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Key indicators

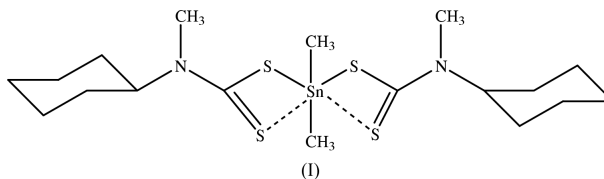
Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.032
 wR factor = 0.081
Data-to-parameter ratio = 23.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis(*N*-cyclohexyl-*N*-methyldithiocarbamato)-
dimethyltin(IV)

The molecule of the title compound, $[\text{Sn}(\text{CH}_3)_2(\text{C}_8\text{H}_{14}\text{NS}_2)_2]$, occupies a special position on a crystallographic mirror plane which coincides with the plane of the dimethyltin group. The severely distorted coordination tetrahedron formed by the four strong bonds of the Sn atom [$\text{Sn}-\text{C} = 2.101(4)$ and $2.108(5)\text{ \AA}$, $\text{Sn}-\text{S} = 2.5169(7)\text{ \AA}$, $\text{C}-\text{Sn}-\text{C} = 137.0(2)^\circ$ and $\text{S}-\text{Sn}-\text{S} = 84.46(3)^\circ$] is expanded to a distorted octahedron due to weak intramolecular $\text{Sn}\cdots\text{S}$ interactions of $2.9785(6)\text{ \AA}$.

Received 3 March 2003
Accepted 12 May 2003
Online 16 May 2003

Comment

The comparison of the geometry of numerous bis(dithiocarbamato)dimethyltin and bis(dithiocarbamato)diphenyltin complexes reveals interesting differences. It turns out that dimethyltin complexes show, in most cases, substantially larger $\text{C}-\text{Sn}-\text{C}$ angles than their diphenyltin analogues [*e.g.* $136.0(1)^\circ$ in $\text{Me}_2\text{Sn}(\text{S}_2\text{CNMe}_2)_2$ (Kimura *et al.*, 1972) and $101.4(6)^\circ$ in $\text{Ph}_2\text{Sn}(\text{S}_2\text{CNEt}_2)_2$ (Lindley & Carr, 1974)]. Furthermore, in diphenyltin complexes, one of the ligands usually chelates the Sn atom symmetrically, whereas the other ligand shows a considerable difference in the $\text{Sn}-\text{S}$ bond distances. By contrast, in dimethyltin complexes, both ligands display the same coordination pattern, with one shorter $\text{Sn}-\text{S}$ bond and one longer $\text{Sn}\cdots\text{S}$ 'secondary' contact.



The geometry of the title compound, (I), is typical for the bis(dithiocarbamato)dimethyltin complexes and illustrates the features outlined above. Just as in its analogue, bis[*N,N*-bis(2-hydroxyethyl)dithiocarbamato]dimethyltin(IV) (Farina *et al.*, 2000), molecule (I) has a crystallographic mirror plane, coinciding with the $\text{C}9/\text{Sn}1/\text{C}10$ plane. The severely distorted coordination tetrahedron formed by the four strong bonds of the Sn atom [$\text{Sn}1-\text{C}9 = 2.101(4)$, $\text{Sn}1-\text{C}10 = 2.108(5)$ and $\text{Sn}1-\text{S}1 = 2.5169(7)\text{ \AA}$; $\text{C}9-\text{Sn}1-\text{C}10 = 137.0(2)^\circ$ and $\text{S}1-\text{Sn}1-\text{S}1^i = 84.46(3)^\circ$; symmetry code: (i) $x, \frac{3}{2}-y, z$] is expanded to a distorted octahedron due to weak intramolecular $\text{Sn}1\cdots\text{S}2$ interactions of $2.9785(6)\text{ \AA}$, the $\text{S}2-\text{Sn}1-\text{S}2^i$ angle being $146.35(2)^\circ$.

The Sn atom shows a very small displacement from the plane of the coordinating atoms S1, S2, S1A and S2A [$0.0048(8)\text{ \AA}$]; the four-membered chelate ring is almost planar and the torsion angle $\text{Sn}1-\text{S}1-\text{C}8-\text{S}2$ is $-6.89(15)^\circ$.

Experimental

To a solution of *N*-methylcyclohexylamine (3.9 ml, 0.04 mol) in ethanol was added, with stirring at 273 K, carbon disulfide (1.8 ml, 0.03 mol). After stirring for 2 h, 3.295 g (0.015 mol) of dimethyltin(IV) chloride (10.00 ml) was added dropwise to the mixture. The mixture was then stirred vigorously for 1 h. The resulting white solid was recrystallized from chloroform.

Crystal data

[Sn(CH₃)₂(C₈H₁₄NS₂)₂]
M_r = 525.40
 Orthorhombic, *Pnma*
a = 13.2000 (9) Å
b = 19.9650 (14) Å
c = 8.9503 (6) Å
V = 2358.7 (3) Å³
Z = 4
D_x = 1.480 Mg m⁻³

Mo *K*α radiation
 Cell parameters from 4467 reflections
 θ = 2.0–27.6°
 μ = 1.44 mm⁻¹
T = 293 (2) K
 Block, light yellow
 0.27 × 0.22 × 0.16 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.696, *T_{max}* = 0.802
 15359 measured reflections

2795 independent reflections
 2441 reflections with *I* > 2σ(*I*)
R_{int} = 0.029
 θ_{\max} = 27.6°
h = −17 → 16
k = −25 → 25
l = −11 → 11

Refinement

Refinement on *F*²
R [*F*² > 2σ(*F*²)] = 0.032
wR (*F*²) = 0.081
S = 1.06
 2795 reflections
 118 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 0.8626P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.74 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.33 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Sn1—S1	2.5169 (7)	S2—C8	1.693 (3)
Sn1—S2	2.9785 (6)	C6—N1	1.482 (3)
Sn1—C9	2.101 (4)	C7—N1	1.457 (3)
Sn1—C10	2.108 (5)	C8—N1	1.330 (3)
S1—C8	1.748 (2)		
S1—Sn1—S1 ¹	84.46 (3)	C10—Sn1—S1	107.28 (10)
S2—Sn1—S2 ¹	146.35 (2)	C8—S1—Sn1	95.09 (8)
C9—Sn1—C10	137.0 (2)	S2—C8—S1	118.81 (13)
C9—Sn1—S1	104.23 (13)		

Symmetry code: (i) *x*, $\frac{3}{2}$ − *y*, *z*.

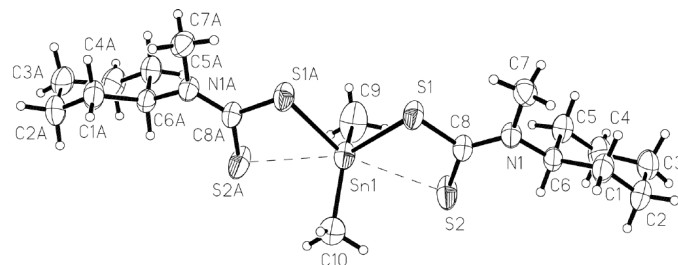


Figure 1

The molecular structure of the title compound, (I), with 50% probability displacement ellipsoids

After their location in a difference map, all H atoms were placed geometrically at ideal positions and allowed to ride on the parent atoms, with C—H = 0.93–0.97 Å. However, the H atoms at C9 and C10 were located in the map, refined initially, and then constrained.

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).

The authors thank the Malaysian Government and Universiti Kebangsaan Malaysia for the research grants IRPA No. 09-02-02-0048-EA144.

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