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Tetramethylammonium bis(2-benzoylbenzoato-κO)triphenylstannate(IV)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.053
wR factor = 0.121
Data-to-parameter ratio = 33.3

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

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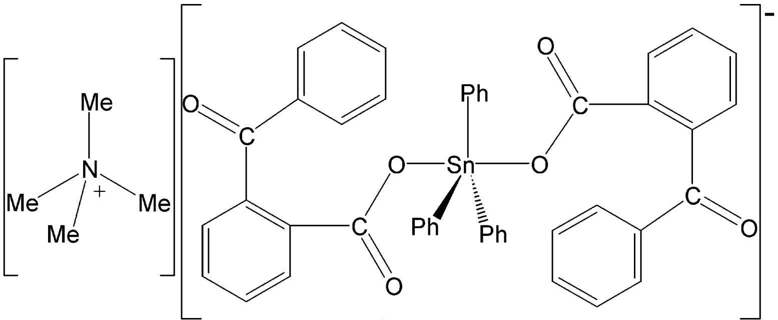
The coordination polyhedron of the five-coordinate Sn atom in the title salt, $(C_4H_{12}N)[Sn(C_6H_5)_3(C_{14}H_9O_3)_2]$, is a *trans*-$C_3SnO_2$ trigonal bipyramid, involving two monodentate 2-benzoylbenzoate ligands and three phenyl groups. The O—Sn—O unit is almost linear [O—Sn—O = 174.56 (8)°].

Comment

The chemistry of organotin compounds, such as the triorganotin carboxylates, is related to their biological properties (Davies & Smith, 1982; Gielen, 1996; Kemmer *et al.*, 2000). The structural chemistry has been reviewed (Tiekink, 1991, 1994; Willem *et al.*, 1998). The class of di(carboxylato)triorganostannates is a class of anionic triorganotin carboxylates; the compounds are expected to be more water soluble because of their ionic nature. Some examples, as listed by the Cambridge Structural Database (2006 release; Allen, 2002) include BELQEO and BELQIS (Ng & Hook, 1999*b*), BEQJAI (Ng & Hook, 1999*a*), and HOSJEE (Ng, 1998); these involve extensive hydrogen-bonding interactions. The first example of a discrete di(carboxylato)triorganostannate is the tetramethylammonium salt of $[Sn(C_2F_3O_2)_2(C_6H_5)_3]$ (Ng & Kumar Das, 1997*b*). Other monomeric examples have since been reported, *viz.* IXINEI (Ng & Rae, 2003), NAKJUF (Ma *et al.*, 2005), RADBEE (Chee *et al.*, 2003) and RESCOH (Ng & Kumar Das, 1997*a*). In the context of our research work on the coordination ability of the carboxylate ligands towards organotin(IV) derivatives, we have reported $[Sn(C_6H_5)_3(C_{14}H_9O_3)]$ (Diop *et al.*, 2007) and have also shown the possibility of complexation with a Lewis base such as triphenylphosphine oxide (Diop *et al.*, 2006). The title compound, (I), a salt, can be considered as the product of the addition of a $C_{14}H_9O_3^-$ anion in the form of its tetramethylammonium salt to $[Sn(C_6H_5)_3(C_{14}H_9O_3)]$.



(I)

The structure of the anion has two monodentate $C_6H_5COC_6H_4COO^-$ units that are covalently bonded to an essentially planar $SnPh_3$ group (Fig. 1). The geometry around the Sn atom is trigonal bipyramidal, with the *ipso* C atoms of the phenyl groups in the equatorial plane. The C11—Sn1—C21 angle is opened up [127.64 (12) Å] with respect to the other two C—Sn—C bond angles [C11—Sn1—C31 = 113.45 (12)° and C21—Sn1—C31 =118.86 (12)°]. The distortion from ideal trigonal–bipyramidal geometry arises from the steric hindrance of the 2-benzoylbenzoate ligands. The tetramethylammoniun cation has only coulombic interactions with the stannate anion.

The Mössbauer spectrum is a slightly asymmetric quadrupole-split doublet with hyperfine parameters (Q.S. = 3.13 and I.S. = 1.52 mm s^{-1}) in the normal range for pentacoordinate triphenyltin(IV) adducts; moreover, the linewidth value (0.95 mm s^{-1}) supports the presence of a single tin center (Davies & Smith, 1982). IR and Raman spectroscopic bands indicate the presence of a carboxylate group that is bonded to a heavy atom ($\Delta\nu = \nu_{asym}OCO - \nu_{sym}OCO = 301\ cm^{-1}$ (Ma *et al.*, 2005; Nakamoto, 1997).

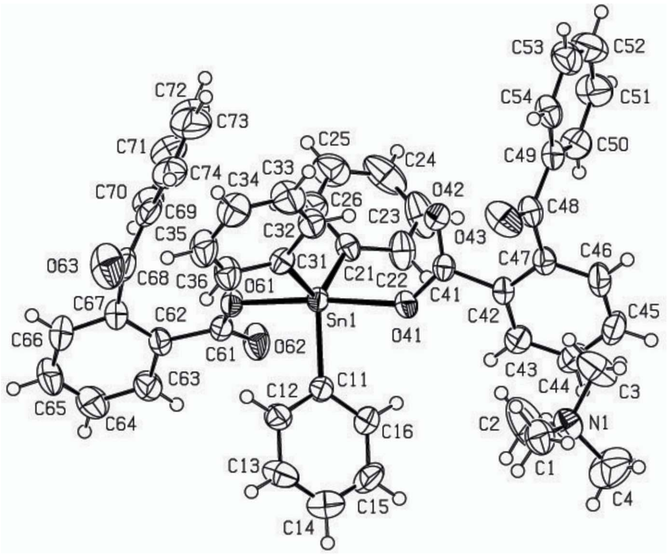


Figure 1
The structure of the anion of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

The salt $[Me_4N][2\text{-}C_6H_5COC_6H_4CO_2]$ was obtained from the neutralization of 2-benzoylbenzoic acid (5 mmol) in ethanol (99.99%, 25 ml) with an aqueous solution of tetramethylammonium hydroxide (5 mmol, 25% in water). The mixture was refluxed for 2 h and the solvent removed *in vacuo*. The crude material was recrystallized from ethanol (25 ml, 99.99%) and dried with P_2O_5 in a desiccator. Compound (I) was obtained by reacting an ethanol solution of the organic salt (5.0 mmol, 25 ml) with a hot ethanol solution (99.99%, 25 ml) of triphenyltin choride (2.5 mmol) in a 2:1 ratio. The mixture was stirred for several hours and slow solvent evaporation gave crystals suitable for X-ray analysis. Presumably, the tetramethylammonium chloride that formed as the by-product had remained in solution.

Crystal data

$(C_4H_{12}N)[Sn(C_6H_5)_3(C_{14}H_9O_3)_2]$
$M_r = 874.56$
Monoclinic, $P2_1/n$
$a = 9.7481\ (11)$ Å
$b = 29.787\ (5)$ Å
$c = 14.704\ (5)$ Å
$\beta = 98.793\ (14)°$
$V = 4219.3\ (16)$ Å^3

$Z = 4$
$D_x = 1.377$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.66$ mm^{-1}
$T = 293\ (2)$ K
Prism, colorless
0.50 × 0.30 × 0.30 mm

Data collection

Enraf–Nonius MACH3 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.735$, $T_{max} = 0.827$
18605 measured reflections

17529 independent reflections
6852 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 34.2°$
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.121$
$S = 0.96$
17529 reflections
527 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.66$ e Å^{-3}
$\Delta\rho_{min} = -1.88$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C11	2.132 (3)	Sn1—O61	2.2092 (19)
Sn1—C21	2.133 (3)	Sn1—O41	2.249 (2)
Sn1—C31	2.136 (3)		
C11—Sn1—C21	127.64 (12)	C31—Sn1—O61	87.39 (10)
C11—Sn1—C31	113.45 (12)	C11—Sn1—O41	83.95 (10)
C21—Sn1—C31	118.86 (12)	C21—Sn1—O41	88.24 (10)
C11—Sn1—O61	90.99 (10)	C31—Sn1—O41	96.43 (10)
C21—Sn1—O61	93.31 (10)	O61—Sn1—O41	174.56 (8)

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å, and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$. The maximum and minimum electron-density peaks are located 0.83 Å from H4C and 0.03 Å from Sn1, respectively.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *GENHKL* (Kretschmar, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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