Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

μ-Isophthalato-bis[triphenyltin(IV)]

Wen-Li Zhang, Jian-Fang Ma* and Hui Jiang

Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China

Correspondence e-mail: jianfangma@yahoo.com.cn

Received 24 January 2006
Accepted 2 February 2006

Key indicators

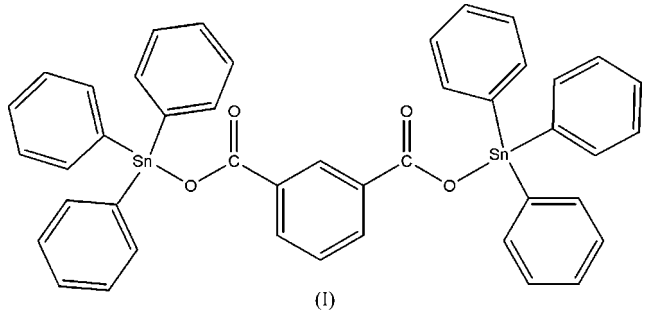
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.042
wR factor = 0.081
Data-to-parameter ratio = 19.6

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

In the title compound, $[Sn_2(C_6H_5)_6(C_8H_4O_4)]$, two triphenyltin groups are bridged by an isophthalate dianion through its two carboxylate groups. Each Sn atom displays a distorted tetrahedral geometry composed of three phenyl groups and one carboxylate O atom from the isophthalate anion.

Comment

Owing to their wide applications, such as PVC stabilizers, agricultural biocides, additives for antifouling paints and catalysts for the production of silicones (Thoonen *et al.*, 2004), organotin compounds have been studied extensively (Lockhart *et al.*, 1987; Teoh *et al.*, 1997; Basu *et al.*, 2005). Organotin compounds show various structures and coordination geometries (Ma *et al.*, 2005; Yin *et al.*, 2005). To further widen the scope of application of organotin compounds, there is a need to prepare new series of organotin complexes. In this paper, the structure of (I) is described.



(I)

As shown in Fig. 1, in the structure of (I) two triphenyltin groups are bridged by one isophthalate, *L*, through its two carboxylate groups. Each Sn atom shows a distorted tetrahedral geometry composed of three phenyl groups and one carboxylate O atom from *L*. The Sn—O distances are similar to reported values (Chee *et al.*, 2003; Tian *et al.*, 2005). In addition, there is a weak Sn···O interaction between Sn1 and O2. The Sn1···O2 distance, 2.724 (3) Å, is longer than the sum of covalent radii (2.13 Å), but is considerably shorter than the sum of van der Waals radii of Sn and O atoms (3.68 Å) (Bondi, 1964). The distortion of the coordination geometry from ideal tetrahedral is reflected in the bond angles about the Sn atom.

Experimental

Isophthalic acid (0.166 g, 1 mmol) was added to a solution of sodium ethoxide (0.136 g, 2 mmol) in ethanol (30 ml). After stirring for 30 min, triphenyltin(IV) chloride (0.77 g, 2 mmol) was added. The mixture was stirred for 12 h at 313 K and then filtered. Light-yellow

crystals of (I) were obtained from the filtrate after it had been allowed to stand for several days at room temperature.

Crystal data

$[Sn_2(C_6H_5)_6(C_8H_4O_4)]$
M_r = 864.13
Monoclinic, $P2_1/n$
a = 10.6434 (12) Å
b = 26.413 (3) Å
c = 13.7552 (15) Å
β = 103.272 (2)°
V = 3763.6 (7) Å^3
Z = 4
D_x = 1.525 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9738 reflections
θ = 2.3–28.5°
μ = 1.37 mm^{-1}
T = 293 (2) K
Block, light yellow
0.43 × 0.31 × 0.29 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.564, T_{max} = 0.680
22965 measured reflections
8843 independent reflections
4724 reflections with $I > 2\sigma(I)$
R_{int} = 0.093
θ_{max} = 28.5°
$h = -10 \rightarrow 14$
$k = -32 \rightarrow 35$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.081
S = 0.96
8843 reflections
451 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.014P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −1.06 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.060 (2)	Sn2—O3	2.036 (3)
Sn1—C7	2.118 (4)	Sn2—C27	2.113 (5)
Sn1—C13	2.126 (4)	Sn2—C39	2.117 (4)
Sn1—C1	2.147 (4)	Sn2—C33	2.128 (4)
O1—Sn1—C7	105.63 (12)	O3—Sn2—C27	112.50 (14)
O1—Sn1—C13	112.19 (12)	O3—Sn2—C39	107.16 (14)
C7—Sn1—C13	118.73 (14)	C27—Sn2—C39	112.93 (16)
O1—Sn1—C1	96.00 (13)	O3—Sn2—C33	94.54 (14)
C7—Sn1—C1	110.80 (13)	C27—Sn2—C33	113.67 (18)
C13—Sn1—C1	111.03 (14)	C39—Sn2—C33	114.47 (16)

H atoms were treated as riding with C—H distances of 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The minimum electron-density peak is loacted 0.96 Å from atom Sn1.

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*.

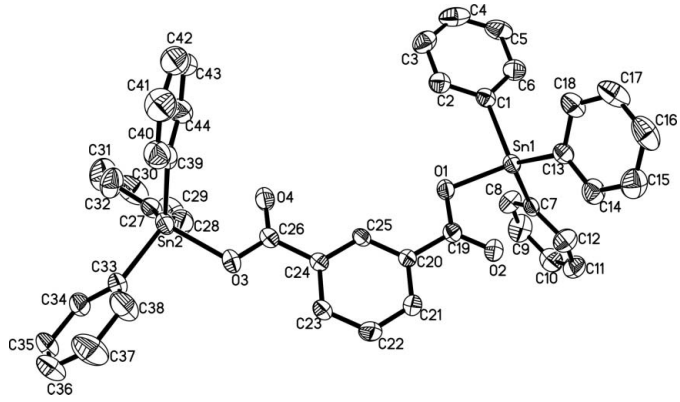


Figure 1
View of the molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted.

We thank the National Natural Science Foundation of China (No. 20471014), the Program for New Century Excellent Talents in Chinese Universities, the Fok Ying Tung Education Foundation and the Science Foundation for Young Teachers of NENU (No. 20050310) for support.

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.
Chee, C. F., Lo, K. M. & Ng, S. W. (2003). *Acta Cryst.* E**59**, m36–m37.
Lockhart, T. P., Calabrese, J. C. & Davidson, F. (1987). *Organometallics*, **6**, 2479–2483.
Ma, C.-L., Zhang, J.-H., Tian, G.-R. & Zhang, R.-F. (2005). *J. Organomet. Chem.* **690**, 519–533.
Sheldrick, G. M. (1990). *SHELXTL-Plus.* Siemens Analytical X-ray Instrument 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.
Thoonen, S. H. L., Deelman, B.-J. & van Koten, G. (2004). *J. Organomet. Chem.* **689**, 2145–2157.
Tian, L.-J., Sun, Y.-X., Yang, M. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m74–m75.
Yin, H.-D., Wang, Q.-B. & Xue, S.-C. (2005). *J. Organomet. Chem.* **690**, 3111–3117.