Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

(3,5-Dinitrobenzoato)tris(2-methyl-2-phenylpropyl)tin(IV)

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The Sn atom of the title compound, $[Sn(C_{10}H_{13})_3(C_7H_3N_2O_6)]$, is four-coordinate and possesses a distorted tetrahedral geometry.

Received 27 June 2005
Accepted 5 July 2005
Online 13 July 2005

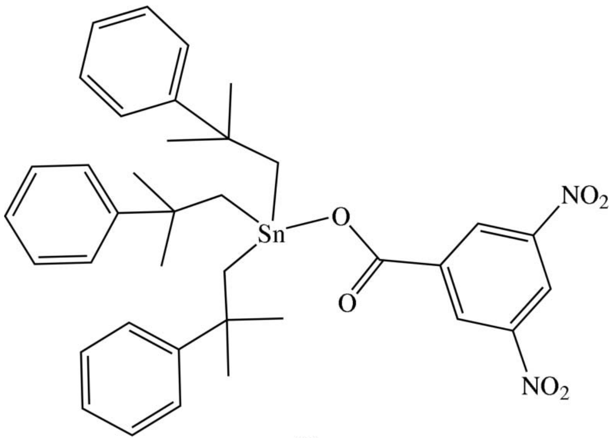
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.047
wR factor = 0.104
Data-to-parameter ratio = 19.1

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

Comment

Tris(2-methyl-2-phenylpropyl)tin carboxylates, $[(C_{10}H_{13})_3Sn(O_2CR)]$, generally possess tetrahedral structures and do not assemble into chain structures *via* carboxylate bridging, due to the crowding of the three bulky groups at the Sn atom (Bao *et al.*, 1998; Bomfim *et al.*, 2002; Tian, Sun, Yang & Ng, 2005; Tian, Sun, Yang & Yang, 2005). In the title compound, (I), tetrahedral coordination is also observed (Fig. 1).



(I)

The Sn1···O2 separation of 3.130 (1) Å indicates there is a weak interaction between these atoms, which distorts the tetrahedral geometry. The monodentate mode of coordination of the carboxylate is also reflected in the disparate O1—C1 and O2—C1 bond lengths of 1.293 (4) and 1.214 (4) Å, respectively. Bond dimensions around the Sn atom (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).

Experimental

Bis[tris(2-phenyl-2-methylpropyl)tin] oxide (1.05 g, 1 mmol) and 3,5-dinitrobenzoic acid (0.42 g, 2 mmol) in benzene (50 ml) were refluxed for 6 h with azeotropic removal of water *via* a Dean–Stark trap. The resulting clear solution was evaporated under reduced pressure. The white solid obtained, (I), was recrystallized from ethanol and crystals of (I) were obtained from hexane by slow evaporation at room temperature (yield 82%, m.p. 402–403 K). Analysis, found: C 61.04, H 5.69, N 3.87%; calculated for $C_{37}H_{42}N_2O_6Sn$: C 60.92, H 5.80, N 3.84%. Spectroscopic analysis: IR (KBr disc): $\nu_{as}(CO_2)$ 1663, $\nu_s(CO_2)$ 1338, $\nu_{as}(NO_2)$ 1543, $\nu_s(NO_2)$ 1381 cm^{-1}; ^{1}H NMR (400 MHz, $CDCl_3$, δ, p.p.m.): 9.49 (3H, *s*, nitrobenzene-H), 7.30–7.09 (15H, *m*, 3 C_6H_5), 1.35 (6H, *s*, 3 CH_2Sn), 1.26 (18H, *s*, 6 CH_3).

Crystal data

$[Sn(C_{10}H_{13})_3(C_7H_3N_2O_6)]$
M_r = 729.42
Monoclinic, $P2_1/n$
a = 9.9262 (8) Å
b = 22.5490 (19) Å
c = 15.8900 (13) Å
β = 96.430 (1)°
V = 3534.2 (5) Å^3
Z = 4
D_x = 1.371 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5905 reflections
θ = 2.2–27.0°
μ = 0.77 mm^{-1}
T = 295 (2) K
Prism, pale yellow
0.30 × 0.13 × 0.12 mm

Data collection

Bruker SMART APEX diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.802, T_{max} = 0.913
30178 measured reflections
8041 independent reflections
7322 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 27.5°
$h = -12 \rightarrow 12$
$k = -29 \rightarrow 29$
$l = -19 \rightarrow 20$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.104
S = 1.19
8041 reflections
421 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0387P)^2 + 2.377P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.73 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.080 (2)	Sn1—C28	2.147 (3)
Sn1—C18	2.144 (3)	Sn1—C8	2.149 (3)
O1—Sn1—C18	101.94 (13)	O1—Sn1—C8	104.51 (11)
O1—Sn1—C28	91.68 (12)	C18—Sn1—C8	117.18 (12)
C18—Sn1—C28	117.18 (14)	C28—Sn1—C8	117.76 (13)

H atoms were placed in calculated positions and included in the refinement in the riding-model approximation, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms, C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms, and C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene H atoms.

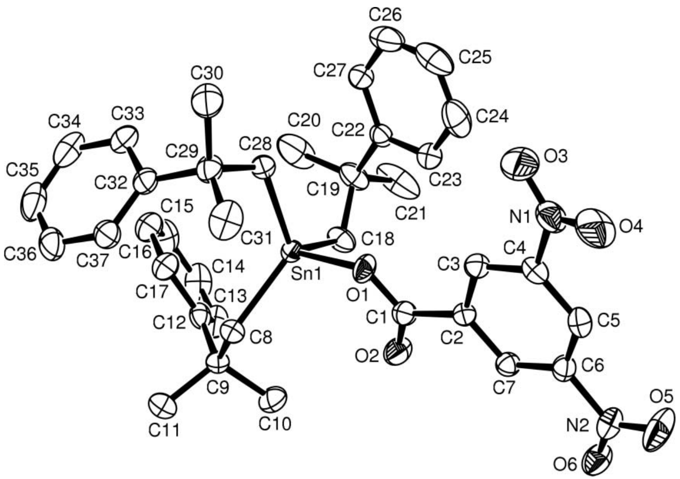


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

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: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Natural Science Foundation of Shandong Province and Qufu Normal University for supporting this work.

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