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(N-Cyclohexyl-N-ethyldithiocarbamato)-triphenyltin(IV)

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The title compound, [Sn(C_6H_5)$_3${$S_2CN(Et)C_6H_{11}$}], has a similar geometry to its methyl analogue, between tetrahedral and distorted trigonal bipyramidal but closer to the latter. The long intramolecular Sn···S interaction of 2.9426 (10) Å is slightly shorter than in its methyl analogue, 3.0134 (8) Å.

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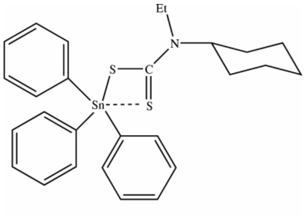
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.025
wR factor = 0.071
Data-to-parameter ratio = 20.5

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

Comment

The structural dimensions of the title compound, (I), are in agreement with the analogues (N-cyclohexyl-N-methyldithiocarbamato)triphenyltin(IV) (Awang *et al.*, 2003), (N-butyl-N-methyldithiocarbamato)triphenyltin (Kana *et al.*, 2001) and (diethyldithiocarbamato)triphenyltin(IV) (Lindley & Carr, 1974). The presence of an ethyl group results in only a slightly shorter weak intermolecular interaction [Sn1···S2 = 2.9426 (10) Å] compared with 3.0134 (8) Å in N-cyclohexyl-N-methyldithiocarbamato)triphenyltin(IV). The geometry of the central Sn atom is also between tetrahedral and trigonal bipyramidal, but closer to the latter with C15—Sn1—C22, C15—Sn1—S1 and C22—Sn1—S1 angles of 114.20 (8), 117.41 (6) and 118.88 (5)°, respectively, in the equatorial positions; the C21—Sn1—S2 angle for the axial positions is 157.11 (6)°.



(I)

Experimental

The title compound was synthesized by addition of carbon disulfide (1.8 ml, 0.03 mol) to an ethanolic solution of N-ethylcyclohexylamine (4 ml, 0.03 mol) and stirring for 1 h at 269 K. After stirring, triphenyltin(IV) chloride (11.6 g, 0.03 mol) solution was added and the solution mixture was further stirred for another 1 h. The white precipitate was filtered off and washed with cold ethanol and dried in vacuum. Some good quality crystals suitable for X-ray analysis were obtained by recrystallization from a 1:1 mixture of ethanol and chloroform.

Crystal data

[Sn(C_6H_5)$_3$($C_9H_{16}NS_2$)]
M_r = 552.34
Triclinic, $P\bar{1}$
a = 10.036 (2) Å
b = 11.435 (3) Å
c = 11.989 (3) Å
α = 105.586 (4)°
β = 105.443 (4)°
γ = 90.646 (4)°
V = 1272.4 (5) Å^3
Z = 2
D_x = 1.442 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6453 reflections
θ = 1.8–27.5°
μ = 1.18 mm^{-1}
T = 293 (2) K
Block, colourless
0.55 × 0.35 × 0.26 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.562$, $T_{\max} = 0.748$
16 186 measured reflections
5793 independent reflections
5492 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.022$
$\theta_{\max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -14 \rightarrow 14$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.025$
$wR(F^2) = 0.071$
$S = 1.05$
5793 reflections
282 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0385P)^2 + 0.5044P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.73$ e Å^{-3}
$\Delta\rho_{\min} = -0.42$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0054 (7)

Table 1
Selected geometric parameters (Å, °).

Sn1—S1	2.4758 (7)	Sn1—C21	2.170 (2)
Sn1—S2	2.9426 (10)	S1—C9	1.750 (2)
Sn1—C15	2.144 (2)	S2—C9	1.690 (2)
Sn1—C22	2.148 (2)		
C15—Sn1—C22	114.20 (8)	C15—Sn1—C21	106.21 (8)
C15—Sn1—S1	117.41 (6)	C22—Sn1—C21	103.04 (8)
C22—Sn1—S1	118.88 (5)	C21—Sn1—S1	92.04 (6)
C21—Sn1—S2	157.11 (6)		

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 distances in the range 0.93–0.97 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ or $1.5U_{\rm eq}({\rm C})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

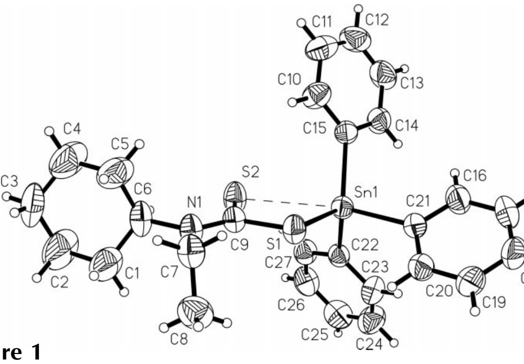


Figure 1
The molecular structure of (I), with 50% probability displacement ellipsoids.

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Acta Cryst. (2003). E**59**, m594–m595 Normah Awang *et al.* • $[{\rm Sn(C_6H_5)_3(C_9H_{16}NS_2)}]$ **m595**