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Bis[*N*-(2-hydroxyethyl)-*N*-methyldithiocarbamato-*S*,*S*′]diphenyltin

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.054
wR factor = 0.146
Data-to-parameter ratio = 23.0

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

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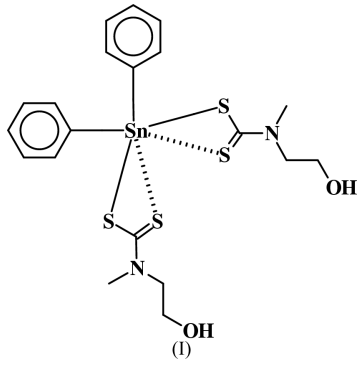
The Sn atom in the title compound, $[Sn(C_6H_5)_2(C_4H_8NOS_2)_2]$, is six-coordinate in a *cis*–C_2SnS_4 octahedral environment.

Comment

Six-coordinate bis-chelated diaryltin compounds generally adopt a *cis*-octahedral geometry (Ng *et al.*, 1987). The bond dimensions of the Sn atom in the title compound, (I), are similar to those found in the symmetrical compound, diphenyltin bis[bis(2-hydroxyethyl)dithiocarbamate] (Farina *et al.*, 2001).



(I)

Experimental

A solution of carbon disulfide in methanol was added to a mixture of diphenyltin dichloride and 2-hydroxyethylmethylamine (1:2 molar stoichiometry) at 277 K. The mixture was stirred to afford a pale-yellow solid, which was collected and recrystallized from a methanol/chloroform mixture to afford the title compound (m.p. 401–402 K). Elemental analysis, found (calculated) for $C_{20}H_{26}N_2O_2S_4Sn$: C 40.40 (41.90), H 4.83 (4.57), N 5.24 (4.89), Sn 20.88% (20.70%).

Crystal data

$[Sn(C_6H_5)_2(C_4H_8NOS_2)_2]$
M_r = 573.36
Monoclinic, *P*2/*c*
a = 8.9931 (1) Å
b = 12.2068 (1) Å
c = 22.6703 (3) Å
β = 92.507 (1)°
V = 2486.29 (5) Å^3
Z = 4
D_x = 1.532 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 8192 reflections
θ = 1.7–28.3°
μ = 1.38 mm^{-1}
T = 298 (2) K
Block, colorless
0.26 × 0.22 × 0.16 mm

Data collection

Siemens CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.715, T_{max} = 0.809
17 084 measured reflections
6025 independent reflections
4060 reflections with $I > 2\sigma(I)$
R_{int} = 0.087
θ_{max} = 28.3°
h = −11 → 11
k = −11 → 16
l = −30 → 22

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.054$	$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	$(\Delta/\sigma)_{max} = 0.001$
$S = 0.98$	$\Delta\rho_{max} = 1.22$ e Å^{-3}
6025 reflections	$\Delta\rho_{min} = -1.77$ e Å^{-3}
262 parameters	

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.164 (5)	Sn1—S2	2.641 (1)
Sn1—C7	2.177 (5)	Sn1—S3	2.550 (1)
Sn1—S1	2.614 (1)	Sn1—S4	2.748 (2)
C1—Sn1—C7	102.7 (2)	C7—Sn1—S4	161.6 (2)
C1—Sn1—S1	95.2 (1)	S1—Sn1—S2	68.2 (1)
C1—Sn1—S2	160.2 (1)	S1—Sn1—S3	152.9 (1)
C1—Sn1—S3	103.2 (1)	S1—Sn1—S4	93.8 (1)
C1—Sn1—S4	87.0 (1)	S2—Sn1—S3	89.4 (1)
C7—Sn1—S1	100.7 (1)	S2—Sn1—S4	83.7 (1)
C7—Sn1—S2	91.3 (1)	S3—Sn1—S4	67.8 (1)
C7—Sn1—S3	94.6 (1)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1a···O2^{i}	0.96	2.26	2.703 (8)	107
O2—H2a···O1^{i}	0.96	2.21	2.703 (8)	110
C15—H15a···S1	0.97	2.44	3.025 (8)	118
C19—H19b···S3	0.97	2.52	2.958 (7)	107

Symmetry code: (i) $1-x, 1-y, 1-z$.

One of the two hydroxyethyl groups is disordered, but this was not resolved. The N—C distance was *DFIX*ed at 1.47±0.01 Å, the C—C distance at 1.54±0.01 Å and the C—O distance at 1.43±0.01 Å; the S1/S2/C13/N1/C14/C15 system was restrained to be planar by *FLAT* 0.01.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

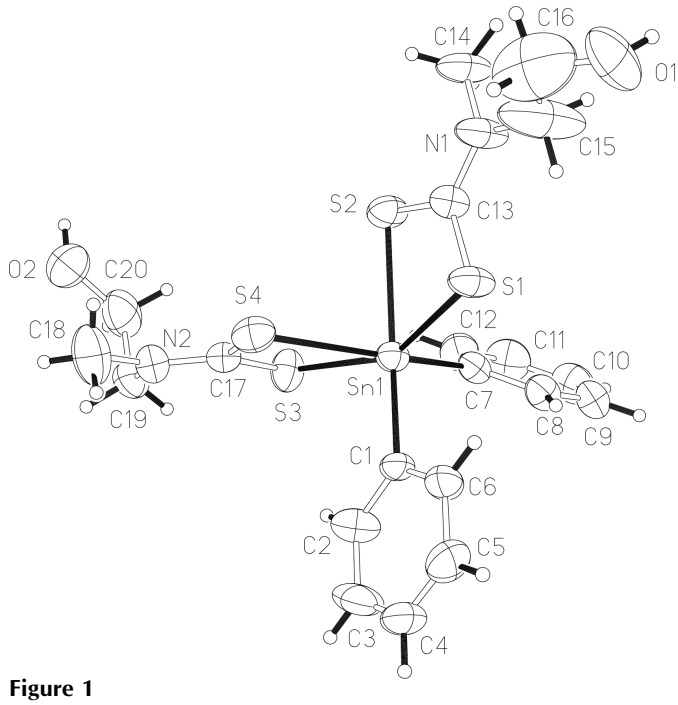


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title compound at the 50% probability level. H atoms are shown as circles of arbitrary radii.

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