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## Structure Reports

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Bis(*N*-isopropyl-*N*-methyldithiocarbamato- $\kappa^2$ S,S')diphenyltin(IV)Amirah Faizah Muthalib,<sup>a</sup> Ibrahim Baba,<sup>a</sup> Yang Farina<sup>a</sup> and Seik Weng Ng<sup>b\*</sup><sup>a</sup>School of Chemical Sciences, Universiti Kebangsaan Malaysia, 43600 Bangi, Malaysia, and <sup>b</sup>Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

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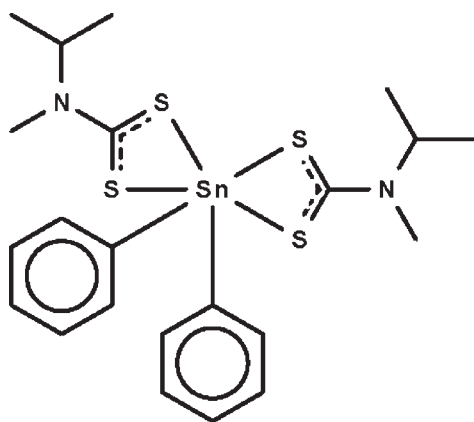
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.005$  Å;  $R$  factor = 0.026;  $wR$  factor = 0.089; data-to-parameter ratio = 20.6.

The dithiocarbamate anions in the title compound,  $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_5\text{H}_{10}\text{NS}_2)_2]$ , chelate to the  $\text{Sn}^{\text{IV}}$  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

 $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_5\text{H}_{10}\text{NS}_2)_2]$  $M_r = 569.41$ Orthorhombic, *Pbcn* $a = 18.8797$  (10) Å $b = 9.2067$  (5) Å $c = 14.5694$  (8) Å $V = 2532.4$  (2) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 1.35$  mm<sup>-1</sup> $T = 293$  K $0.35 \times 0.35 \times 0.20$  mm

## Data collection

Bruker SMART APEX diffractometer

Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{\text{min}} = 0.649$ ,  $T_{\text{max}} = 0.774$ 

15127 measured reflections

2785 independent reflections

2291 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.022$ 

## 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

 $\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>

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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## supporting information

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

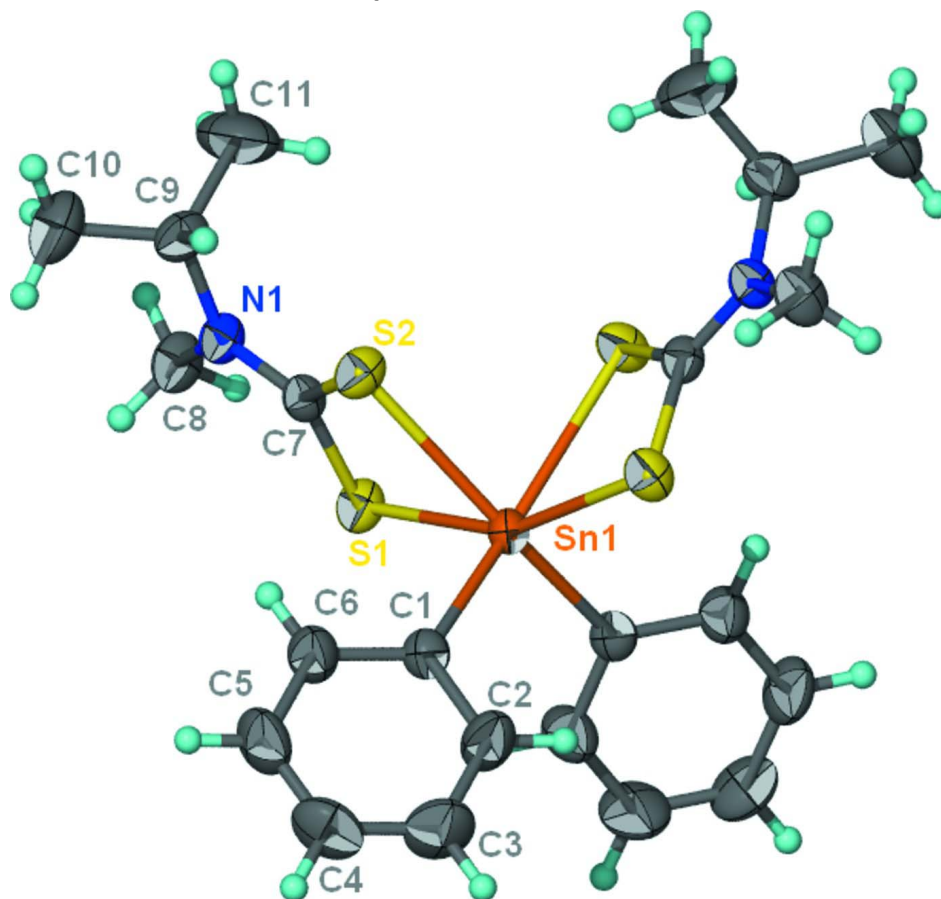
Amirah Faizah Muthalib, Ibrahim Baba, Yang Farina and Seik Weng Ng

**S1. 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.

**S2. 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 1.2–1.5 $U_{eq}(C)$ .



**Figure 1**

Displacement ellipsoid plot (Barbour, 2001) of  $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_5\text{H}_{10}\text{NS}_2)_2]$  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<sub>6</sub>H<sub>5</sub>)<sub>2</sub>(C<sub>3</sub>H<sub>7</sub>NS<sub>2</sub>)<sub>2</sub>] $M_r = 569.41$ Orthorhombic, *Pbcn*

Hall symbol: -P 2n 2ab

 $a = 18.8797$  (10) Å $b = 9.2067$  (5) Å $c = 14.5694$  (8) Å $V = 2532.4$  (2) Å<sup>3</sup> $Z = 4$  $F(000) = 1160$  $D_x = 1.493$  Mg m<sup>-3</sup>Mo *K* $\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 6898 reflections

 $\theta = 2.4$ – $28.3^\circ$  $\mu = 1.35$  mm<sup>-1</sup> $T = 293$  K

Block, colourless

 $0.35 \times 0.35 \times 0.20$  mm*Data collection*Bruker SMART APEX  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 $\omega$  scansAbsorption correction: multi-scan  
(*SADABS*; Sheldrick, 1996) $T_{\min} = 0.649$ ,  $T_{\max} = 0.774$ 

15127 measured reflections

2785 independent reflections

2291 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.022$  $\theta_{\text{max}} = 27.5^\circ$ ,  $\theta_{\text{min}} = 2.2^\circ$  $h = -22 \rightarrow 22$  $k = -11 \rightarrow 11$  $l = -13 \rightarrow 18$ *Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.026$  $wR(F^2) = 0.089$  $S = 1.10$ 

2785 reflections

135 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methodsSecondary atom site location: difference Fourier  
mapHydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.044P)^2 + 2.0829P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.001$  $\Delta\rho_{\text{max}} = 0.29$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.30$  e Å<sup>-3</sup>*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å<sup>2</sup>)*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
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<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
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 <sup>i</sup>	2.167 (3)	C4—C5	1.364 (6)
Sn1—C1	2.167 (3)	C4—H4	0.93
Sn1—S1 <sup>i</sup>	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 <sup>i</sup>	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 <sup>i</sup> —Sn1—C1	101.13 (15)	C4—C5—H5	119.9
C1 <sup>i</sup> —Sn1—S1 <sup>i</sup>	99.94 (8)	C6—C5—H5	119.9
C1—Sn1—S1 <sup>i</sup>	94.10 (7)	C1—C6—C5	121.1 (3)
C1 <sup>i</sup> —Sn1—S1	94.10 (7)	C1—C6—H6	119.4
C1—Sn1—S1	99.94 (8)	C5—C6—H6	119.4
S1 <sup>i</sup> —Sn1—S1	157.84 (4)	N1—C7—S2	122.3 (2)
C1 <sup>i</sup> —Sn1—S2	159.15 (7)	N1—C7—S1	120.20 (19)
C1—Sn1—S2	92.55 (8)	S2—C7—S1	117.49 (15)
S1 <sup>i</sup> —Sn1—S2	94.64 (2)	N1—C8—H8A	109.5
S1—Sn1—S2	67.84 (2)	N1—C8—H8B	109.5
C1 <sup>i</sup> —Sn1—S2 <sup>i</sup>	92.55 (8)	H8A—C8—H8B	109.5
C1—Sn1—S2 <sup>i</sup>	159.15 (7)	N1—C8—H8C	109.5
S1 <sup>i</sup> —Sn1—S2 <sup>i</sup>	67.84 (2)	H8A—C8—H8C	109.5
S1—Sn1—S2 <sup>i</sup>	94.64 (2)	H8B—C8—H8C	109.5
S2—Sn1—S2 <sup>i</sup>	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 <sup>i</sup> —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 <sup>i</sup> —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 <sup>i</sup> —Sn1—S1—C7	-73.43 (9)	C3—C4—C5—C6	1.9 (6)
C1 <sup>i</sup> —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 <sup>i</sup> —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 <sup>i</sup> —Sn1—S2—C7	96.66 (9)	C9—N1—C7—S2	7.8 (4)
C1 <sup>i</sup> —Sn1—C1—C2	41.2 (2)	C8—N1—C7—S1	-0.2 (4)
S1 <sup>i</sup> —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 <sup>i</sup> —Sn1—C1—C2	-88.8 (3)	Sn1—S1—C7—N1	174.6 (2)
C1 <sup>i</sup> —Sn1—C1—C6	-135.0 (3)	Sn1—S1—C7—S2	-4.77 (15)
S1 <sup>i</sup> —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 <sup>i</sup> —Sn1—C1—C6	94.9 (3)	C8—N1—C9—C11	-76.4 (4)

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