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(2-Benzoylbenzoato)triphenyltin(IV)

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Key indicators

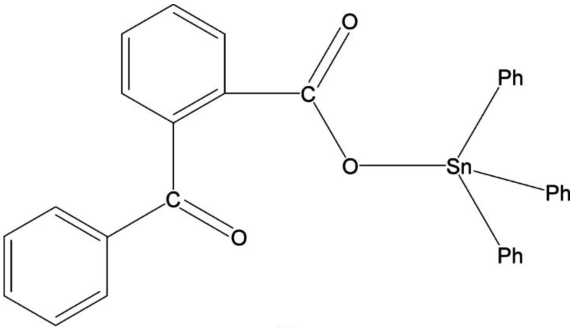
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.034
wR factor = 0.095
Data-to-parameter ratio = 17.9

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

The structure of the title compound, [Sn(C_6H_5)$_3$($C_{14}H_9O_3$)], consists of monomeric species featuring a distorted tetrahedral environment around the Sn centre. The tetrahedral angles are non-equivalent, owing to the relatively close approach of a carboxylate O atom.

Comment

The chemistry of organotin(IV) complexes incorporating carboxylate ligands has attracted ever increasing attention, partly owing to their biological and pharmaceutical applications (Davies & Smith, 1982; Gielen, 1996; Kemmer *et al.*, 2000) and, from a chemical point of view, due to the versatile molecular structure and supramolecular architecture exhibited by these complexes (Tiekink, 1991, 1994; Willem *et al.*, 1998). In the present study, we have synthesized and characterized an isomer of the previously reported 2-benzoylbenzoatotriphenyltin(IV) derivative (Khoo *et al.*, 1995). This latter structure is polymeric and contains *trans* O_2SnC_3 units, the ketonic O atom being involved in the polymerization of the compound.



(I)

The molecule of the title compound, (I), consists of a $C_6H_5COC_6H_4COO^-$ anion, coordinated in monodentate mode to an $SnPh_3$ group (Fig. 1). The Sn centre is in a tetrahedral environment (Table 1), with a weak intramolecular interaction between the Sn centre and atom O3 of the carboxylate group [Sn···O3 = 2.689 (2) Å]. As in a similar structure, the relatively close intramolecular Sn···O interaction, within the sum of the van der Waals radii for these atoms (Tiekink *et al.*, 1995), is not indicative of significant bonding interactions between the respective pair of atoms. The relatively close approach of atom O3 to Sn, however, causes some distortion from ideal geometry. The molecule adopts a *C*-type structure in the classification of Tiekink (Tiekink, 1991) and the Sn atom, linked to three phenyl rings

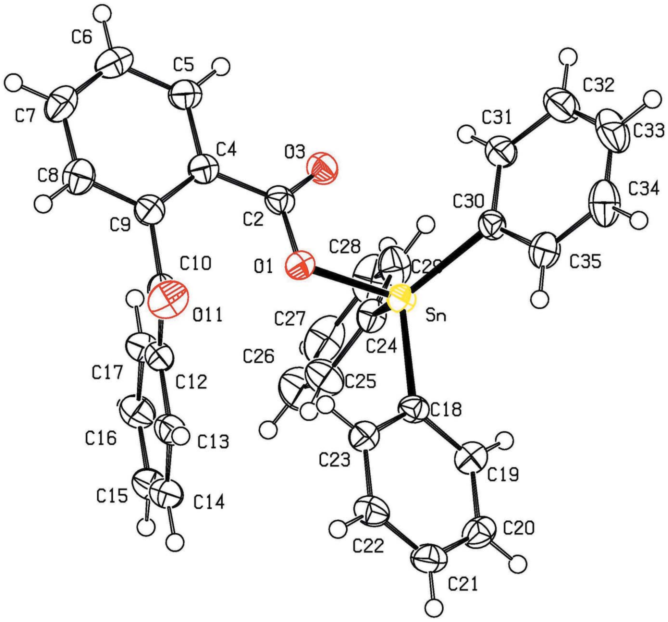


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

and one O atom of the 2-benzoylbenzoate ligand, has a distorted tetrahedral geometry, in which the tetrahedral angles range from 105.83 (9) to 121.82 (10)°.

The enlargement of the C30—Sn—C24 [121.82 (10)°] angle can be attributed to the relatively close approach of atom O3 of the carboxylate group to the Sn centre. The variations in the C—Sn—C angles and Sn—C bonds may be traced to the distortion of the tetrahedral environment. Similar behaviour of the carboxylate ligands has also been reported in $(CH_3NH)C_6H_4COOSnPh_3$ and $(C_6H_{11})_2CHCOOSnPh_3$ (Rénamy *et al.*, 2004). The Sn1—O1 [2.0885 (18) Å] bond length is of the order of those reported for some triphenyltin(IV) esters of salicylic acid, *o*-anisic acid and *p*-methylthiobenzoic acid (Vollano *et al.*, 1984).

Spectroscopic data have also supported the structure of (I). The Mössbauer parameters (QS = 2.49 mm s^{-1}) and the IR absorption frequencies ($\Delta\nu = \nu_{asym}$OCO − ν_{sym}OCO = 255 cm^{-1}) are consistent with, respectively, a tetrahedral environment around the Sn centre (Davies & Smith, 1982) and a monodentate carboxylate ligand (Khoo *et al.*, 1995; Nakamoto, 1997). This can be explained by the large differences in the Sn···O interactions. The Sn···O3 contact is very long and may not cause a significant change in the spectroscopic data.

Experimental

$[Cy_2NH_2][-C_6H_5COC_6H_4CO_2]$, (II), was obtained from the neutralization of 2-benzoylbenzoic acid ($C_6H_5COC_6H_4CO_2H$; 2.35 g, 10.4 mmol) with dicyclohexylamine (Cy_2NH; 1.882 g, 10.4 mmol) in water (5 ml). The mixture was stirred for several hours and the solvent was then removed *in vacuo*. Recrystallization from ethanol (25 ml, 99.99%) gave compound (II). Compound (I) was obtained by reacting an ethanol solution **(Volume?)** of (II) (99.99%) with Ph_3SnCl (2.5 mmol) in a 1:1 ratio. The mixture was stirred for several hours and slow solvent evaporation gave crystals suitable for X-ray analysis.

Crystal data

$[Sn(C_6H_5)_3(C_{14}H_9O_3)]$
M_r = 575.20
Monoclinic, $P2_1/c$
a = 8.761 (3) Å
b = 17.363 (5) Å
c = 17.752 (5) Å
β = 109.73 (2)°
V = 2541.9 (13) $Å^3$

Z = 4
D_x = 1.503 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.04 mm^{-1}
T = 294 (2) K
Parallelipiped, colourless
0.32 × 0.30 × 0.26 mm

Data collection

Marresearch MAR345 image-plate diffractometer
φ scans
Absorption correction: none
64928 measured reflections

5835 independent reflections
5667 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
S = 1.10
5835 reflections
326 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0462P)^2 + 3.3458P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.87 e $Å^{-3}$
$\Delta\rho_{min}$ = −0.77 e $Å^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0275 (11)

Table 1
Selected geometric parameters (Å, °).

Sn—O1	2.0885 (18)	O1—C2	1.314 (3)
Sn—C30	2.118 (2)	C2—O3	1.237 (3)
Sn—C24	2.123 (2)	C10—O11	1.219 (3)
Sn—C18	2.138 (2)		
O1—Sn—C30	109.75 (8)	O1—Sn—C18	98.06 (8)
O1—Sn—C24	105.82 (9)	C30—Sn—C18	110.82 (10)
C30—Sn—C24	121.82 (10)	C24—Sn—C18	107.86 (10)

H atoms were positioned geometrically, with C—H = 0.93 Å, and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *MAR software* (Klein, 1998); cell refinement: *marHKL* (Klein & Bartels, 2000); data reduction: *marHKL*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1998); software used to prepare material for publication: *SHELXL97*.

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