μ-3-Mercaptobenzoato-κ²O:S-bis(triphenyltin)

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Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.006 Å
R factor = 0.027
wR factor = 0.071
Data-to-parameter ratio = 15.3

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

The title complex, [Sn$_2$(C$_6$H$_5$)$_6$(C$_7$H$_4$O$_2$S)$_2$], is a binuclear triphenyltin derivate bridged by a 3-mercaptobenzoate anion. Both Sn atoms are four-coordinate and display distorted tetrahedral geometry.

Comment

In recent years, organotin complexes have been attracting more and more attention for their wide industrial applications and biological activities (Duboy & Roy, 2003). In order to explore the relationships between the properties and structures, a larger number of organotin complexes have been prepared (Gielen, 2002). We report here the structure of the title binuclear Sn^{IV} complex, (I).

(I)
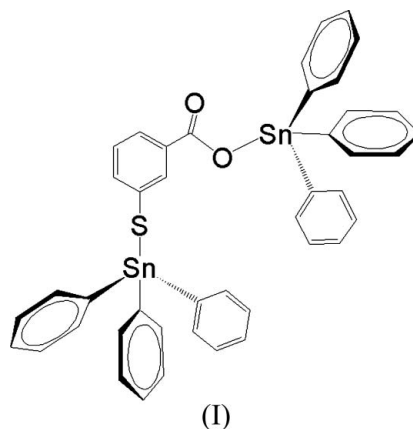
The molecular structure of (I) is shown in Fig. 1. The mercaptobenzoate anion bridges the Sn1 and Sn2 atoms to form the binuclear complex. Both Sn1 and Sn2 are four coordinated in a distorted tetrahedron. The Sn—S and Sn—O bond distances (Table 1) are comparable to those found in [O,S-bis(triphenyltin(IV)-2-mercaptobenzoate] (Ng *et al.*, 1989) and in (o-aminobenzoato-O)-triphenyltin (Swisher *et al.*, 1984), respectively. The bond angles at the Sn2 atom range from 95.39 (12) to 114.37 (13)°, showing the degree of distortion from a tetrahedron.

Although the Sn2···O2 separation of 2.871 (3) Å is significantly shorter than the sum of van der Waals radii for Sn and O atoms, the normal C1—O1—Sn2 bond angle of 112.7 (2)° suggests no bonding between atoms Sn2 and O2 (Li *et al.*, 2005).

Experimental

The reaction was carried out under nitrogen atmosphere. 3-Mercaptobenzoic acid (0.154 g, 1 mmol) was added to a solution of
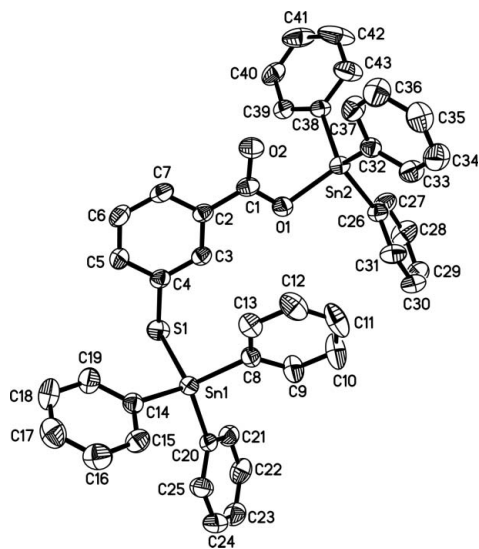
Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

benzene (20 ml) with sodium ethoxide (0.136 g, 2 mmol). After stirring for 10 min, triphenyltin chloride (0.770 g, 2 mmol) was added to the mixture. The mixture was kept at 313 K for 12 h. After cooling to room temperature, the solution was filtered. The solvent of the filtrate was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from ethanol. Colorless single crystals of (I) were obtained after 1 d. Yield 0.724 g, 85%. M.p. 414 K. Analysis calculated for $C_{43}H_{34}O_2SSn_2$: C 60.60, H 4.02%; found: C 60.55, H 4.05%.

Crystal data

$[Sn_2(C_6H_5)_6(C_7H_4O_2S)_2]$	$D_x = 1.510$ Mg m^{-3}
$M_r = 852.14$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 8267
$a = 10.383$ (3) Å	reflections
$b = 17.997$ (5) Å	$\theta = 2.3–26.2°$
$c = 20.207$ (6) Å	$\mu = 1.42$ mm^{-1}
$\beta = 96.928$ (5)°	$T = 298$ (2) K
$V = 3748$ (2) Å^3	Block, colorless
$Z = 4$	$0.48 \times 0.25 \times 0.21$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	6639 independent reflections
φ and ω scans	5151 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.021$
$T_{min} = 0.548$, $T_{max} = 0.754$	$\theta_{max} = 25.0°$
19694 measured reflections	$h = -11 \rightarrow 12$
	$k = -21 \rightarrow 21$
	$l = -24 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.027$	$+ 1.9228P]$
$wR(F^2) = 0.071$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.002$
6639 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
433 parameters	$\Delta\rho_{min} = -0.32$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—S1	2.4295 (11)	Sn2—O1	2.049 (2)
Sn1—C8	2.128 (3)	Sn2—C26	2.133 (3)
Sn1—C14	2.133 (3)	Sn2—C32	2.118 (3)
Sn1—C20	2.138 (3)	Sn2—C38	2.122 (3)
C8—Sn1—C14	113.79 (13)	O1—Sn2—C32	112.13 (12)
C8—Sn1—C20	108.63 (13)	O1—Sn2—C38	107.09 (12)
C14—Sn1—C20	112.32 (13)	C32—Sn2—C38	114.37 (13)
C8—Sn1—S1	108.91 (9)	O1—Sn2—C26	95.39 (12)
C14—Sn1—S1	106.66 (10)	C32—Sn2—C26	114.17 (14)
C20—Sn1—S1	106.19 (9)	C38—Sn2—C26	111.94 (13)

H atoms were placed geometrically with C–H = 0.93 Å and treated as riding on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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