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*Crystallographic report*

# Crystal and molecular structure of triphenyltin thiazole-2-carboxylate

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**The tin atom in the title compound is in a distorted $C_3O$ tetrahedral geometry, as the carboxylate ligand is effectively monodentate. Copyright © 2004 John Wiley & Sons, Ltd.**

**KEYWORDS:** crystal structure; triphenyltin; thiazole-2-carboxylate

## COMMENT

The monomeric structure of $Ph_3SnO_2CC_3H_2NS$, Fig. 1, is essentially tetrahedral, as the Sn···O2 separation of 2.771(2) Å is not considered to represent a significant bonding interaction. The structure is one of the two major motifs for $R_3Sn(O2CR')$, the other being polymeric with a trigonal bipyramidal geometry for ti.[1,2] The observed values are similar to those found for related species, such as triphenyltin thiophenyl-2-carboxylate,[3] tricyclohexyltin *N*-methylindole-3-acetate,[4] and tricyclohexyltin 2-[(*E*)-2-(2-hydroxy-5-methylphenyl)-1-diazenyl]benzoate.[5]

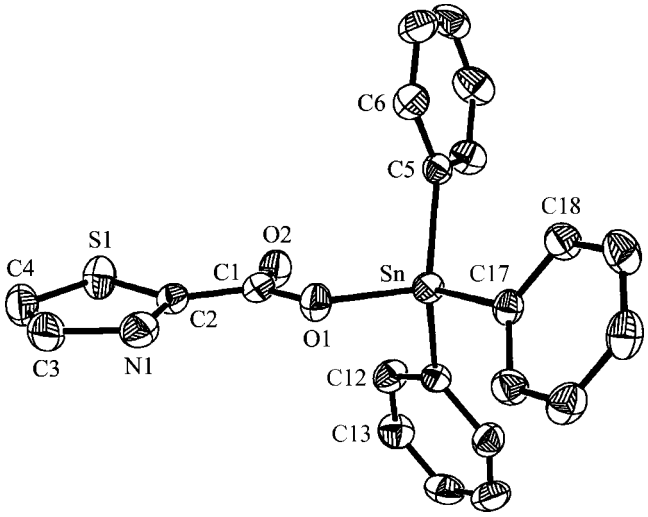


**Figure 1.** The molecular structure of $Ph_3SnO_2CC_3H_2NS$; hydrogen atoms have been omitted for clarity. Key geometric parametric parameters: Sn–O1 2.082(2), Sn–C5 2.123(3), Sn–C11 2.118(3), Sn–C17 2.139(3), Sn···O2 2.771(2) Å; O1–Sn–C5 109.23(10), O1–Sn–C11 108.15(10), O1–Sn–C17 94.32(9), C5–Sn–C11 118.08(11), C5–Sn–C17 110.70(1), C11–Sn–C17 113.61(1)°.

## EXPERIMENTAL

The salt $SNC_3H_2CO_2Na$ (1.2 mmol) was added to a benzene (10 ml) solution of $Ph_3SnCl$ (1.0 mmol) and stirred for 15 h at 40 °C. The precipitated salts were removed by filtration and the clear solution thus obtained was evaporated under vacuum to leave a white solid. The product was recrystallized from a dichloromethane–hexane solution to give colorless crystals; m.p. 78–80 °C. IR (KBr), $\upsilon$: 3061, 3025, 1620, 1426, 542, 448 $cm^{-1}$. Intensity data were collected at 301 K on a Bruker Smart 1000 CCD for a colorless block $0.40 \times 0.50 \times 0.60$ $mm^3$. $C_{22}H_{17}NO_2SSn$, $M = 478.12$, monoclinic, $P2_1/n$, $a = 13.433(4)$, $b = 11.766(4)$, $c = 14.247(4)$ Å, $\beta = 116.498(4)°$, $V = 2015.3(11)$ $Å^3$, $Z = 4$, 4096 unique data ($\theta_{max} = 26.5°$), 3387 data with $I \geq 2\sigma(I)$. $R = 0.027$ (obs. data), $wR = 0.063$ (all data).

Programs used: SHELXL and ORTEP. CCDC deposition number: 179921.

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