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Bis(*N*-ethyl-*N*-methyldithiocarbamato-κ^2S,S')diphenyltin(IV)

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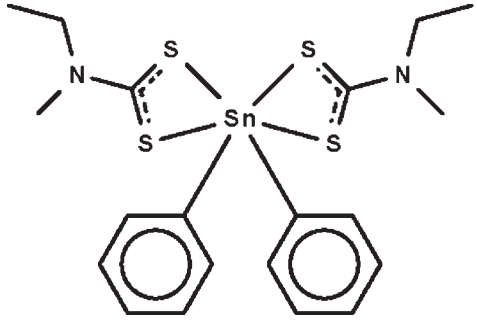
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.022; wR factor = 0.058; data-to-parameter ratio = 22.3.

The dithiocarbamate anions in the title compound, $[Sn(C_6H_5)_2(C_4H_8NS_2)_2]$, chelate to the Sn^{IV} atom, which is six-coordinated in a skew-trapezoidal-bipyramidal geometry. The molecule lies across a twofold rotation axis.

Related literature

For other diphenyltin bis(dithiocarbamate) compounds, see: Alcock *et al.* (1992); Farina *et al.* (2001*a*,*b*); Hook *et al.* (1994). For a discussion of the geometry of tin in diorganotin bis-chelates, see: Ng *et al.* (1987).



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_4H_8NS_2)_2]$
M_r = 541.36
Monoclinic, $C2/c$
a = 17.7925 (11) Å
b = 7.0928 (5) Å
c = 18.8889 (12) Å
β = 91.2716 (9)°
V = 2383.2 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 293 K
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.634, T_{max} = 0.814
9577 measured reflections
2739 independent reflections
2493 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.04
2739 reflections
123 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.1239 (19)	Sn1—S2	3.0167 (5)
Sn1—S1	2.5043 (5)		
C1—Sn1—C1^{i}	128.41 (11)		

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI5040).

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supporting information

Acta Cryst. (2010). E**66**, m355 [doi:10.1107/S1600536810007427]

Bis(*N*-ethyl-*N*-methyldithiocarbamato-$\kappa^2 S,S'$)diphenyltin(IV)

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S1. Experimental

Diphenyltin dichloride (10 mmol), ethylmethylamine (10 mmol) and carbon disulfide (10 mmol) were reacted in ethanol (50 ml) at 277 K to produce a white solid. The mixture was stirred for 1 h. The solid was collected and recrystallized from ethanol.

S2. Refinement

H atoms were placed in calculated positions (C–H = 0.93 to 0.96 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2–1.5U_{eq}(C).

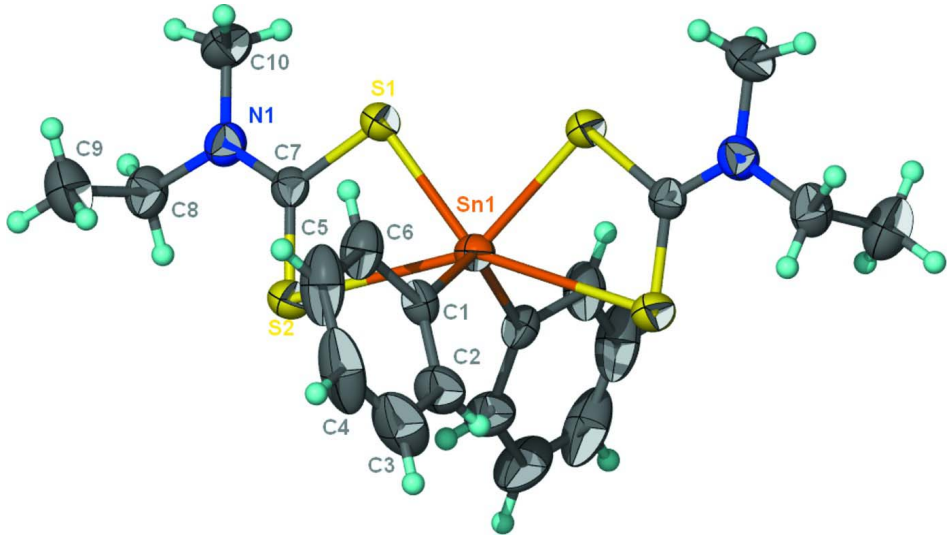

Figure 1

Displacement ellipsoid plot (Barbour, 2001) of $[Sn(C_6H_5)_2(C_4H_8NS_2)_2]$ at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry operation (1 - x, y, 3/2 - z).

Bis(*N*-ethyl-*N*-methyldithiocarbamato-$\kappa^2 S,S'$)diphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_2(C_4H_8NS_2)_2]$
M_r = 541.36
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 17.7925 (11) Å
b = 7.0928 (5) Å
c = 18.8889 (12) Å
β = 91.2716 (9)°
V = 2383.2 (3) Å^3
Z = 4
F(000) = 1096
D_x = 1.509 Mg m^{-3}
Mo *K*α radiation, λ = 0.71073 Å
Cell parameters from 5306 reflections

θ = 2.2–28.2°
μ = 1.43 mm^{-1}
T = 293 K

Block, colourless
0.35 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.634, T_{max} = 0.814

9577 measured reflections
2739 independent reflections
2493 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 2.2°
h = −20→22
k = −9→9
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.022
$wR(F^2)$ = 0.058
S = 1.04
2739 reflections
123 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 0.7977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.5000	0.38413 (2)	0.7500	0.04035 (7)
S1	0.45891 (3)	0.65032 (7)	0.67111 (3)	0.04919 (13)
S2	0.42774 (4)	0.27299 (7)	0.61016 (3)	0.05418 (14)
N1	0.41100 (11)	0.5964 (2)	0.53945 (9)	0.0507 (4)
C1	0.40305 (11)	0.2538 (3)	0.79172 (9)	0.0443 (4)
C2	0.40685 (16)	0.0719 (4)	0.81763 (14)	0.0662 (6)
H2	0.4526	0.0086	0.8191	0.079*
C3	0.3429 (2)	−0.0169 (5)	0.84136 (16)	0.0955 (11)
H3	0.3455	−0.1399	0.8583	0.115*
C4	0.2756 (2)	0.0781 (7)	0.83971 (16)	0.1033 (14)
H4	0.2327	0.0193	0.8563	0.124*
C5	0.27101 (15)	0.2563 (6)	0.81423 (15)	0.0919 (11)
H5	0.2250	0.3185	0.8127	0.110*
C6	0.33506 (13)	0.3464 (4)	0.79027 (13)	0.0645 (6)
H6	0.3319	0.4693	0.7733	0.077*
C7	0.43002 (10)	0.5087 (3)	0.59980 (10)	0.0414 (4)
C8	0.38489 (14)	0.4917 (4)	0.47687 (11)	0.0607 (6)
H8A	0.4069	0.3666	0.4777	0.073*
H8B	0.4016	0.5554	0.4346	0.073*
C9	0.30029 (16)	0.4746 (5)	0.47381 (15)	0.0858 (9)
H9A	0.2852	0.4060	0.4321	0.129*
H9B	0.2783	0.5982	0.4724	0.129*

H9C	0.2836	0.4088	0.5150	0.129*
C10	0.41159 (17)	0.8023 (3)	0.53227 (13)	0.0695 (7)
H10A	0.3976	0.8361	0.4846	0.104*
H10B	0.4611	0.8492	0.5432	0.104*
H10C	0.3764	0.8564	0.5643	0.104*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03637 (11)	0.03690 (11)	0.04792 (12)	0.000	0.00416 (7)	0.000
S1	0.0589 (3)	0.0391 (2)	0.0490 (3)	−0.0011 (2)	−0.0102 (2)	−0.0020 (2)
S2	0.0672 (4)	0.0414 (3)	0.0535 (3)	0.0006 (2)	−0.0079 (2)	−0.0050 (2)
N1	0.0552 (11)	0.0531 (10)	0.0437 (9)	0.0031 (8)	−0.0019 (8)	0.0021 (7)
C1	0.0397 (10)	0.0543 (11)	0.0390 (9)	−0.0084 (9)	0.0005 (7)	−0.0025 (8)
C2	0.0691 (16)	0.0583 (14)	0.0713 (15)	−0.0173 (12)	0.0015 (12)	0.0073 (11)
C3	0.112 (3)	0.097 (2)	0.0778 (19)	−0.060 (2)	−0.0050 (18)	0.0196 (17)
C4	0.072 (2)	0.182 (4)	0.0552 (15)	−0.066 (2)	0.0015 (14)	0.0113 (19)
C5	0.0418 (14)	0.171 (4)	0.0633 (16)	−0.0129 (19)	0.0031 (11)	−0.001 (2)
C6	0.0431 (12)	0.0930 (18)	0.0575 (13)	0.0025 (12)	0.0011 (10)	0.0039 (12)
C7	0.0349 (10)	0.0461 (10)	0.0431 (9)	0.0031 (8)	0.0006 (7)	−0.0019 (8)
C8	0.0657 (15)	0.0760 (16)	0.0402 (10)	0.0081 (12)	−0.0037 (10)	−0.0055 (11)
C9	0.076 (2)	0.108 (2)	0.0727 (17)	−0.0121 (18)	−0.0087 (14)	−0.0172 (17)
C10	0.089 (2)	0.0547 (13)	0.0646 (14)	0.0013 (13)	−0.0086 (13)	0.0156 (11)

Geometric parameters (Å, º)

Sn1—C1	2.1239 (19)	C3—H3	0.93
Sn1—C1^{i}	2.1239 (19)	C4—C5	1.354 (5)
Sn1—S1^{i}	2.5043 (5)	C4—H4	0.93
Sn1—S1	2.5043 (5)	C5—C6	1.391 (4)
Sn1—S2	3.0167 (5)	C5—H5	0.93
S1—C7	1.7485 (19)	C6—H6	0.93
S2—C7	1.684 (2)	C8—C9	1.510 (4)
N1—C7	1.336 (2)	C8—H8A	0.97
N1—C10	1.467 (3)	C8—H8B	0.97
N1—C8	1.463 (3)	C9—H9A	0.96
C1—C6	1.376 (3)	C9—H9B	0.96
C1—C2	1.382 (3)	C9—H9C	0.96
C2—C3	1.383 (4)	C10—H10A	0.96
C2—H2	0.93	C10—H10B	0.96
C3—C4	1.374 (5)	C10—H10C	0.96
C1—Sn1—C1^{i}	128.41 (11)	C4—C5—C6	120.1 (3)
C1—Sn1—S1^{i}	109.64 (5)	C4—C5—H5	119.9
C1^{i}—Sn1—S1^{i}	108.67 (6)	C6—C5—H5	119.9
C1—Sn1—S1	108.67 (6)	C1—C6—C5	120.0 (3)
C1^{i}—Sn1—S1	109.64 (5)	C1—C6—H6	120.0
S1^{i}—Sn1—S1	82.14 (2)	C5—C6—H6	120.0

C1—Sn1—S2	82.95 (5)	N1—C7—S2	123.74 (15)
C1^{i}—Sn1—S2	83.99 (5)	N1—C7—S1	117.02 (15)
S1^{i}—Sn1—S2	146.217 (16)	S2—C7—S1	119.24 (11)
S1—Sn1—S2	64.079 (15)	N1—C8—C9	111.7 (2)
C7—S1—Sn1	95.86 (7)	N1—C8—H8A	109.3
C7—S2—Sn1	80.30 (6)	C9—C8—H8A	109.3
C7—N1—C10	122.72 (18)	N1—C8—H8B	109.3
C7—N1—C8	121.53 (19)	C9—C8—H8B	109.3
C10—N1—C8	115.70 (18)	H8A—C8—H8B	107.9
C6—C1—C2	119.3 (2)	C8—C9—H9A	109.5
C6—C1—Sn1	120.37 (17)	C8—C9—H9B	109.5
C2—C1—Sn1	120.29 (17)	H9A—C9—H9B	109.5
C1—C2—C3	120.4 (3)	C8—C9—H9C	109.5
C1—C2—H2	119.8	H9A—C9—H9C	109.5
C3—C2—H2	119.8	H9B—C9—H9C	109.5
C4—C3—C2	119.5 (3)	N1—C10—H10A	109.5
C4—C3—H3	120.2	N1—C10—H10B	109.5
C2—C3—H3	120.2	H10A—C10—H10B	109.5
C5—C4—C3	120.7 (3)	N1—C10—H10C	109.5
C5—C4—H4	119.6	H10A—C10—H10C	109.5
C3—C4—H4	119.6	H10B—C10—H10C	109.5

C1—Sn1—S1—C7	−76.24 (8)	Sn1—C1—C2—C3	−176.6 (2)
C1^{i}—Sn1—S1—C7	68.53 (9)	C1—C2—C3—C4	−0.7 (4)
S1^{i}—Sn1—S1—C7	175.62 (7)	C2—C3—C4—C5	0.9 (5)
S2—Sn1—S1—C7	−4.19 (6)	C3—C4—C5—C6	−0.9 (5)
C1—Sn1—S2—C7	119.15 (9)	C2—C1—C6—C5	−0.5 (3)
C1^{i}—Sn1—S2—C7	−110.88 (9)	Sn1—C1—C6—C5	176.56 (19)
S1^{i}—Sn1—S2—C7	4.05 (8)	C4—C5—C6—C1	0.7 (4)
S1—Sn1—S2—C7	4.39 (7)	C10—N1—C7—S2	178.37 (19)
C1^{i}—Sn1—C1—C6	−153.86 (19)	C8—N1—C7—S2	1.1 (3)
S1^{i}—Sn1—C1—C6	70.36 (18)	C10—N1—C7—S1	−1.8 (3)
S1—Sn1—C1—C6	−17.76 (18)	C8—N1—C7—S1	−179.01 (16)
S2—Sn1—C1—C6	−77.32 (17)	Sn1—S2—C7—N1	173.36 (18)
C1^{i}—Sn1—C1—C2	23.16 (16)	Sn1—S2—C7—S1	−6.49 (10)
S1^{i}—Sn1—C1—C2	−112.61 (17)	Sn1—S1—C7—N1	−172.10 (15)
S1—Sn1—C1—C2	159.26 (16)	Sn1—S1—C7—S2	7.75 (12)
S2—Sn1—C1—C2	99.71 (17)	C7—N1—C8—C9	92.6 (3)
C6—C1—C2—C3	0.5 (4)	C10—N1—C8—C9	−84.8 (3)

Symmetry code: (i) $-x+1, y, -z+3/2$.