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Crystallographic report

Chlorodiphenyltin(IV) piperidine-1-carbodithioate

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A trigonal bipyramidal C_2ClS_2 coordination geometry for tin is found in $Ph_2Sn(S_2CN(CH_2)_5)Cl$.

KEYWORDS: crystal structure; organotin; piperidinedithiocarbamate

COMMENT

The tin atom in $Ph_2Sn(S_2CN(CH_2)_5)Cl$ (Fig. 1) is five-coordinated within a C_2ClS_2 donor set that is best described as trigonal bipyramidal with the S1 and chlorine in the axial positions (Cl–Sn–S1 is 154.68(2)°) as for the literature precedent.[1]

EXPERIMENTAL

$Ph_2Sn(S_2CN(CH_2)_5)Cl$ was prepared by stirring $C_5H_{11}N$, CS_2 and Ph_2SnCl_2 (1 : 1 : 1) at 273 K in ethanol as per the literature method.[2] The solid product obtained was recrystallized from chloroform; m.p. 439–441 K. IR (KBr): ν(C–S) 1065, ν(Sn–C) 287, ν(Sn–S) 448, ν(Sn–Cl) 362 cm^{-1}. Intensity data were collected at 173(2) K on a Nonius KappaCCD diffractometer. $C_{18}H_{20}ClNS_2Sn$, $M = 468.61$, orthorhombic, $P2_12_12_1$, $a = 10.281(1)$, $b = 12.118(2)$, $c = 15.440(3)$ Å, $V = 1923.6(5)$ $Å^3$, $Z = 4$, 4400 reflections ($\theta_{max} = 27.5°$), $R = 0.022$ (4092 data with $I \geq 2\sigma(I)$), $wR = 0.050$ (all data); Flack parameter: −0.029(17). Programs used: SHELXL-97 and ORTEP II. CCDC deposition number: 247555.

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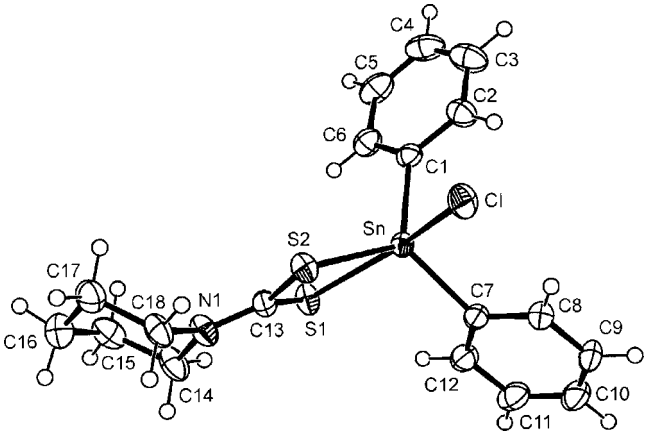

Figure 1. Molecular structure of $Ph_2Sn(S_2CN(CH_2)_5)Cl$. Key geometric parameters: Sn–Cl 2.4766(6), Sn–S1 2.628(7), Sn–S2 2.4736(7), Sn–C1 2.134(2), Sn–C7 2.146(2) Å; Cl–Sn–S1 154.68(2), S1–Sn–S2 70.47(2), C1–Sn–C7 114.36(9)°.

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