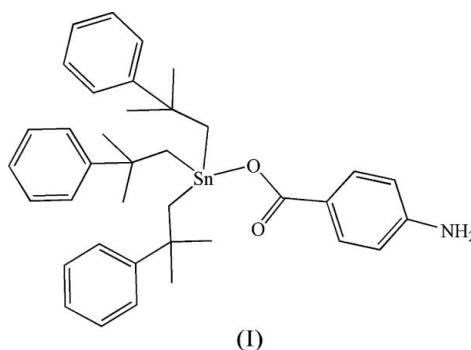
The title compound, $[\text{Sn}(\text{C}_{10}\text{H}_{13})_3(\text{C}_7\text{H}_6\text{NO}_2)]$, crystallizes with two independent molecules in the asymmetric unit. The Sn atom is four-coordinate and has a distorted SnC_3O tetrahedral geometry. $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds help to establish the crystal packing.

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Comment

Tris(2-methyl-2-phenylpropyl)tin carboxylates, $[(\text{C}_{10}\text{H}_{13})_3\text{Sn}(\text{O}_2\text{CR})]$, usually possess tetrahedrally coordinated Sn atoms and do not auto-associate into chain structures *via* carboxylate bridging, owing to the crowding of the three bulky organic groups at the Sn atom (Bao *et al.*, 1998; Bomfim *et al.*, 2002; Tian, Sun, Yang & Yang, 2005; Tian, Sun, Yang & Ng, 2005). In the title compound, (I), tetrahedral Sn coordination is also observed (Fig. 1). This compound crystallizes with two independent molecules in the asymmetric unit; they do not differ significantly from each other.



The $\text{Sn}1\cdots\text{O}2$ and $\text{Sn}1'\cdots\text{O}2'$ separations of 3.068 (4) and 3.122 (4) Å, respectively, indicate there are weak interactions between these atoms, which distort the tetrahedral SnOC_3 geometry. Otherwise, the bond dimensions around the Sn atoms (Table 1) are similar to those found in other reported tris(2-methyl-2-phenylpropyl)tin carboxylates, such as tris(2-methyl-2-phenylpropyl)tin phenoxyacetate (Bao *et al.*, 1998), acetate (Bomfim *et al.*, 2002), 3-pyridinecarboxylate (Tian, Sun, Yang & Yang, 2005) and bis[tris(2-methyl-2-phenylpropyl)tin(IV)] phthalate (Tian, Sun, Yang & Ng, 2005). The carboxylate C—O bond lengths indicate localization of the negative charges. The crystal packing for (I) is consolidated by two $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2).

Experimental

Bis[tris(2-phenyl-2-methylpropyl)tin] oxide (1.05 g, 1 mmol) and 4-aminobenzoic acid (0.27 g, 2 mmol) in benzene (50 ml) were refluxed for 4 h with azeotropic removal of water *via* a Dean–Stark

trap. The resulting clear solution was evaporated under reduced pressure. The white solid obtained was recrystallized from methanol and crystals of (I) were obtained from hexane–chloroform (1:1 v/v) by slow evaporation at 298 K (yield 72%, m.p. 362–363 K). Analysis found: C 68.04, H 6.79, N 2.17%; calculated for $C_{37}H_{45}NO_2Sn$: C 67.90, H 6.93, N 2.14%. IR (KBr disc): $\nu_{as}(\text{COO})$ 1641, $\nu_s(\text{COO})$ 1347 cm^{-1} .

Crystal data

$[\text{Sn}(\text{C}_{10}\text{H}_{13})_3(\text{C}_7\text{H}_6\text{NO}_2)]$
 $M_r = 654.43$
 Orthorhombic, $P2_12_12_1$
 $a = 13.165$ (1) Å
 $b = 13.4984$ (10) Å
 $c = 38.507$ (3) Å
 $V = 6842.9$ (9) Å³

$Z = 8$
 $D_x = 1.270$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.78$ mm⁻¹
 $T = 295$ (2) K
 Block, colorless
 $0.38 \times 0.35 \times 0.30$ mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{\min} = 0.757$, $T_{\max} = 0.800$

55565 measured reflections
 14187 independent reflections
 12378 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.032$
 $\theta_{\text{max}} = 26.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.105$
 $S = 1.16$
 14187 reflections
 739 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0374P)^2 + 4.2443P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.79$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.80$ e Å⁻³
 Absolute structure: Flack (1983), 6368 Friedel pairs
 Flack parameter: 0.02 (2)

Table 1

Selected geometric parameters (Å, °).

Sn1—O1	2.061 (3)	Sn1'—O1'	2.063 (3)
Sn1—C11	2.133 (6)	Sn1'—C21'	2.142 (5)
Sn1—C21	2.147 (5)	Sn1'—C1'	2.144 (6)
Sn1—C1	2.158 (5)	Sn1'—C11'	2.146 (5)
C31—O1	1.292 (6)	C31'—O1'	1.286 (6)
C31—O2	1.225 (6)	C31'—O2'	1.215 (6)
O1—Sn1—C11	109.6 (2)	O1'—Sn1'—C21'	93.01 (18)
O1—Sn1—C21	92.33 (18)	O1'—Sn1'—C1'	101.26 (18)
C11—Sn1—C21	115.4 (2)	C21'—Sn1'—C1'	115.9 (2)
O1—Sn1—C1	103.05 (18)	O1'—Sn1'—C11'	110.06 (19)
C11—Sn1—C1	116.8 (2)	C21'—Sn1'—C11'	115.6 (2)
C21—Sn1—C1	115.53 (19)	C1'—Sn1'—C11'	116.8 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1C ⁱ ⋯O2 ⁱ	0.86	2.09	2.932 (6)	168
N1'—H1C' ⁱ ⋯O2' ⁱⁱ	0.86	2.07	2.921 (7)	173

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

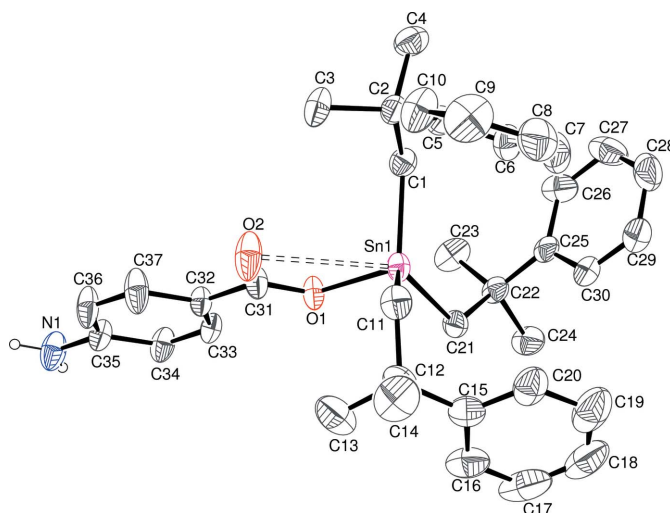


Figure 1

The structure of the Sn1 molecule in (I), showing 30% displacement ellipsoids (arbitrary spheres for the H atoms). The long Sn1⋯O2 interaction is shown by dashed lines. The structure of the Sn1' molecule is virtually identical.

H atoms were placed in calculated positions (N—H = 0.86 Å and C—H = 0.93–0.97 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$ or $1.5U_{\text{eq}}(\text{methyl carrier})$.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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