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(*N*-Ethyl-*N*-propyldithiocarbamato)triphenyltin(IV)

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Key indicators

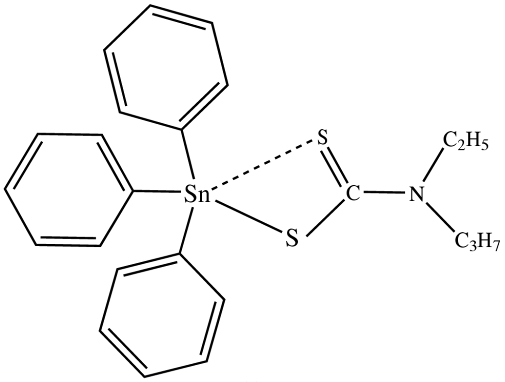
Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.005 Å
R factor = 0.028
wR factor = 0.063
Data-to-parameter ratio = 19.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, [Sn(C_6H_5)$_3$($C_6H_{12}NS_2$)], has a long-range intramolecular Sn···S interaction of 3.0950 (10) Å, which allows the geometry of the Sn atom to be close to trigonal bipyramidal, with an axial C—Sn—S bond angle of 156.50 (6)°. The structural dimensions of the molecule are comparable with those of other triphenyltin–dithiocarbamate complexes.

Comment

Several triphenyltin–dithiocarbamate complexes have been reported to have a geometry of the central Sn atom between tetrahedral and trigonal bipyrimidal due to the presence of a long interaction between the Sn atom and the uncoordinated S atom of the dithiocarbamate ligand. (*N*-Cyclohexyl-*N*-methyldithiocarbamato)triphenyltin(IV) (Awang *et al.*, 2003), (*n*-butyl-*N*-methyldithiocarbamato)triphenyltin(IV) (Kana *et al.*, 2001), (diethyldithiocarbamato)triphenyltin(IV) (Lindley & Carr, 1974) and (*N*-cyclohexyl-*N*-ethyldithiocarbamato)-triphenyltin(IV) (Awang *et al.*, 2003) are typical examples where the geometry of the central Sn atom in the complexes is close to trigonal bipyramidal. The title compound, (I) (Fig. 1), is analogous to those complexes and shows similar structural dimensions (Table 1) with a long intramolecular Sn1···S2 interaction of 3.0950 (10) Å, comparable with those in (*N*-cyclohexyl-*N*-methyldithiocarbamato)triphenyltin(IV) [3.0134 (8) Å]. The geometry of the Sn atom is also close to trigonal bipyramidal, with C2—Sn1—C19, C19—Sn1—S1 and C12—Sn1—S1 angles of 116.49 (3), 120.29 (7) and 110.95 (7)°, respectively, in the equatorial positions. The C18—Sn1—S2 angle for the axial position is 156.50 (6)°. Other bond lengths and angles of the ligand are in the normal ranges (Allen *et al.*, 1987).



(I)

Experimental

The title compound was synthesized by the addition of carbon disulfide (1.2 ml, 0.02 mol) to an ethanol solution of ethylpropylamine (1.743 g, 0.02 mol); the resulting solution was stirred for 1 h at 269 K. Triphenyltin(IV) chloride (3.84 g, 0.01 mol) was then added and the mixture was stirred for another 1 h. The white precipitate which formed was filtered off and washed with cold ethanol and dried in a vacuum. Good quality crystals were obtained by recrystallization from a mixture of ethanol and dichloromethane (1:2 *v*/*v*).

Crystal data

$[Sn(C_6H_5)_3(C_6H_{12}NS_2)]$
$M_r = 512.28$
Monoclinic, $P2_1/n$
$a = 9.4395$ (18) Å
$b = 26.225$ (5) Å
$c = 9.8059$ (19) Å
$\beta = 98.954$ (3)°
$V = 2397.9$ (8) Å^3
$Z = 4$

$D_x = 1.419$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 983 reflections
$\theta = 2.2$–26.5°
$\mu = 1.25$ mm^{-1}
$T = 273$ (2) K
Block, colourless
0.38 × 0.29 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.648$, $T_{max} = 0.825$
13 102 measured reflections

4928 independent reflections
4481 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 26.5°$
$h = -11 \rightarrow 11$
$k = -22 \rightarrow 32$
$l = -12 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.063$
$S = 1.14$
4928 reflections
255 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0247P)^2 + 0.9515P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.45$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—S1	2.4600 (7)	S1—C1	1.757 (2)
Sn1—S2	3.0950 (10)	S2—C1	1.679 (3)
Sn1—C12	2.132 (2)	N1—C1	1.328 (3)
Sn1—C19	2.134 (2)	N1—C4	1.469 (3)
Sn1—C18	2.154 (2)	N1—C2	1.478 (3)
C12—Sn1—C19	116.49 (9)	C19—Sn1—S1	120.29 (7)
C12—Sn1—C18	106.03 (9)	C12—Sn1—S1	110.95 (7)
C19—Sn1—C18	105.89 (9)	C18—Sn1—S2	156.50 (6)
C18—Sn1—S1	93.23 (6)		

After their location in a difference map, all H atoms were positioned geometrically and allowed to ride on their parent C atoms, with C—H = 0.93–0.97 Å, and $U_{iso}(H) = 1.5U_{eq}(C)$ for CH_3 and $1.2U_{eq}(C)$ for CH_2 and CH.

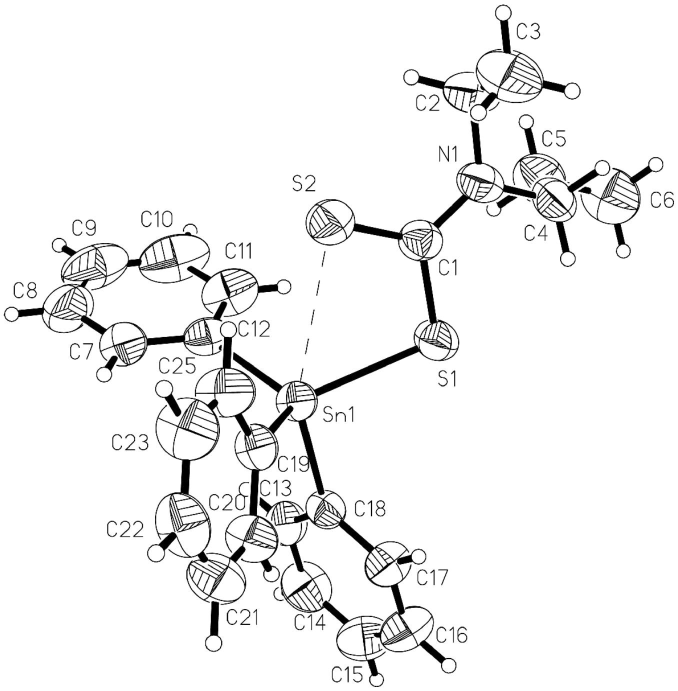


Figure 1
The molecular structure of (I) shown with 50% probability displacement ellipsoids. The dashed line indicates the long Sn···S interaction.

Data collection: *SMART* (Siemens, 1997); cell refinement: *SAINT* (Siemens, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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