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(4-Biphenylacetato)tricyclohexyltin(IV)

Lai-Jin Tian,[a]* Yu-Xi Sun,[a] Yi-Zhen Gao[a] and Guo-Ming Yang[b]

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

Correspondence e-mail: laijintian@163.com

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.005 Å
R factor = 0.030
wR factor = 0.081
Data-to-parameter ratio = 16.3

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

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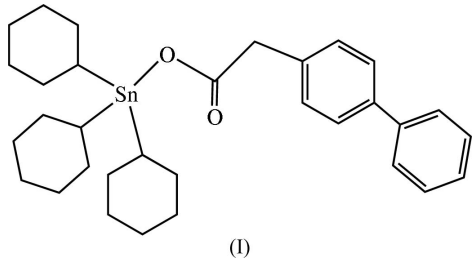
The Sn atom of the title compound, $[Sn(C_6H_{11})_3(C_{14}H_{11}O_2)]$, is four-coordinate and possesses a distorted tetrahedral geometry.

Comment

Tricyclohexyltin carboxylates, $[(C_6H_{11})_3Sn(O_2CR)]$, generally have a tetrahedral structure and do not auto-associate into chain structures *via* carboxylate bridging, due to the crowding of the three bulky cyclohexyl groups at the Sn atom (Chandrasekhar *et al.*, 2002; Tiekink, 1991, 1994).



(I)

4-Biphenylacetic acid is a non-steroidal anti-inflammatory drug (Bundgaard & Nielsen, 1988) and in its tricyclohexyltin ester, (I), the Sn atom is four-coordinate and possesses a distorted tetrahedral geometry (Fig. 1). The Sn···O2 separation of 2.900 (2) Å is not indicative of a significant interaction between these atoms. The major stereochemical role of atom O2 is to distort the tetrahedral geometry by opening up the C7—Sn1—C13 angle to 121.90 (11)° and reducing the O1—Sn1—C1 angle to 93.81 (9)°. The monodentate mode of coordination of 4-biphenylacetate is reflected in the disparate O1—C19 and O2—C19 bond lengths of 1.292 (4) and 1.206 (4) Å, respectively. The four bond lengths to Sn (Table 1)

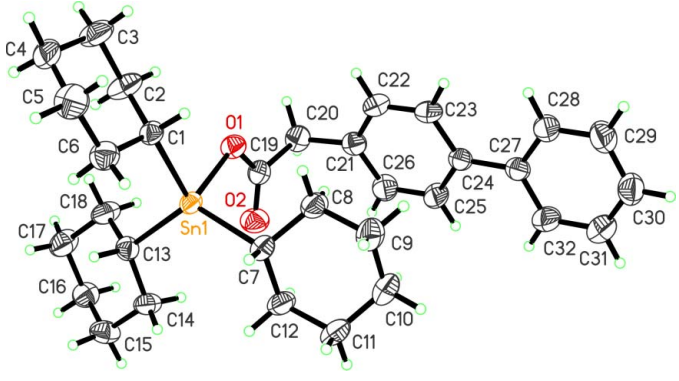


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

are similar to those found in other reported tricyclohexyltin carboxylates, such as tricyclohexyltin indole-3-acetate (Molloy *et al.*, 1986), trifluoroacetate (Calogero *et al.*, 1980), *N*-phthaloylglycinate (Ng & Kumar Das, 1997*a*), (*N*,*N*-diethylthiocarbamoylthio)acetate (Ng & Kumar Das, 1997*b*) and 2-(4-chlorophenyl)-3-methylbutyrate (Song *et al.*, 2003).

Experimental

Tricyclohexyltin hydroxide (0.577 g, 1.5 mmol) and 4-biphenylacetic acid (0.318 g, 1.5 mmol) in benzene (60 ml) were refluxed for 6 h with azeotropic removal of water *via* a Dean–Stark trap. The resulting clear solution was evaporated under vacuum. The white solid obtained, the title compound, was recrystallized from ethanol and crystals of (I) were obtained from a methanol solution of the compound (yield 81.7%, m.p. 351–352 K). Analysis, found: C 66.34, H 7.49%; calculated for $C_{32}H_{44}O_2Sn$: C 66.33, H 7.65%.

Crystal data

$[Sn(C_6H_{11})_3(C_{14}H_{11}O_2)]$
$M_r = 579.36$
Triclinic, $P\overline{1}$
$a = 9.3181$ (12) Å
$b = 11.6211$ (15) Å
$c = 13.9327$ (18) Å
$\alpha = 87.052$ (2)°
$\beta = 76.227$ (2)°
$\gamma = 77.460$ (2)°
$V = 1430.4$ (3) Å^3
$Z = 2$
$D_x = 1.345$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 885 reflections
$\theta = 3.0$–22.9°
$\mu = 0.92$ mm^{-1}
$T = 295$ (2) K
Block, colourless
0.32 × 0.22 × 0.15 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.758$, $T_{max} = 0.875$
7734 measured reflections
5165 independent reflections
4834 reflections with $I > 2\sigma(I)$
$R_{int} = 0.018$
$\theta_{max} = 25.5°$
$h = -11 \rightarrow 11$
$k = -14 \rightarrow 9$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.081$
$S = 1.05$
5165 reflections
316 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.6525P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.93$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.089 (2)	Sn1—C7	2.165 (3)
Sn1—C13	2.162 (3)	Sn1—C1	2.168 (3)
O1—Sn1—C13	110.51 (10)	O1—Sn1—C1	93.81 (9)
O1—Sn1—C7	103.00 (10)	C13—Sn1—C1	111.80 (11)
C13—Sn1—C7	121.90 (11)	C7—Sn1—C1	111.69 (11)

H atoms were placed in calculated positions and refined in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}$(carrier C). Constrained C—H distances were 0.93 for aromatic CH, 0.97 for methylene CH_2 and 0.98 Å for methine CH.

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: *XP* (Bruker, 2002); software used to prepare material for publication: *SHELXL97*.

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