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

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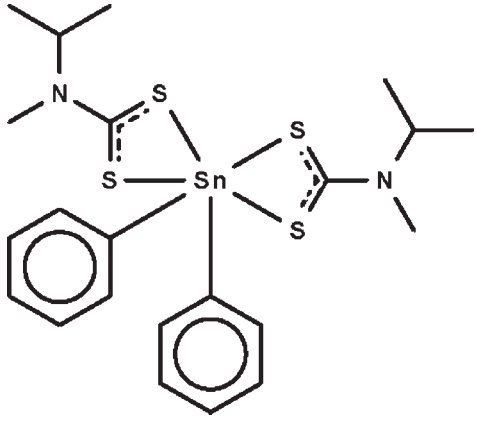
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.026; wR factor = 0.089; data-to-parameter ratio = 20.6.

The dithiocarbamate anions in the title compound, $[Sn(C_6H_5)_2(C_5H_{10}NS_2)_2]$, 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 bischelates, see: Ng *et al.* (1987).



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_5H_{10}NS_2)_2]$ M_r = 569.41
Orthorhombic, *Pbcn*
a = 18.8797 (10) Å
b = 9.2067 (5) Å
c = 14.5694 (8) Å
V = 2532.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.35 mm^{-1}
T = 293 K
0.35 × 0.35 × 0.20 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.649, T_{max} = 0.774
15127 measured reflections
2785 independent reflections
2291 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.089
S = 1.10
2785 reflections
135 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C1	2.167 (3)	Sn1—S2	2.6910 (8)
Sn1—S1	2.5820 (7)		

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: CI5039).

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supplementary materials

Acta Cryst. (2010). E**66**, m354 [**doi:10.1107/S1600536810007415**]

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

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Experimental

Diphenyltin dichloride (10 mmol), isopropylmethylamine (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.

Refinement

H atoms were placed in calculated positions (C–H = 0.93–0.98 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2-1.5U_{eq}(C).

Figures

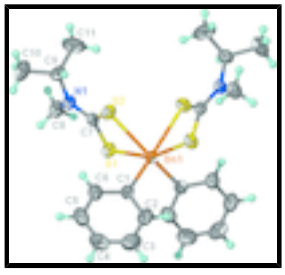

Fig. 1. Displacement ellipsoid plot (Barbour, 2001) of $[Sn(C_6H_5)_2(C_5H_{10}NS_2)_2]$ at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Unlabelled atoms are related to labelled atoms by the symmetry operation (1 - x, y, 1/2 - z).

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

Crystal data

$[Sn(C_6H_5)_2(C_5H_{10}NS_2)_2]$	$F(000)$ = 1160
M_r = 569.41	D_x = 1.493 Mg m^{-3}
Orthorhombic, *Pbcn*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -P 2n 2ab	Cell parameters from 6898 reflections
a = 18.8797 (10) Å	θ = 2.4–28.3°
b = 9.2067 (5) Å	μ = 1.35 mm^{-1}
c = 14.5694 (8) Å	*T* = 293 K
V = 2532.4 (2) Å^3	Block, colourless
Z = 4	0.35 × 0.35 × 0.20 mm

Data collection

Bruker SMART APEX	2785 independent reflections

diffractometer	
Radiation source: fine-focus sealed tube	2291 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.022$
ω scans	$\theta_{max} = 27.5°$, $\theta_{min} = 2.2°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -22\rightarrow22$
$T_{min} = 0.649$, $T_{max} = 0.774$	$k = -11\rightarrow11$
15127 measured reflections	$l = -13\rightarrow18$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.026$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.089$	H-atom parameters constrained
$S = 1.10$	$w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 2.0829P]$ where $P = (F_o^2 + 2F_c^2)/3$
2785 reflections	$(\Delta/\sigma)_{max} = 0.001$
135 parameters	$\Delta\rho_{max} = 0.29$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.30$ 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	0.71348 (3)	0.2500	0.03365 (10)
S1	0.44810 (4)	0.65957 (8)	0.41039 (4)	0.04395 (18)
S2	0.40918 (5)	0.48826 (9)	0.24740 (4)	0.04373 (19)
N1	0.36739 (12)	0.4240 (3)	0.41754 (14)	0.0388 (5)
C1	0.42071 (15)	0.8630 (3)	0.19862 (19)	0.0404 (6)
C2	0.44326 (19)	0.9844 (4)	0.1519 (3)	0.0648 (10)
H2	0.4911	0.9945	0.1382	0.078*
C3	0.3962 (2)	1.0925 (4)	0.1246 (3)	0.0802 (12)
H3	0.4128	1.1745	0.0941	0.096*
C4	0.3258 (2)	1.0776 (4)	0.1429 (3)	0.0722 (11)
H4	0.2943	1.1505	0.1258	0.087*
C5	0.3015 (2)	0.9560 (4)	0.1861 (3)	0.0692 (10)
H5	0.2533	0.9448	0.1969	0.083*
C6	0.34853 (18)	0.8492 (4)	0.2139 (2)	0.0544 (8)
H6	0.3314	0.7668	0.2434	0.065*
C7	0.40355 (14)	0.5130 (3)	0.36386 (17)	0.0356 (5)
C8	0.36473 (18)	0.4480 (4)	0.51766 (19)	0.0518 (8)
H8A	0.4088	0.4889	0.5379	0.078*
H8B	0.3568	0.3571	0.5482	0.078*
H8C	0.3268	0.5137	0.5319	0.078*
C9	0.33678 (18)	0.2865 (3)	0.3824 (2)	0.0486 (7)
H9	0.3324	0.2958	0.3156	0.058*

C10	0.2637 (2)	0.2584 (5)	0.4203 (3)	0.0784 (12)
H10A	0.2425	0.1787	0.3880	0.118*
H10B	0.2351	0.3437	0.4128	0.118*
H10C	0.2672	0.2350	0.4844	0.118*
C11	0.3871 (3)	0.1643 (5)	0.4012 (4)	0.1013 (17)
H11A	0.3723	0.0795	0.3681	0.152*
H11B	0.3875	0.1436	0.4658	0.152*
H11C	0.4339	0.1916	0.3818	0.152*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03059 (17)	0.03725 (15)	0.03310 (15)	0.000	0.00153 (9)	0.000
S1	0.0463 (4)	0.0523 (4)	0.0332 (3)	−0.0086 (3)	0.0028 (3)	−0.0052 (3)
S2	0.0555 (5)	0.0467 (4)	0.0290 (3)	−0.0106 (3)	0.0052 (3)	−0.0015 (3)
N1	0.0427 (13)	0.0454 (12)	0.0282 (10)	−0.0041 (10)	0.0043 (9)	0.0025 (9)
C1	0.0377 (16)	0.0452 (14)	0.0383 (14)	−0.0004 (11)	−0.0031 (11)	−0.0004 (11)
C2	0.050 (2)	0.063 (2)	0.082 (2)	−0.0027 (17)	−0.0015 (18)	0.0269 (19)
C3	0.085 (3)	0.062 (2)	0.093 (3)	0.006 (2)	−0.007 (2)	0.037 (2)
C4	0.072 (3)	0.072 (2)	0.073 (2)	0.029 (2)	−0.021 (2)	0.0082 (19)
C5	0.042 (2)	0.082 (3)	0.084 (3)	0.0168 (18)	−0.0038 (18)	0.008 (2)
C6	0.0450 (19)	0.0591 (19)	0.0591 (19)	0.0038 (15)	0.0025 (15)	0.0092 (16)
C7	0.0346 (14)	0.0408 (13)	0.0315 (12)	0.0029 (11)	0.0014 (10)	0.0024 (10)
C8	0.057 (2)	0.0659 (19)	0.0327 (13)	−0.0092 (16)	0.0060 (13)	0.0025 (13)
C9	0.060 (2)	0.0449 (16)	0.0413 (15)	−0.0084 (13)	0.0040 (14)	0.0043 (12)
C10	0.058 (3)	0.090 (3)	0.087 (3)	−0.026 (2)	0.004 (2)	0.004 (2)
C11	0.103 (4)	0.052 (2)	0.148 (5)	0.016 (2)	−0.014 (3)	−0.014 (3)

Geometric parameters (Å, °)

Sn1—C1^{i}	2.167 (3)	C4—C5	1.364 (6)
Sn1—C1	2.167 (3)	C4—H4	0.93
Sn1—S1^{i}	2.5820 (7)	C5—C6	1.386 (5)
Sn1—S1	2.5820 (7)	C5—H5	0.93
Sn1—S2	2.6910 (8)	C6—H6	0.93
Sn1—S2^{i}	2.6909 (8)	C8—H8A	0.96
S1—C7	1.728 (3)	C8—H8B	0.96
S2—C7	1.715 (3)	C8—H8C	0.96
N1—C7	1.323 (3)	C9—C10	1.508 (5)
N1—C8	1.476 (3)	C9—C11	1.498 (5)
N1—C9	1.483 (4)	C9—H9	0.98
C1—C2	1.376 (4)	C10—H10A	0.96
C1—C6	1.387 (4)	C10—H10B	0.96
C2—C3	1.392 (5)	C10—H10C	0.96
C2—H2	0.93	C11—H11A	0.96
C3—C4	1.362 (6)	C11—H11B	0.96
C3—H3	0.93	C11—H11C	0.96
C1^{i}—Sn1—C1	101.13 (15)	C4—C5—H5	119.9

C1^{i}—Sn1—S1^{i}	99.94 (8)	C6—C5—H5	119.9
C1—Sn1—S1^{i}	94.10 (7)	C1—C6—C5	121.1 (3)
C1^{i}—Sn1—S1	94.10 (7)	C1—C6—H6	119.4
C1—Sn1—S1	99.94 (8)	C5—C6—H6	119.4
S1^{i}—Sn1—S1	157.84 (4)	N1—C7—S2	122.3 (2)
C1^{i}—Sn1—S2	159.15 (7)	N1—C7—S1	120.20 (19)
C1—Sn1—S2	92.55 (8)	S2—C7—S1	117.49 (15)
S1^{i}—Sn1—S2	94.64 (2)	N1—C8—H8A	109.5
S1—Sn1—S2	67.84 (2)	N1—C8—H8B	109.5
C1^{i}—Sn1—S2^{i}	92.55 (8)	H8A—C8—H8B	109.5
C1—Sn1—S2^{i}	159.15 (7)	N1—C8—H8C	109.5
S1^{i}—Sn1—S2^{i}	67.84 (2)	H8A—C8—H8C	109.5
S1—Sn1—S2^{i}	94.64 (2)	H8B—C8—H8C	109.5
S2—Sn1—S2^{i}	79.19 (4)	N1—C9—C10	112.1 (3)
C7—S1—Sn1	88.84 (9)	N1—C9—C11	109.3 (3)
C7—S2—Sn1	85.58 (10)	C10—C9—C11	112.6 (3)
C7—N1—C8	120.6 (2)	N1—C9—H9	107.5
C7—N1—C9	121.7 (2)	C10—C9—H9	107.5
C8—N1—C9	117.1 (2)	C11—C9—H9	107.5
C2—C1—C6	117.3 (3)	C9—C10—H10A	109.5
C2—C1—Sn1	118.2 (2)	C9—C10—H10B	109.5
C6—C1—Sn1	124.4 (2)	H10A—C10—H10B	109.5
C1—C2—C3	121.7 (3)	C9—C10—H10C	109.5
C1—C2—H2	119.2	H10A—C10—H10C	109.5
C3—C2—H2	119.2	H10B—C10—H10C	109.5
C4—C3—C2	119.6 (4)	C9—C11—H11A	109.5
C4—C3—H3	120.2	C9—C11—H11B	109.5
C2—C3—H3	120.2	H11A—C11—H11B	109.5
C3—C4—C5	120.1 (3)	C9—C11—H11C	109.5
C3—C4—H4	120.0	H11A—C11—H11C	109.5
C5—C4—H4	120.0	H11B—C11—H11C	109.5
C4—C5—C6	120.2 (3)		
C1^{i}—Sn1—S1—C7	−166.32 (12)	C6—C1—C2—C3	2.9 (6)
C1—Sn1—S1—C7	91.61 (12)	Sn1—C1—C2—C3	−173.6 (3)
S1^{i}—Sn1—S1—C7	−36.91 (9)	C1—C2—C3—C4	−1.2 (7)
S2—Sn1—S1—C7	2.91 (9)	C2—C3—C4—C5	−1.3 (7)
S2^{i}—Sn1—S1—C7	−73.43 (9)	C3—C4—C5—C6	1.9 (6)
C1^{i}—Sn1—S2—C7	28.6 (2)	C2—C1—C6—C5	−2.2 (5)
C1—Sn1—S2—C7	−102.64 (12)	Sn1—C1—C6—C5	174.0 (3)
S1^{i}—Sn1—S2—C7	163.03 (9)	C4—C5—C6—C1	−0.1 (6)
S1—Sn1—S2—C7	−2.94 (9)	C8—N1—C7—S2	179.1 (2)
S2^{i}—Sn1—S2—C7	96.66 (9)	C9—N1—C7—S2	7.8 (4)
C1^{i}—Sn1—C1—C2	41.2 (2)	C8—N1—C7—S1	−0.2 (4)
S1^{i}—Sn1—C1—C2	−59.7 (3)	C9—N1—C7—S1	−171.5 (2)
S1—Sn1—C1—C2	137.5 (3)	Sn1—S2—C7—N1	−174.7 (2)

S2—Sn1—C1—C2	−154.6 (3)	Sn1—S2—C7—S1	4.59 (14)
S2^{i}—Sn1—C1—C2	−88.8 (3)	Sn1—S1—C7—N1	174.6 (2)
C1^{i}—Sn1—C1—C6	−135.0 (3)	Sn1—S1—C7—S2	−4.77 (15)
S1^{i}—Sn1—C1—C6	124.0 (3)	C7—N1—C9—C10	−139.3 (3)
S1—Sn1—C1—C6	−38.8 (3)	C8—N1—C9—C10	49.2 (4)
S2—Sn1—C1—C6	29.2 (3)	C7—N1—C9—C11	95.2 (4)
S2^{i}—Sn1—C1—C6	94.9 (3)	C8—N1—C9—C11	−76.4 (4)

Symmetry codes: (i) −*x*+1, *y*, −*z*+1/2.

Fig. 1