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[4-(Diethylamino)benzoato-κ*O*]triphenyltin(IV)

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Key indicators

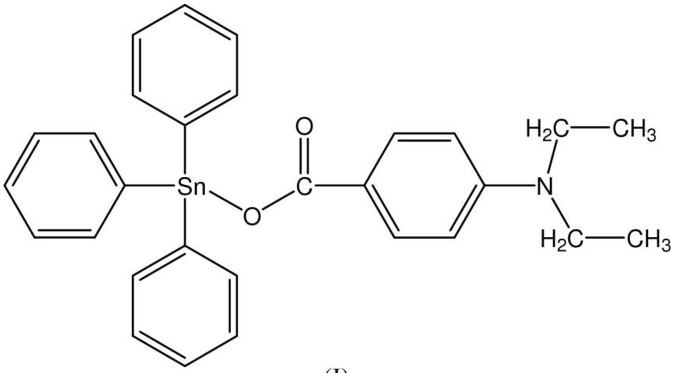
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.027
wR factor = 0.072
Data-to-parameter ratio = 43.8

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

The Sn atom in the title compound, $[Sn(C_6H_5)_3(C_{11}H_{14}NO_2)]$, shows tetrahedral coordination. The asymmetric unit has two independent molecules; the crystal structure is stabilized by C—H···O and C—H···π interactions.

Comment

Recent *in vitro* antitumour and antibacterial activity studies of organotin(IV) carboxylate compounds have revealed their effectiveness as antitumour drugs (Willem *et al.*, 1997, Gielen *et al.*, 2000, Tian *et al.*, 2005). Moreover, among the organotin(IV) carboxylate compounds, triorganotin(IV) carboxylates display the highest biological activity (Novelli *et al.*, 1999). Generally, triphenyltin(IV) carboxylate complexes are commonly found as monomeric structures with four-coordinate distorted tetrahedral or five-coordinate trigonal–bipyramidal geometry (Baul *et al.*, 2001; Yeap & Teoh, 2003; Win *et al.*, 2006). In a recent study, the coordination geometry of (3,5-dinitrobenzoato)triphenyltin(IV) was found to be distorted tetrahedral and due to the long range interaction of the carboxylate anion coordinated to Sn in an isobidentate manner (Win *et al.*, 2006). Based on a crystallography structural study, the title complex, (I), is monomeric with two molecules in the asymmetric unit.



(I)

The ligand bond lengths and angles in (I) have normal values (Allen *et al.*, 1987), comparable to a related structure (Win *et al.*, 2006); bond lengths and angles for the Sn coordination are given in Table 1. In molecule *A*, the dihedral angles between C1*A*–C6*A* and C7*A*–C12*A*, C7*A*–C12*A* and C13*A*–C18*A*, and C1*A*–C6*A* and C13*A*–C18*A* are 45.36 (7), 61.01 (7) and 28.62 (6)°, respectively. In molecule B, the dihedral angles between C1*B*–C6*B* and C7*B*–C12*B*, C7*B*–C12*B* and C13*B*–C18*B*, and C1*B*–C6*B* and C13*B*–C18*B* are 62.64 (7), 64.60 (7) and 53.21 (7)°, respectively.

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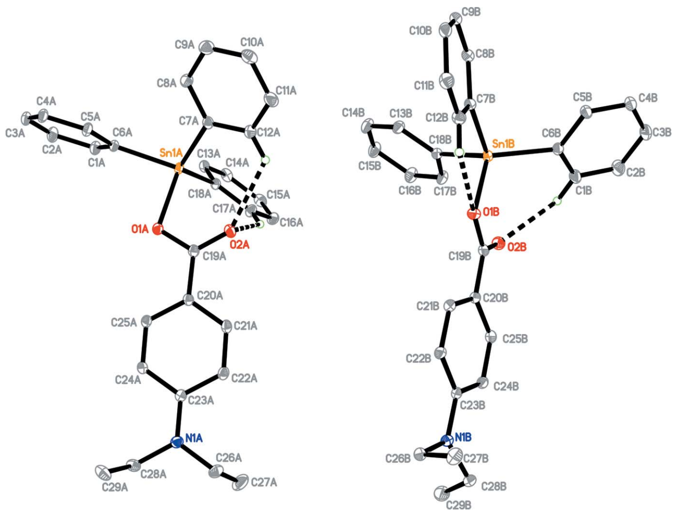

Figure 1
The asymmetric unit of (I), showing 30% probability displacement ellipsoids and the atomic numbering. The intramolecular hydrogen bonds are shown as dashed lines. H atoms not involved in the hydrogen bonds have been omitted.

Intramolecular C1*B*—H1*BA*···O2*B*, C12*A*—H12*A*···O2*A* and C17*A*—H17*A*···O2*A* hydrogen bonds generate *S*(7) ring motifs, while the C12*B*—H12*B*···O1*B* hydrogen bond generates an *S*(5) ring motif (Table 2) (Bernstein *et al.*, 1995). The crystal structure is stabilized by C—H···O and C—H···π interactions (Table 2).

Experimental

The complex 4-(diethylaminobenzoato)triphenyltin(IV) was obtained by heating under reflux a 1:1 molar mixture of triphenyltin(IV) hydroxide (1.10 g, 3 mmol) and 4-(diethylamino)benzoic acid (0.58 g, 3 mmol) in acetonitrile (50 ml) for 2 h. A clear transparent solution was isolated by filtration and kept in a bottle. After 4 d, some colourless crystals (1.30 g, 79.9% yield) were obtained (m.p. 386.7–387.0 K). Analysis found: C 64.28, H 5.00, N 2.63, Sn 21.31%; calculated for $C_{29}H_{29}NO_2Sn$: C 64.24, H 5.39, N 2.58, Sn 21.89%. FT-IR from a KBr disc (cm^{-1}): ν(COO)$_{as}$ 1603, ν(COO)$_s$ 1347, ν(O—Sn—O) 617, ν(Sn—O) 448.

Crystal data

$[Sn(C_6H_5)_3(C_{11}H_{14}NO_2)]$
$M_r = 542.22$
Triclinic, $P\bar{1}$
$a = 10.8876$ (3) Å
$b = 13.0407$ (3) Å
$c = 17.8896$ (5) Å
$\alpha = 84.632$ (1)°
$\beta = 82.117$ (1)°
$\gamma = 84.260$ (1)°
$V = 2495.16$ (11) Å^3
$Z = 4$
$D_x = 1.443$ Mg m^{-3}
Mo *K*α radiation
$\mu = 1.05$ mm^{-1}
$T = 100.0$ (1) K
Block, colourless
0.41 × 0.36 × 0.31 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.646$, $T_{max} = 0.735$
104338 measured reflections
26062 independent reflections
21490 reflections with $I > 2\sigma(I)$
$R_{int} = 0.032$
$\theta_{max} = 37.5°$

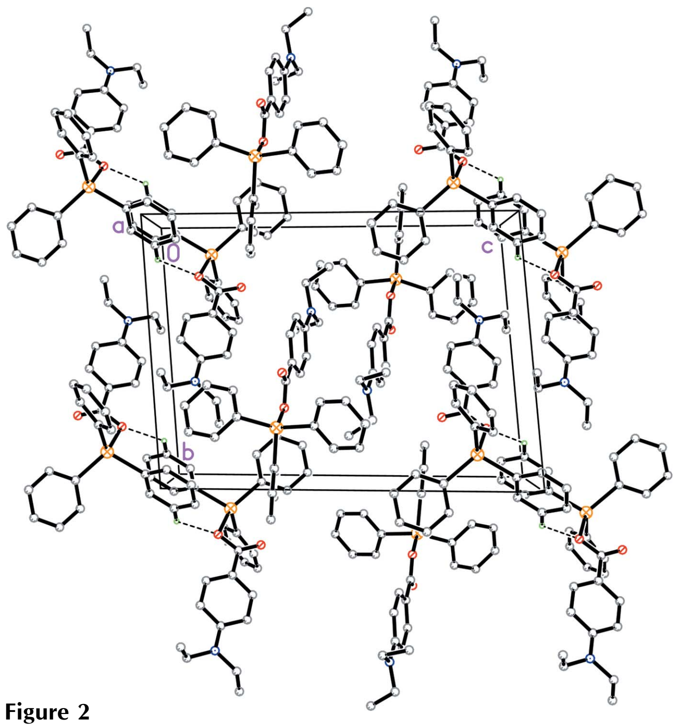

Figure 2
The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in the hydrogen bonding have been omitted.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.072$
$S = 1.04$
26062 reflections
595 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2 + 0.7386P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.40$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1*A*—O1*A*	2.0686 (9)	Sn1*B*—O1*B*	2.0639 (9)
Sn1*A*—C18*A*	2.1285 (11)	Sn1*B*—C18*B*	2.1240 (12)
Sn1*A*—C7*A*	2.1365 (13)	Sn1*B*—C6*B*	2.1301 (12)
Sn1*A*—C6*A*	2.1413 (12)	Sn1*B*—C7*B*	2.1362 (12)
O1*A*—Sn1*A*—C18*A*	105.41 (4)	O1*B*—Sn1*B*—C18*B*	108.36 (4)
C18*A*—Sn1*A*—C7*A*	117.81 (4)	O1*B*—Sn1*B*—C6*B*	114.95 (4)
O1*A*—Sn1*A*—C6*A*	94.13 (4)	C18*B*—Sn1*B*—C7*B*	108.42 (5)
C7*A*—Sn1*A*—C6*A*	108.11 (5)	C6*B*—Sn1*B*—C7*B*	111.40 (5)

Table 2
Hydrogen-bond geometry (Å, °).

*Cg*1, *Cg*2, *Cg*3, *Cg*4, *Cg*5 and *Cg*6 are centroids of the C1*B*–C6*B*, C13*B*–C18*B*, C1*A*–C6*A*, C13*A*–C18*A*, C20*A*–C25*A* and C20*B*–C25*B* rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4*A*—H4*AA*···O1*A*^{i}	0.93	2.55	3.239 (2)	132
C1*B*—H1*BA*···O2*B*	0.93	2.52	3.121 (2)	123
C12*A*—H12*A*···O2*A*	0.93	2.43	3.080 (2)	127
C12*B*—H12*B*···O1*B*	0.93	2.55	3.120 (2)	120
C17*A*—H17*A*···O2*A*	0.93	2.35	3.082 (2)	135
C8*A*—H8*AA*···*Cg*1^{ii}	0.93	3.15	3.795 (2)	128
C10*A*—H10*A*···*Cg*2^{ii}	0.93	3.06	3.462 (2)	108

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4*B*—H4*BA*···*Cg*3^{ii}	0.93	2.85	3.567 (2)	135
C9*B*—H9*BA*···*Cg*4^{ii}	0.93	2.59	3.327 (1)	137
C15*A*—H15*A*···*Cg*5^{iii}	0.93	2.85	3.661 (1)	146
C22*A*—H22*A*···*Cg*6^{iv}	0.93	3.13	3.653 (1)	118
C26*B*—H26*C*···*Cg*2^{iv}	0.97	2.88	3.723 (1)	146
C29*A*—H29*A*···*Cg*4^{v}	0.96	2.87	3.799 (2)	162

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x, -y, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+1, -z+1$; (v) $-x+1, -y+1, -z$.

H atoms were positioned geometrically and treated as riding, with C—H = 0.93-0.97 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) or 1.5$U_{\rm eq}$(methyl C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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