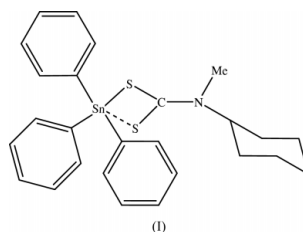


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Key indicators

Single-crystal X-ray study
 $T = 273$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.025
 wR factor = 0.070
Data-to-parameter ratio = 20.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*(N-Cyclohexyl-N-methyldithiocarbamato)-*
triphenyltin(IV)The title compound, $\text{Ph}_3\text{Sn}[\text{S}_2\text{CN}(\text{Me})\text{C}_6\text{H}_{11}]$, has an isobidentate ligand, with the tin coordination geometry intermediate between tetrahedral and distorted trigonal bipyramidal, owing to the presence of a long intramolecular $\text{Sn} \cdots \text{S}$ interaction of 3.0134 (8) Å.

Comment

(Dithiocarbamato)diorganotin complexes such as bis(dimethyldithiocarbamato)dimethyltin (Kimura *et al.*, 1972) and bis(diethyldithiocarbamato)diphenyltin (Lindley & Carr, 1974) are known to show an expansion and distortion of their coordination geometries due to weak intramolecular $\text{Sn} \cdots \text{S}$ interactions. The nature of the ligands and the substituents at the tin atom also have an influence on the coordination environment in the complex.

The title compound, (I), a triorganotin system with an unsymmetrical ligand, is isostructural to (*N*-butyl-*N*-methyldithiocarbamato)triphenyltin(IV), $\text{Ph}_3\text{Sn}[\text{S}_2\text{CN}(\text{CH}_3)(\text{C}_4\text{H}_9)]$ (Kana *et al.*, 2001), and (diethyldithiocarbamato)triphenyltin(IV) (Lindley & Carr, 1974). The isobidentate nature of the chelation, with $\text{Sn1}-\text{S1} = 2.4558$ (6) Å and a weak intramolecular $\text{Sn1} \cdots \text{S2}$ interaction of 3.0134 (8) Å [2.4631 (9) and 3.084 (1) Å respectively in $\text{Ph}_3\text{Sn}(\text{S}_2\text{CN}(\text{CH}_3)\text{C}_4\text{H}_9)]$, leads to a coordination geometry intermediate between tetrahedral and distorted trigonal bipyramidal. The angles $\text{C6}-\text{Sn1}-\text{S1}$, $\text{C6}-\text{Sn1}-\text{C18}$ and $\text{C18}-\text{Sn1}-\text{S1}$ [116.14 (5), 116.63 (8) and 116.28(6) Å, respectively] are close to 120°, as expected at equatorial positions, and the $\text{C12}-\text{Sn1}-\text{S2}$ angle for the axial positions is 158.43 (6)°. Other bond parameters of the dithiocarbamate ligand are normal and similar to those in bis(*N*-cyclohexyl-*N*-methyldithiocarbamato)dimethyltin(IV), which has a severely distorted octahedral geometry (Awang *et al.*, 2003.)

Experimental

The title compound was synthesized by the addition of carbon disulfide, CS_2 (1.8 ml, 0.03 mol), to an ethanolic solution of *N*-methylcyclohexylamine (4 ml, 0.03 mol) with stirring for one hour at 269 K. Triphenyltin(IV) chloride (11.6 g, 0.03 mol) solution was then added and the solution mixture was stirred for another hour. The

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resulting white precipitate was filtered, washed with cold ethanol and dried *in vacuo*. Crystals suitable for X-ray analysis were obtained by recrystallization from a 1:1 mixture of ethanol and chloroform.

Crystal data

[Sn(C₈H₁₄NS₂)(C₆H₅)₃]

$M_r = 538.31$

Triclinic, $P\bar{1}$

$a = 9.7951(17) \text{ \AA}$

$b = 11.342(2) \text{ \AA}$

$c = 11.952(2) \text{ \AA}$

$\alpha = 75.037(3)^\circ$

$\beta = 75.962(3)^\circ$

$\gamma = 89.058(3)^\circ$

$V = 1242.9(4) \text{ \AA}^3$

$Z = 2$

$D_x = 1.438 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation

Cell parameters from 6115 reflections

$\theta = 1.8\text{--}27.6^\circ$

$\mu = 1.21 \text{ mm}^{-1}$

$T = 273(2) \text{ K}$

Block, white

$0.53 \times 0.42 \times 0.26 \text{ mm}$

Data collection

Bruker SMART APEX CCD area-detector diffractometer

ω scans

Absorption correction: multi-scan

SADABS (Sheldrick, 1996)

$T_{\min} = 0.566$, $T_{\max} = 0.744$

15537 measured reflections

5658 independent reflections

5341 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.020$

$\theta_{\text{max}} = 27.6^\circ$

$h = -12 \rightarrow 12$

$k = -14 \rightarrow 14$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

$R[F^2 > 2\sigma(F^2)] = 0.025$

$wR(F^2) = 0.070$

$S = 1.06$

5658 reflections

271 parameters

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.3014P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} < 0.001$

$\Delta\rho_{\text{max}} = 0.53 \text{ e \AA}^{-3}$

$\Delta\rho_{\text{min}} = -0.41 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Sn1—S1	2.4558 (6)	S1—C19	1.753 (2)
Sn1—S2	3.0134 (8)	S2—C19	1.680 (2)
Sn1—C6	2.136 (2)	N1—C19	1.317 (3)
Sn1—C12	2.155 (2)	N1—C20	1.457 (3)
Sn1—C18	2.125 (2)	N1—C21	1.482 (3)
C6—Sn1—S1	116.14 (5)	C18—Sn1—C12	106.24 (8)
C18—Sn1—C6	116.63 (8)	C6—Sn1—C12	102.95 (8)
C18—Sn1—S1	116.28 (6)	C12—Sn1—S1	94.08 (6)
C12—Sn1—S2	158.43 (6)	C19—S1—Sn1	96.88 (7)

After their location in a difference Fourier map, all H-atoms were included in the refinement in geometrically calculated positions, and allowed to ride on the parent C atoms, with C—H = 0.93–0.98 \AA , respectively.

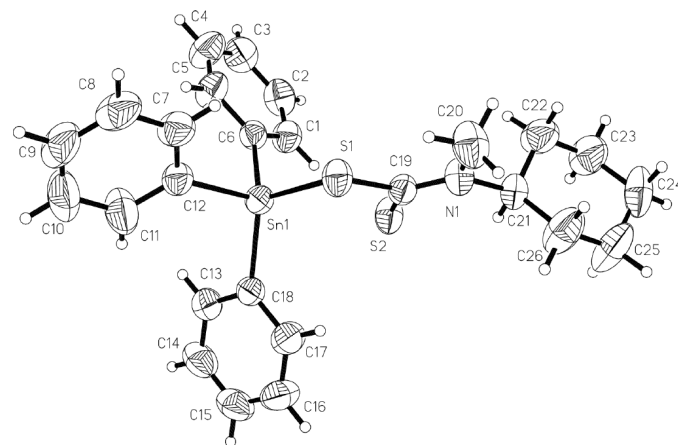


Figure 1

Molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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, 1990).

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