Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Tris(2-methyl-2-phenylpropyl)(4-nitrophenolato)tin(IV)

Guo-Ming Yang,[a] Guo-Xia Tan,[b] Yang-Jun Ding[b] and Jun Wu[a]*

[a]Department of Chemistry, Zhejiang University, Hangzhou 310027, People's Republic of China, and [b]Department of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China

Correspondence e-mail: wujunchem@163.com

Received 27 April 2006
Accepted 28 April 2006

The Sn atom of the monomeric title compound, $[Sn(C_{10}H_{13})_3(C_6H_4NO_3)]$, adopts a distorted $SnOC_3$ tetrahedral geometry.

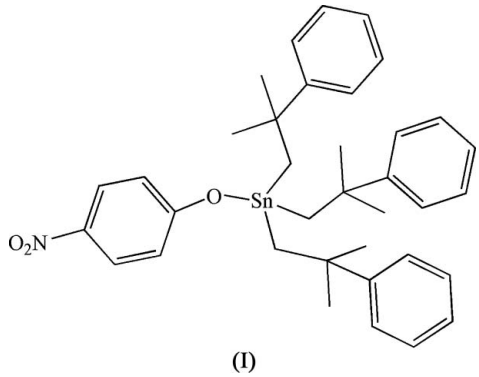
Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.004 Å
R factor = 0.024
wR factor = 0.062
Data-to-parameter ratio = 18.1

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

Comment

The condensation reaction of tris(2-methyl-2-phenylpropyl)tin oxide (fenbutatin oxide) (Zimmer *et al.*, 1966), an industrial miticide, with phenols has been little reported in the literature. One example (Zhang *et al.*, 2002) resulted in the formation of a $SnOC_3$ tetrahedral centre.



(I)

In the title compound, (I), the Sn atom is also tetrahedrally coordinated (Fig. 1). This is different from Me_3SnOMe (Domingos & Sheldrick, 1974), in which almost planar trimethyltin groups are linked by two methoxy ligands, forming infinite one-dimensional zigzag chains with a nearly ideally trigonal–bipyramidal coordinated Sn atom, presumably due to the crowding of the four bulky groups at the Sn atom in (I). The Sn—C distances in (I) are clustered in the narrow range 2.1415 (13)–2.1584 (18) Å (Table 1) and are in agreement with the values [2.140 (3)–2.158 (3) Å] reported for tris(2-methyl-2-phenylpropyl)tin *N*-phthaloylglycinate (Tian *et al.*, 2006), but slightly longer than those [2.105 (4)–2.114 (4) Å] in tris(2-methyl-2-phenylpropyl)tin pentachlorophenolate (Zhang *et al.*, 2002).

Experimental

The title compound was synthesized by condensing bis[tri(2-phenyl-2-methylpropyl)tin] oxide (1.05 g, 1 mmol) with 4-nitrophenol (0.28 g, 2 mmol) in toluene (50 ml). Water was removed with a Dean–Stark water separator and the condensation was complete in about 5 h. The resulting clear solution was evaporated under vacuum. The white solid obtained was recrystallized from ethanol and crystals of (I) were obtained from cyclohexane by slow evaporation at 298 K (yield 73.5%, m.p. 361–362 K). Analysis found: C 65.62, H 6.37, N 2.09%; calculated for $C_{36}H_{43}NO_3Sn$: C 65.87, H 6.60, N 2.13%. IR

(KBr disc): $\nu_{as}(NO_2)$ 1549, $\nu_s(NO_2)$ 1386, ν(SnO) 559 cm^{-1}. ^1H NMR (500 MHz, $CDCl_3$): δ 8.18, 6.59 (4H, *dd*, nitrobenzene H), 7.32–7.07 (15H, *m*, $3C_6H_5$), 1.19 (18H, *s*, $6CH_3$), 1.15 (6H, *s*, $3CH_2Sn$).

Crystal data

$[Sn(C_{10}H_{13})_3(C_6H_4NO_3)]$	V = 1649.51 (12) Å^3
M_r = 656.40	Z = 2
Triclinic, $P\overline{1}$	D_x = 1.322 Mg m^{-3}
a = 9.9002 (4) Å	Mo $K\alpha$ radiation
b = 12.1230 (5) Å	μ = 0.81 mm^{-1}
c = 14.4012 (6) Å	T = 273 (2) K
α = 86.585 (1)°	Plate, pale yellow
β = 75.938 (1)°	0.32 × 0.25 × 0.09 mm
γ = 79.725 (1)°	

Data collection

Bruker SMART APEX CCD diffractometer	17940 measured reflections
	6787 independent reflections
φ and ω scans	6450 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	R_{int} = 0.018
	θ_{max} = 26.5°
T_{min} = 0.782, T_{max} = 0.931	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2 + 0.293P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.024	
$wR(F^2)$ = 0.062	
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
6787 reflections	$\Delta\rho_{max}$ = 0.33 e Å^{-3}
376 parameters	$\Delta\rho_{min}$ = −0.29 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.0454 (13)	Sn1—C7	2.1504 (18)
Sn1—C27	2.1415 (17)	Sn1—C17	2.1584 (18)
O1—Sn1—C27	95.05 (6)	O1—Sn1—C17	104.58 (7)
O1—Sn1—C7	101.12 (7)	C27—Sn1—C17	114.52 (7)
C27—Sn1—C7	117.47 (7)	C7—Sn1—C17	118.62 (7)

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

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*.

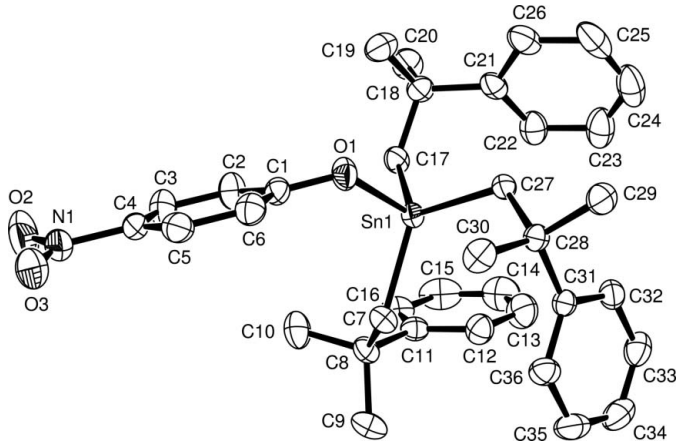


Figure 1
The structure of (I), showing 30% displacement ellipsoids. H atoms have been omitted for clarity.

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

References

Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Domingos, A. M. & Sheldrick, G. M. (1974). *Acta Cryst.* B**30**, 519–521.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Tian, L.-J., Yu, F.-Y., Sun, Y.-X. & Liu, X.-C. (2006). *Acta Cryst.* E**62**, m488–m489.
Zhang, Z.-G., Huang, Y.-Q., Zou, Y., Zhang, S.-K. & Xie, Q.-L. (2002). *Chem. J. Chin. Univ.* **23**, 399–402.
Zimmer, H., Homberg, O. A. & Jayawant, M. (1966). *J. Org. Chem.* **31**, 3857–3860.