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Bis[*N*,*N*-bis(2-hydroxyethyl)dithiocarbamato-*S*,*S*′]-diphenyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.048
wR factor = 0.112
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.

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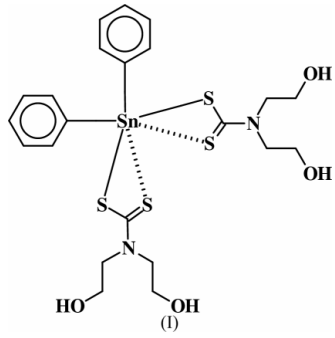
The Sn atom in the title compound, $[Sn(C_6H_5)_2(C_5H_{10}NO_2S_2)_2]$, is six-coordinate in a *cis*-C_2SnS_4 octahedral environment.

Comment

Six-coordinate bis-chelated diaryltin compounds generally adopt a *cis*-octahedral geometry (Ng *et al.*, 1987). In diphenyltin bis(diethyldithiocarbamate), (II), the chelation by one dithiocarbamate group is relatively symmetrical [Sn—S = 2.613 (5) and 2.637 (5) Å] whereas the chelation by the other is not [Sn—S = 2.548 (5) and 2.790 (6) Å]; the C—Sn—C angle is opened up to 101.4 (6) Å (Lindley & Carr, 1974). The bond dimensions in the title compound, (I), are similar to those in (II); in (I), the hydroxyl groups of each dithiocarbamate ligand are hydrogen bonded to each other. Adjacent molecules are linked by hydrogen bonds into a linear chain structure. The *cis* geometry contrasts with the skew-trapezoidal geometry [C—Sn—C = 139.3 (2)°] adopted by the dimethyltin homolog (Yang Farina *et al.*, 2000).



(I)

Experimental

A solution of carbon disulfide in methanol was added to a mixture of diphenyltin dichloride and diethanolamine (1:2 molar ratio) at 277 K. The mixture was stirred to afford a pale-yellow solid, which was recrystallized from a 3:2 methanol–chloroform mixture to afford (I) (m.p. 402–403 K). Elemental analysis, found (calculated) for $C_{22}H_{30}N_2O_4S_4Sn$: C 42.7 (41.7), H 4.6 (4.8), N 4.5 (4.4), Sn 18.3% (18.7%).

Crystal data

$[Sn(C_6H_5)_2(C_5H_{10}NO_2S_2)_2]$
M_r = 633.41
Triclinic, $P\overline{1}$
a = 9.0118 (2) Å
b = 12.4051 (1) Å
c = 12.6024 (2) Å
α = 86.889 (1)°
β = 69.575 (1)°
γ = 88.293 (1)°
V = 1318.24 (4) Å^3
Z = 2
D_x = 1.596 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 7568 reflections
θ = 1.6–29.5°
μ = 1.32 mm^{-1}
T = 298 (2) K
Block, colorless
0.40 × 0.22 × 0.20 mm

Data collection

Siemens CCD area-detector diffractometer
ω scans
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)
T_{min} = 0.621, T_{max} = 0.779
9804 measured reflections
6443 independent reflections
5242 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 29.5°
$h = -12 \rightarrow 10$
$k = -17 \rightarrow 16$
$l = -17 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.112
S = 0.98
6443 reflections
314 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.31 e Å^{-3}
$\Delta\rho_{min}$ = −1.91 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.156 (4)	Sn1—S2	2.624 (1)
Sn1—C7	2.160 (4)	Sn1—S3	2.540 (1)
Sn1—S1	2.606 (1)	Sn1—S4	2.827 (1)
C1—Sn1—C7	104.9 (1)	C7—Sn1—S4	160.3 (1)
C1—Sn1—S1	94.2 (1)	S1—Sn1—S2	68.3 (1)
C1—Sn1—S2	154.8 (1)	S1—Sn1—S3	158.4 (1)
C1—Sn1—S3	101.6 (1)	S1—Sn1—S4	101.0 (1)
C1—Sn1—S4	83.8 (1)	S2—Sn1—S3	91.8 (1)
C7—Sn1—S1	96.0 (1)	S2—Sn1—S4	82.1 (1)
C7—Sn1—S2	95.2 (1)	S3—Sn1—S4	66.6 (1)
C7—Sn1—S3	94.1 (1)		

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*a*···O2	0.77 (6)	1.90 (6)	2.660 (5)	167 (7)
O2—H2*a*···O4^{i}	0.80 (5)	1.90 (5)	2.692 (5)	173 (5)
O3—H3*a*···O1^{ii}	0.76 (4)	1.98 (5)	2.736 (5)	179 (4)
O4—H4*a*···O3	0.80 (5)	1.95 (5)	2.710 (5)	159 (5)

Symmetry codes: (i) $-x, 1-y, 1-z$; (ii) $1-x, 1-y, 1-z$.

The hydroxyl H atoms were located and refined.

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.

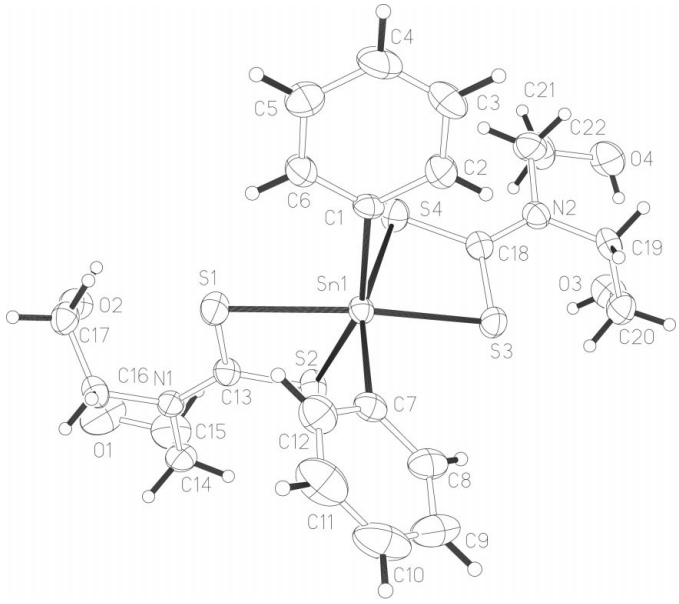


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title compound with ellipsoids at the 50% probability level. H atoms are shown as circles of arbitrary radii.

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References

Yang Farina, A. A., Othman, A. H., Baba, I., Sivakumar, K., Fun, H.-K. & Ng, S. W. (2000). *Acta Cryst.* C**56**, e84-e85.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Lindley, P. F. & Carr, P. (1974). *J. Cryst. Mol. Struct.* **4**, 173–185.
Ng, S. W., Chen, W., Kumar Das, V. G. & Mak, T. C. W. (1987). *J. Organomet. Chem.* **334**, 295–305.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Siemens (1996). *SAINT* and *SMART*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.