

## Tricyclohexyl(4-nitrophenoxyacetato)tin(IV)

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## Key indicators

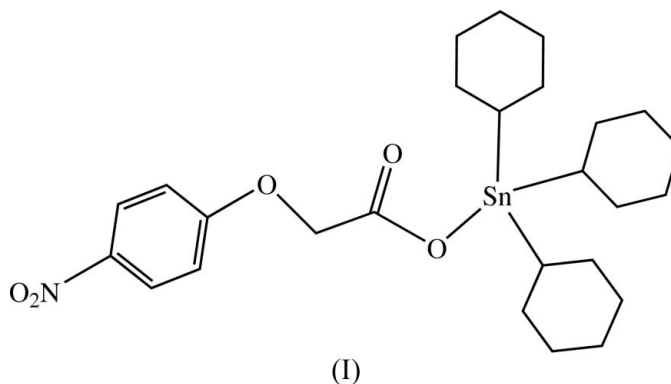
Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å  
 $R$  factor = 0.032  
 $wR$  factor = 0.076  
Data-to-parameter ratio = 18.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The coordination geometry about the Sn atom in the title compound,  $[\text{Sn}(\text{C}_6\text{H}_{11})_3(\text{C}_8\text{H}_6\text{NO}_5)]$ , is best described as highly distorted tetrahedral. There is an intermolecular interaction,  $2.769(2)$  Å, between the Sn atom and the carbonyl O atom of the carboxylate group of an adjacent molecule.

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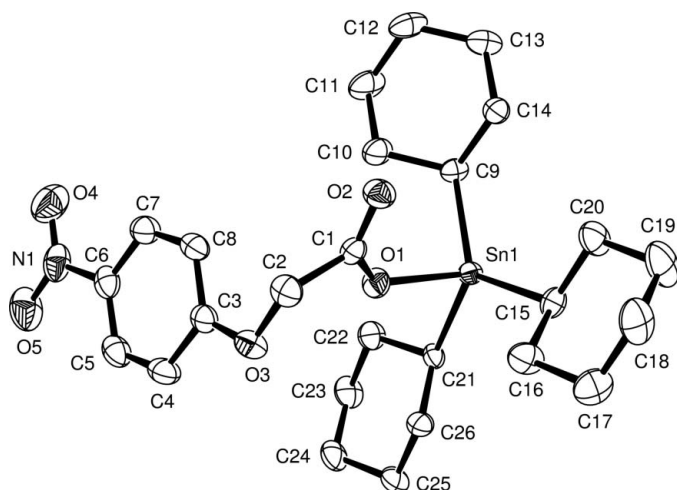
## Comment

Tricyclohexyltin carboxylates,  $(\text{C}_6\text{H}_{11})_3\text{Sn}(\text{O}_2\text{CR})$ , generally have a tetrahedral structure and do not auto-associate into chain structures *via* carboxylate bridging, due to the effects of the three bulky organic groups at Sn (Chandrasekhar *et al.*, 2002; Tiekink, 1991, 1994). 4-Nitrophenoxyacetic acid, whose crystal structure has been reported previously (Kumar & Rao, 1980), is a pesticide intermediate used in the synthesis of fungicides and plant-growth regulators (Xue & Zou, 1999). We present here the crystal structure analysis of its tricyclohexyltin ester, (I).

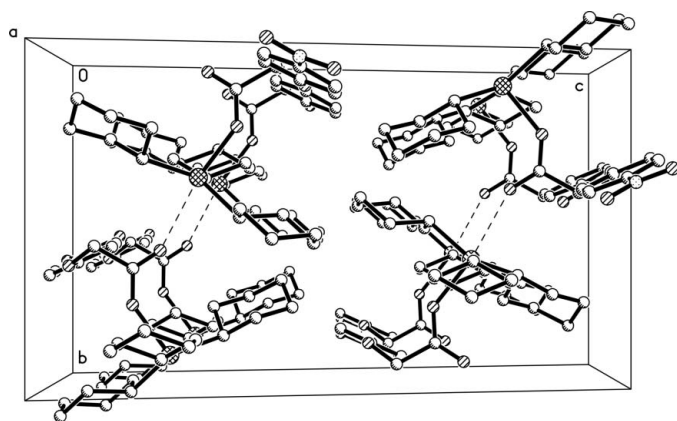


In (I), the Sn atom is best described as having a highly distorted tetrahedral geometry, the range of angles subtended at Sn being  $89.83(9)$ – $124.93(11)^\circ$  (Fig. 1, Table 1). An  $\text{Sn}1 \cdots \text{O}2^i$  intermolecular contact of  $2.769(2)$  Å [symmetry code: (i)  $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$ ] is not considered to be a significant bonding interaction (Willem *et al.*, 1998). If the  $\text{Sn}1 \cdots \text{O}2^i$  interaction were considered as a significant bonding interaction, then (I) would be described as a five-coordinate complex with the Sn atom having a *trans*- $R_3\text{SnO}_2$  trigonal-bipyramidal geometry. In that case, atoms C9, C15 and C21 would define the trigonal plane and a one-dimensional polymer would be formed through the apical positions occupied by O1 and O2 (Fig. 2). However, in this description, the Sn atom would lie  $0.238(2)$  Å out of the trigonal plane.

Atom  $\text{O}2^i$  exerts a steric influence on atom Sn1 from the opposite side of atom O1, and thus contributes to the distort-



**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.



**Figure 2**  
The crystal packing of (I), viewed along the *a* axis. Dashed lines indicate Sn...O interactions. H atoms have been omitted.

tion of the tetrahedral geometry around the Sn atom, by opening up the C—Sn1—C angles and contracting the O1—Sn1—C angles. The Sn1...O2 separation of 3.523 (3) Å, and the Sn1—O1 distance of 2.1317 (19) Å, are longer than those found in previously reported tricyclohexyltin carboxylates, such as tricyclohexyltin indole-3-acetate (Molloy *et al.*, 1986), trifluoroacetate (Calogero *et al.*, 1980), *N*-phthaloylglycinate (Ng & Kumar Das, 1997*a*), (*N,N*-diethylthiocarbamoylthio)acetate (Ng & Kumar Das, 1997*b*), 2-[2-(2-hydroxy-5-methylphenyl)-1-diazenyl]benzoate (Willem *et al.*, 1998), 2-(4-chlorophenyl)-3-methylbutyrate (Song *et al.*, 2003) and 4-biphenylacetate (Tian *et al.*, 2005). However, the three Sn—C distances in (I) are similar to those of the carboxylate structures mentioned above (Table 1).

## Experimental

Tricyclohexyltin hydroxide (0.577 g, 1.5 mmol) and 4-nitrophenoxycarboxylic acid (0.30 g, 1.5 mmol) in toluene (60 ml) were refluxed for 4 h

with azeotropic removal of water *via* a Dean–Stark trap. The resulting clear solution was evaporated to dryness under a vacuum. The pale-yellow solid obtained, (I), was recrystallized from ethanol and crystals of (I) were obtained from hexane–chloroform (1:1) by slow evaporation at 298 K (yield 70.3%; m.p. 358–359 K). Analysis, found: C 55.22, H 6.69, N 2.37%; calculated for C<sub>26</sub>H<sub>39</sub>NO<sub>5</sub>Sn: C 55.34, H 6.97, N 2.48%.

## Crystal data

[Sn(C<sub>6</sub>H<sub>11</sub>)<sub>3</sub>(C<sub>8</sub>H<sub>6</sub>NO<sub>5</sub>)]  
*M<sub>r</sub>* = 564.27  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 10.8892 (15) Å  
*b* = 11.7837 (16) Å  
*c* = 20.768 (3) Å  
 $\beta$  = 101.456 (2)°  
*V* = 2611.8 (6) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.435 Mg m<sup>-3</sup>  
 Mo K $\alpha$  radiation  
 Cell parameters from 5699 reflections  
 $\theta$  = 2.5–27.6°  
 $\mu$  = 1.01 mm<sup>-1</sup>  
*T* = 295 (2) K  
 Prism, pale yellow  
 0.22 × 0.09 × 0.09 mm

## Data collection

Bruker SMART APEX area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Bruker, 2002)  
*T<sub>min</sub>* = 0.808, *T<sub>max</sub>* = 0.914  
 20503 measured reflections

5390 independent reflections  
 4395 reflections with *I* > 2 $\sigma$ (*I*)  
*R<sub>int</sub>* = 0.040  
 $\theta_{max}$  = 26.5°  
*h* = -13 → 13  
*k* = -14 → 14  
*l* = -26 → 25

## Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.032  
*wR*(*F*<sup>2</sup>) = 0.076  
*S* = 1.02  
 5390 reflections  
 298 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.037P)^2 + 0.0495P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.50 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.41 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Sn1—O1	2.1317 (19)	Sn1—O2 <sup>i</sup>	2.769 (2)
Sn1—C21	2.144 (2)	O1—C1	1.274 (3)
Sn1—C9	2.152 (3)	O2—C1	1.217 (3)
Sn1—C15	2.155 (3)		
O1—Sn1—C21	89.83 (9)	C9—Sn1—C15	124.93 (11)
O1—Sn1—C9	99.86 (9)	O1—Sn1—O2 <sup>i</sup>	170.61 (11)
C21—Sn1—C9	116.16 (10)	C21—Sn1—O2 <sup>i</sup>	81.49 (9)
O1—Sn1—C15	98.68 (9)	C9—Sn1—O2 <sup>i</sup>	87.27 (9)
C21—Sn1—C15	115.26 (11)	C15—Sn1—O2 <sup>i</sup>	81.95 (9)

Symmetry code: (i)  $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$ .

H atoms were placed in calculated positions and refined in the riding-model approximation, with  $U_{iso}(\text{H}) = 1.2U_{eq}(\text{carrier C})$ . Constrained C—H distances were 0.93 for aromatic CH, 0.97 for methylene CH<sub>2</sub> and 0.98 Å for methine CH.

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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