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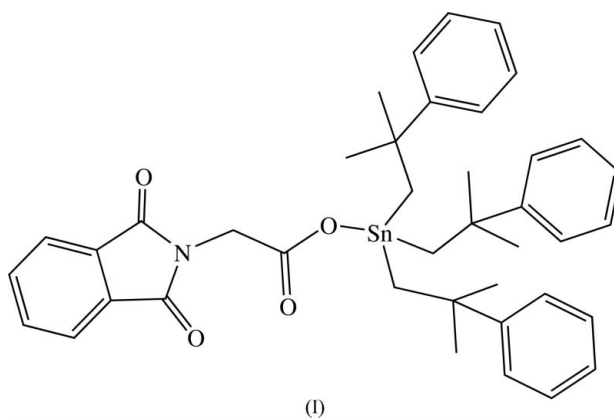
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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.037
 wR factor = 0.091
Data-to-parameter ratio = 17.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Tris(2-methyl-2-phenylpropyl)(2-phthalimido-
acetato- κO)tin(IV)The Sn atom of the title compound, $[\text{Sn}(\text{C}_{10}\text{H}_{13})_3(\text{C}_{10}\text{H}_6\text{NO}_4)]$, is four-coordinate and possesses a distorted tetrahedral geometry.Received 3 January 2006
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Comment

N-Phthaloylglycine, whose crystal structure has been reported (Feeder & Jones, 1996), is a protected amino acid. The crystal structures of several triorganotin esters containing the ligand have revealed some interesting features (Ng *et al.*, 1990, 1994; Ng & Kumar Das, 1997; Lo *et al.*, 1997). In triphenyltin *N*-phthaloylglycinate, six molecules are bridged by carboxylate groups to form a cyclic hexamer (Ng *et al.*, 1990). In the tricyclohexyltin analogue, the molecules are linked into a helical chain through amido-O atoms (Ng & Kumar Das, 1997). In aquatributyltin *N*-phthaloylglycinate (Ng *et al.*, 1994) and aqua(*p*-chlorophenyl)diphenyltin *N*-phthaloylglycinate (Lo *et al.*, 1997), the Sn atoms exist in a distorted trigonal-bipyramidal geometry, with a coordinated water molecule occupying an axial site.



In the title compound, (I), the Sn atom is four-coordinate and possesses a distorted tetrahedral geometry (Fig. 1). The $\text{Sn}\cdots\text{O}1$ separation of 3.055 (2) Å indicates there is a weak interaction between these atoms, which distorts the tetrahedral geometry. The monodentate mode of coordination of *N*-phthaloylglycinate is reflected in the disparate $\text{C}1-\text{O}1$ and $\text{C}1-\text{O}2$ bond lengths of 1.211 (3) and 1.293 (3) Å, respectively. The $\text{Sn}-\text{C}$ distances lie within the narrow range of 2.140 (3)–2.158 (3) Å (Table 1) and are in agreement with values reported in related structures, such as the phenoxyacetate (Bao *et al.*, 1998), pyridine-3-carboxylate (Tian, Sun, Yang & Yang, 2005) and 3,5-dinitrobenzoate (Tian, Yu *et al.*, 2005) salts of tris(2-methyl-2-phenylpropyl)tin, and bis[tris(2-methyl-2-phenylpropyl)tin(IV)] phthalate (Tian, Sun, Yang &

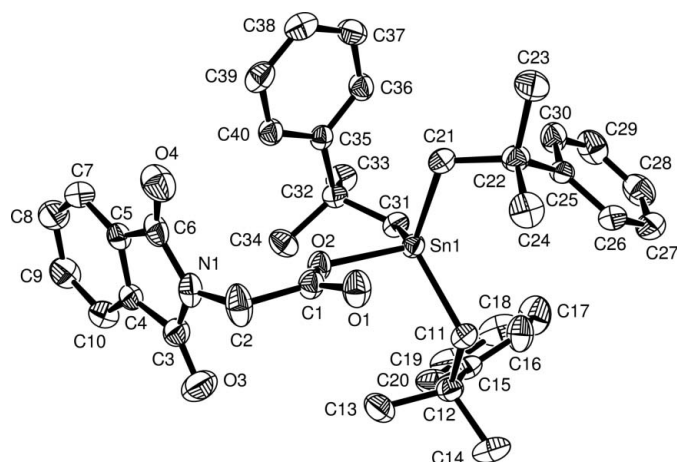


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

Ng, 2005). The Sn—O bond length in (I) is similar to that found in the carboxylate structures mentioned above.

Experimental

Bis[tris(2-methyl-2-phenylpropyl)tin] oxide (1.05 g, 1 mmol) and *N*-phthaloylglycine (0.41 g, 2 mmol) in toluene (50 ml) were refluxed for 5 h with azeotropic removal of water *via* a Dean–Stark trap. The resulting clear solution was evaporated under reduced pressure. The white solid obtained, (I), was purified by recrystallization from methanol, and crystals of (I) were obtained from a chloroform–hexane (1:1, *v/v*) solution by slow evaporation at 298 K (yield 80.6%, m.p. 386–387 K). Analysis, found: C 66.26, H 6.09, N 1.97%; calculated for $C_{40}H_{45}NO_4Sn$: C 66.50, H 6.28, N 1.94%. IR (KBr disc): $\nu_{as}(CO_2)$ 1672, $\nu_s(CO_2)$ 1321 cm^{-1} .

Crystal data

$[Sn(C_{10}H_{13})_3(C_{10}H_6NO_4)]$
 $M_r = 722.46$
 Monoclinic, $P2_1/c$
 $a = 10.0019$ (12) Å
 $b = 10.9043$ (13) Å
 $c = 33.233$ (4) Å
 $\beta = 96.101$ (2)°
 $V = 3604.0$ (7) Å³
 $Z = 4$

$D_x = 1.331$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 5308 reflections
 $\theta = 2.2$ – 25.7 °
 $\mu = 0.75$ mm⁻¹
 $T = 295$ (2) K
 Block, colourless
 0.19 × 0.18 × 0.18 mm

Data collection

Bruker SMART APEX area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
 $T_{min} = 0.871$, $T_{max} = 0.877$
 26020 measured reflections

7409 independent reflections
 6457 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.024$
 $\theta_{max} = 26.5$ °
 $h = -12 \rightarrow 12$
 $k = -13 \rightarrow 13$
 $l = -41 \rightarrow 41$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.091$
 $S = 1.10$
 7409 reflections
 415 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 1.4856P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.68$ e Å⁻³
 $\Delta\rho_{min} = -0.59$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Sn1—O2	2.0720 (18)	Sn1—C21	2.140 (3)
Sn1—C11	2.150 (3)	Sn1—C31	2.158 (3)
O2—Sn1—C11	102.83 (10)	C11—Sn1—C21	117.99 (11)
O2—Sn1—C21	102.59 (10)	C11—Sn1—C31	114.70 (11)
O2—Sn1—C31	102.15 (10)	C21—Sn1—C31	113.59 (12)

H atoms were placed in calculated positions and refined in the riding-model approximation, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for aromatic H atoms, C—H = 0.96 Å and $U_{iso}(H) = 1.5U_{eq}(C)$ for methyl H atoms, and C—H = 0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$ for methylene H atoms.

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: ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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