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Crystallographic report

Chlorodimethyltin(IV) piperidine-1-carbodithioate

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$Me_2Sn(S_2CN(CH_2)_5)Cl$ contains five-coordinated tin with a bidentate dithiocarbamate ligand spanning equatorial and axial positions in a distorted trigonal bipyramidal geometry. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; organotin; piperidinedithiocarbamate

COMMENT

$Me_2Sn(S_2CN(CH_2)_5)Cl$ (Fig. 1), features an asymmetrically chelating dithiocarbamate ligand. The tin atom, in accord with literature expectation,[1] is five-coordinated within a C_2ClS_2 donor set that is best described as trigonal-bipyramidal with the S1 and C1 atoms in axial positions, defining a bond angle of 154.56(2)°.

EXPERIMENTAL

$Me_2Sn(S_2CN(CH_2)_5)Cl$ was prepared by stirring 1 : 1 : 1 quantities of $C_5H_{11}N$, CS_2 and Me_2SnCl_2 at 273 K in ethanol, using the reported method.[2] The resulting residue was recrystallized from chloroform, giving colourless crystals; m.p. 371 K. IR (KBr): ν(C–S) 1112, ν(Sn–C) 557, ν(Sn–S) 435, ν(Sn–Cl) 362 cm^{-1}. Data were collected at 173(2) K on a Nonius KappaCCD diffractometer. $C_8H_{16}ClNS_2Sn$, $M = 344.48$, monoclinic, $P2_1/c$, $a = 10.817(3)$, $b = 10.044(2)$, $c = 12.508(4)$ Å, $\beta = 106.734(12)°$, $V = 1301.4(6)$ Å^3, $Z = 4$, $R = 0.023$ (2678 data with $I \geq 2\sigma(I)$), $wR = 0.056$ (all 2952 data). Programs used: SHELXL-97 and ORTEP II. CCDC deposition number: 247554.

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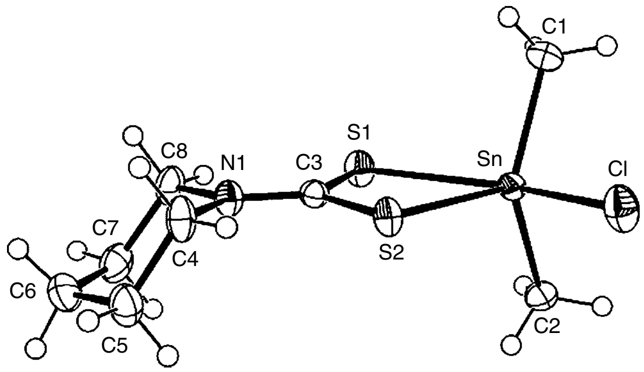

Figure 1. Molecular structure of $Me_2Sn(S_2CN(CH_2)_5)Cl$. Key geometric parameters: Sn–Cl 2.4929(8), Sn–S1 2.7114(8), Sn–S2 2.4838(8), Sn–C1 2.119(3), Sn–C2 2.116(2) Å; Cl–Sn–S1 154.56(2), S1–Sn–S2 68.656(19), C1–Sn–C2 130.93(11)°.

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