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Crystallographic report

Diphenyltin(IV) *N*-salicylidenevalinate

Han Dong Yin* and Qi Bao Wang

Department of Chemistry, Liaocheng University, Liaocheng 252059, People's Republic of China

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The title compound, {$Ph_2Sn[2\text{-}OC_6H_4CH{=}NCHCH(CH_3)_2COO]$}, is a five-coordinated monomer with trigonal bipyramidal tin and with the axial positions occupied by oxygen atoms derived from the tridentate ligand. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; tin; carboxylate; amino acid derivative

COMMENT

Recently organotin esters *N*-arylidene-amino acids have attracted considerable attention owing to their biological activity.[1,2] The structure of {$Ph_2Sn[2\text{-}OC_6H_4CH{=}NCHCH(CH_3)_2COO]$}, Fig. 1, is monomeric, features a distorted trigonal bipyramidal geometry for tin with oxygen atoms in axial positions, and is similar to [$Ph_2Sn(2\text{-}OC_6H_4C(CH_3){=}NCH_2COO)$].[3]

EXPERIMENTAL

To a benzene suspension of Ph_2SnO (0.288 g; 1 mmol) was added a benzene solution of *N*-salicylidenevaline (0.221 g; 1 mmol). The mixture was heated under reflux with stirring for about 7 h. The clear solution thus obtained was evaporated under vacuum to leave a yellow solid, which was recrystallized from a dichloromethane–hexane solution to give yellow crystals, m.p. 193 °C (dec.). IR (KBr): 3036, 2952, 1671, 1601, 1434, 1236, 576, 472, 445 cm^{-1}. Intensity data were collected at 298(2) K on a Bruker Smart 1000 CCD for a block 0.25 × 0.31 × 0.42 mm^3. $C_{24}H_{23}NO_3Sn$, $M = 492.12$, monoclinic, $P2_1/c$, $a = 8.534(2)$, $b = 10.171(2)$, $c = 24.696(6)$ Å, $\beta = 97.631(3)°$, $V = 2124.7(9)$ $Å^3$, $Z = 4$, 3738 unique data ($\theta_{max} = 25.0°$), $R = 0.020$, $wR = 0.052$. Programs used: SHELXL and ORTEP. CCDC deposition number: 232635.

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*Correspondence to: Han Dong Yin, Department of Chemistry, Liaocheng University, Liaocheng, 252059, People's Republic of China.
E-mail: handongyin@lctu.edu.cn
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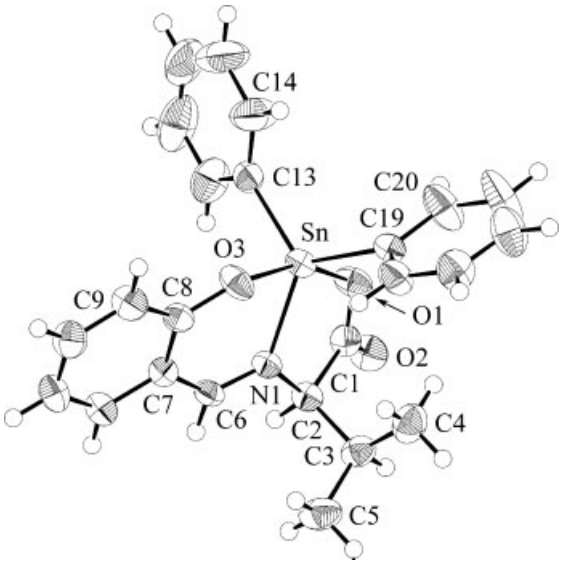

Figure 1. The molecular structure of {$Ph_2Sn[2\text{-}OC_6H_4CH{=}NCHCH(CH_3)_2COO]$}. Key geometric parameters: Sn–O1 2.139(2), Sn–O3 2.086(2), Sn–N1 2.156(2), Sn–C13 2.112(2), Sn–C19 2.112(2) Å; O1–Sn–O3 158.28(6), O1–Sn–N1 75.28(6), O1–Sn–C13 92.40(8), O1–Sn–C19 96.98(8), O3–Sn–N1 83.02(8), O3–Sn–C13 98.74(8), O3–Sn–C19 93.77(8), N1–Sn–C13 118.20(8), N1–Sn–C19 122.26(8), C13–Sn–C19 119.24(9)°.

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