

## Di-*n*-butylbis(*N*-*n*-butyl-*N*-ethyldithiocarbamato- $\kappa$ S)tin(IV)

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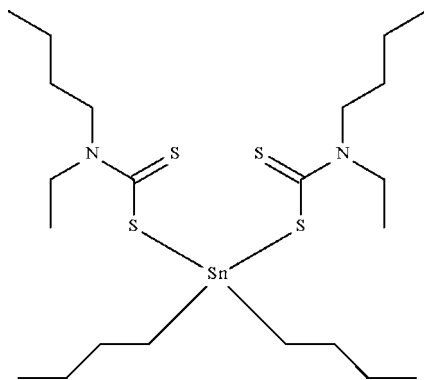
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Key indicators: single-crystal X-ray study;  $T = 123$  K; mean  $\sigma(\text{N}-\text{C}) = 0.012$  Å; some non-H atoms missing; disorder in main residue;  $R$  factor = 0.066;  $wR$  factor = 0.239; data-to-parameter ratio = 15.8.

The Sn atom in the title compound,  $[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_7\text{H}_{14}\text{NS}_2)_2]$ , exists in a tetrahedral  $\text{C}_2\text{S}_2\text{Sn}$  coordination geometry. The geometry is distorted towards skew-trapezoidal-bipyramidal owing to the proximity of the double-bond S atoms [ $\text{Sn}-\text{S} = 2.521$  (2) and  $\text{Sn}\cdots\text{S} = 2.933$  (2) Å]. The Sn atom lies on a special position of  $mm2$  site symmetry and the tin-bound *n*-butyl chain is disordered about a mirror plane. The ethyl and *n*-butyl groups of the dithiocarbamate unit are disordered about another mirror plane.

### Related literature

For other di-*n*-butyltin dithiocarbamates, see: Farina *et al.* (2000); Lokaj *et al.* (1986); Menezes *et al.* (2005); Vrabel *et al.* (1992*a,b*); Vrabel & Kello (1993); Zia-ur-Rehman *et al.* (2006). For a review of the applications and structures of tin dithiocarbamates, see: Tiekink (2008).



### Experimental

#### Crystal data

$[\text{Sn}(\text{C}_4\text{H}_9)_2(\text{C}_7\text{H}_{14}\text{NS}_2)_2]$   
 $M_r = 585.54$   
 Orthorhombic,  $Pmmn$   
 $a = 11.1317$  (2) Å  
 $b = 19.4349$  (3) Å  
 $c = 7.7262$  (1) Å

$V = 1671.51$  (5) Å<sup>3</sup>  
 $Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.02$  mm<sup>-1</sup>  
 $T = 123$  K  
 $0.30 \times 0.25 \times 0.20$  mm

#### Data collection

Bruker SMART APEX  
 diffractometer  
 Absorption correction: multi-scan  
 (SADABS; Sheldrick, 1996)  
 $T_{\text{min}} = 0.749$ ,  $T_{\text{max}} = 0.821$

11224 measured reflections  
 2072 independent reflections  
 1667 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.066$   
 $wR(F^2) = 0.239$   
 $S = 1.11$   
 2072 reflections  
 131 parameters

55 restraints  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 1.03$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.66$  e Å<sup>-3</sup>

Data collection: APEX2 (Bruker, 2008); cell refinement: SAINT (Bruker, 2008); 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, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2428).

### References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.  
 Bruker (2008). APEX2 and SAINT. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Farina, Y., Baba, I., Othman, A. H. & Ng, S. W. (2000). *Main Group Met. Chem.* **23**, 795–796.  
 Lokaj, J., Kello, E., Kettmann, V., Vrabel, V. & Rattay, V. (1986). *Collect. Czech. Chem. Commun.* **51**, 2521–2527.  
 Menezes, D. C., Vieira, F. T., de Lima, G. M., Porto, A. O., Cortes, M. E., Ardisson, J. D. & Albrecht-Schmitt, T. E. (2005). *Eur. J. Med. Chem.* **40**, 1277–1282.  
 Sheldrick, G. M. (1996). SADABS. University of Gottingen, Germany.  
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.  
 Tiekink, E. R. T. (2008). *Appl. Organomet. Chem.* **22**, 533–550.  
 Vrabel, V. & Kello, E. (1993). *Acta Cryst.* **C49**, 873–875.  
 Vrabel, V., Lokaj, J., Kello, E., Garaj, J., Batsanov, A. C. & Struchkov, Yu. T. (1992*b*). *Acta Cryst.* **C48**, 633–635.  
 Vrabel, V., Lokaj, J., Kello, E., Rattay, V., Batsanov, A. C. & Struchkov, Yu. T. (1992*a*). *Acta Cryst.* **C48**, 627–629.  
 Westrip, S. P. (2009). publCIF. In preparation.  
 Zia-ur-Rehman, Shahzadi, S., Ali, S., Badshah, A. & Jin, G.-X. (2006). *J. Iran. Chem. Soc.* **3**, 157–160.

**supplementary materials**

*Acta Cryst.* (2009). E65, m594 [ doi:10.1107/S1600536809014883 ]

## Di-*n*-butylbis(*N*-*n*-butyl-*N*-ethylthiocarbamato- $\kappa$ S)tin(IV)

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### Experimental

Carbon disulfide (4 ml, 0.06 mol) was added to *n*-butylisopropylamine (8 ml, 0.06 mol) in ethanol (50 ml) at 277 K. Dibutyltin dichloride (9.1 g, 0.03 mol) dissolved in ethanol (50 ml) was added. The white solid that precipitated was collected and recrystallized from ethanol.

### Refinement

The tin-bound butyl chain was allowed to refined off the mirror plane, as were the ethyl and butyl groups of the dithiocarbamate anion. 1,2-Related carbon-carbon distances were restrained to  $1.54 \pm 0.01$  Å and the 1,3-related ones to  $2.51 \pm 0.02$  Å. The N1–C6 and N1–C6' pair of distances were restrained to 0.01 Å as were the N1–C8 and N1–C8' pair. The temperature factors of the primed atoms were restrained to those of the unprimed ones; the anisotropic displacement parameters of the primed atoms were restrained to be nearly isotropic.

Carbon-bound H-atoms were placed in calculated positions (C–H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with  $U(\text{H})$  set to 1.2 to 1.5 $U(\text{C})$ . The final difference Fourier map had a large peak in the vicinity of the C9' atom.

### Figures

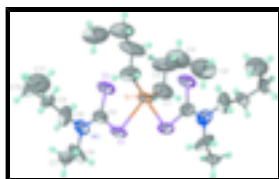


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of dibutylbis(*N*-*n*-butyl-*N*-ethylbutyldithiocarbamato)tin at the 70% probability level; the disorder is not shown. Unlabelled atoms are related by a 2-fold axis. Hydrogen atoms are drawn as spheres of arbitrary radius.

## Di-*n*-butylbis(*N*-*n*-butyl-*N*-ethylthiocarbamato- $\kappa$ S)tin(IV)

### Crystal data

[Sn(C<sub>4</sub>H<sub>9</sub>)<sub>2</sub>(C<sub>7</sub>H<sub>14</sub>NS<sub>2</sub>)<sub>2</sub>]

$M_r = 585.54$

Orthorhombic, *Pmmn*

Hall symbol: -P 2ab 2a

$a = 11.1317$  (2) Å

$b = 19.4349$  (3) Å

$c = 7.7262$  (1) Å

$V = 1671.51$  (5) Å<sup>3</sup>

$F_{000} = 612$

$D_x = 1.163$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 5407 reflections

$\theta = 2.8$ – $28.2^\circ$

$\mu = 1.02$  mm<sup>-1</sup>

$T = 123$  K

Block, colorless

# supplementary materials

$Z = 2$   $0.30 \times 0.25 \times 0.20$  mm

## Data collection

Bruker SMART APEX diffractometer	2072 independent reflections
Radiation source: fine-focus sealed tube	1667 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.024$
$T = 123$ K	$\theta_{\text{max}} = 27.5^\circ$
$\omega$ scans	$\theta_{\text{min}} = 2.1^\circ$
Absorption correction: Multi-scan (SADABS; Sheldrick, 1996)	$h = -14 \rightarrow 14$
$T_{\text{min}} = 0.749$ , $T_{\text{max}} = 0.821$	$k = -24 \rightarrow 25$
11224 measured reflections	$l = -10 \rightarrow 9$

## Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.239$	$w = 1/[\sigma^2(F_o^2) + (0.1484P)^2 + 2.8257P]$
$S = 1.11$	where $P = (F_o^2 + 2F_c^2)/3$
2072 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
131 parameters	$\Delta\rho_{\text{max}} = 1.03 \text{ e } \text{\AA}^{-3}$
55 restraints	$\Delta\rho_{\text{min}} = -0.66 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none

## Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.7500	0.2500	0.43290 (7)	0.0602 (4)	
S1	0.7500	0.33480 (11)	0.6798 (2)	0.0659 (6)	
S2	0.7500	0.39534 (11)	0.3309 (3)	0.0852 (9)	
N1	0.7500	0.4700 (4)	0.6210 (11)	0.0661 (18)	
C1	0.5831 (12)	0.257 (4)	0.3153 (12)	0.085 (10)	0.50
H1A	0.5315	0.2190	0.3580	0.102*	0.50
H1B	0.5448	0.3008	0.3488	0.102*	0.50
C2	0.5905 (11)	0.2529 (13)	0.1171 (11)	0.100 (5)	0.50
H2A	0.6437	0.2901	0.0752	0.120*	0.50
H2B	0.6277	0.2085	0.0843	0.120*	0.50
C3	0.4697 (14)	0.2591 (17)	0.0264 (19)	0.107 (9)	0.50
H3A	0.4814	0.2581	-0.1006	0.129*	0.50
H3B	0.4314	0.3034	0.0573	0.129*	0.50
C4	0.3882 (18)	0.1990 (16)	0.082 (3)	0.130 (9)	0.50
H4A	0.3075	0.2058	0.0345	0.195*	0.50

H4B	0.3839	0.1973	0.2087	0.195*	0.50
H4C	0.4215	0.1557	0.0384	0.195*	0.50
C5	0.7500	0.4065 (5)	0.5500 (10)	0.0576 (18)	
C6	0.744 (3)	0.4806 (13)	0.8169 (16)	0.085 (4)	0.25
H6A	0.7181	0.5282	0.8426	0.102*	0.25
H6B	0.6849	0.4485	0.8678	0.102*	0.25
C7	0.865 (3)	0.4679 (13)	0.8947 (16)	0.049 (4)	0.25
H7A	0.8610	0.4755	1.0200	0.074*	0.25
H7B	0.9235	0.4996	0.8437	0.074*	0.25
H7C	0.8896	0.4204	0.8716	0.074*	0.25
C6'	0.732 (3)	0.4781 (19)	0.8168 (18)	0.085 (4)	0.25
H6'1	0.6980	0.4354	0.8668	0.102*	0.25
H6'2	0.6764	0.5166	0.8415	0.102*	0.25
C7'	0.857 (3)	0.4929 (13)	0.895 (3)	0.049 (4)	0.25
H7'1	0.8499	0.4994	1.0199	0.074*	0.25
H7'2	0.8904	0.5346	0.8419	0.074*	0.25
H7'3	0.9108	0.4539	0.8711	0.074*	0.25
C8	0.7479 (19)	0.5360 (8)	0.521 (3)	0.083 (4)	0.50
H8A	0.7211	0.5739	0.5971	0.100*	0.25
H8B	0.6901	0.5321	0.4240	0.100*	0.25
C9	0.8705 (19)	0.5520 (8)	0.451 (3)	0.047 (4)	0.25
H9A	0.8942	0.5147	0.3706	0.056*	0.25
H9B	0.9283	0.5519	0.5483	0.056*	0.25
C10	0.8813 (14)	0.6206 (8)	0.356 (3)	0.042 (3)	0.25
H10A	0.9489	0.6186	0.2727	0.050*	0.25
H10B	0.8979	0.6579	0.4398	0.050*	0.25
C11	0.764 (3)	0.6359 (14)	0.259 (4)	0.102 (6)	0.25
H11A	0.7647	0.6837	0.2178	0.153*	0.25
H11B	0.6955	0.6291	0.3365	0.153*	0.25
H11C	0.7567	0.6048	0.1592	0.153*	0.25
C8'	0.734 (3)	0.5340 (12)	0.513 (5)	0.083 (4)	0.25
H8C	0.6770	0.5655	0.5725	0.100*	0.25
H8D	0.6985	0.5215	0.3999	0.100*	0.25
C9'	0.8539 (19)	0.5710 (11)	0.485 (3)	0.047 (4)	0.25
H9C	0.8873	0.5851	0.5982	0.056*	0.25
H9D	0.9114	0.5388	0.4302	0.056*	0.25
C10'	0.8399 (14)	0.6346 (8)	0.370 (3)	0.042 (3)	0.25
H10C	0.8562	0.6218	0.2482	0.050*	0.25
H10D	0.8999	0.6696	0.4046	0.050*	0.25
C11'	0.7130 (18)	0.6661 (16)	0.383 (4)	0.102 (6)	0.25
H11D	0.7018	0.6997	0.2898	0.153*	0.25
H11E	0.7037	0.6889	0.4951	0.153*	0.25
H11F	0.6528	0.6295	0.3717	0.153*	0.25

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn1	0.1059 (7)	0.0502 (5)	0.0245 (4)	0.000	0.000	0.000

## supplementary materials

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S1	0.1097 (17)	0.0588 (11)	0.0292 (8)	0.000	0.000	-0.0063 (7)
S2	0.172 (3)	0.0471 (11)	0.0367 (9)	0.000	0.000	-0.0001 (8)
N1	0.080 (4)	0.055 (4)	0.064 (4)	0.000	0.000	-0.018 (3)
C1	0.112 (9)	0.08 (3)	0.062 (6)	0.03 (2)	-0.015 (6)	-0.007 (11)
C2	0.135 (11)	0.112 (11)	0.053 (5)	0.075 (14)	0.011 (7)	0.029 (11)
C3	0.145 (13)	0.11 (2)	0.070 (7)	0.041 (19)	-0.030 (9)	0.006 (12)
C4	0.137 (18)	0.16 (2)	0.089 (13)	0.024 (18)	-0.032 (12)	0.002 (13)
C5	0.073 (5)	0.057 (4)	0.043 (4)	0.000	0.000	-0.006 (3)
C6	0.086 (8)	0.091 (6)	0.077 (6)	0.000 (8)	-0.029 (8)	-0.042 (5)
C7	0.048 (5)	0.066 (11)	0.034 (4)	0.002 (9)	-0.017 (4)	0.016 (6)
C6'	0.086 (8)	0.091 (6)	0.077 (6)	0.000 (8)	-0.029 (8)	-0.042 (5)
C7'	0.048 (5)	0.066 (11)	0.034 (4)	0.002 (9)	-0.017 (4)	0.016 (6)
C8	0.068 (7)	0.063 (5)	0.118 (7)	-0.021 (8)	0.010 (9)	0.001 (5)
C9	0.040 (6)	0.057 (8)	0.044 (7)	0.002 (6)	0.011 (5)	0.013 (7)
C10	0.031 (8)	0.035 (6)	0.058 (6)	0.010 (5)	0.014 (6)	0.005 (5)
C11	0.119 (11)	0.092 (9)	0.095 (9)	0.039 (9)	-0.007 (8)	0.002 (7)
C8'	0.068 (7)	0.063 (5)	0.118 (7)	-0.021 (8)	0.010 (9)	0.001 (5)
C9'	0.040 (6)	0.057 (8)	0.044 (7)	0.002 (6)	0.011 (5)	0.013 (7)
C10'	0.031 (8)	0.035 (6)	0.058 (6)	0.010 (5)	0.014 (6)	0.005 (5)
C11'	0.119 (11)	0.092 (9)	0.095 (9)	0.039 (9)	-0.007 (8)	0.002 (7)

### *Geometric parameters (Å, °)*

Sn1—C1	2.073 (13)	C7—H7B	0.9800
Sn1—C1 <sup>i</sup>	2.073 (13)	C7—H7C	0.9800
Sn1—C1 <sup>ii</sup>	2.073 (13)	C6'—C7'	1.545 (10)
Sn1—C1 <sup>iii</sup>	2.073 (13)	C6'—H6'1	0.9900
Sn1—S1	2.5211 (19)	C6'—H6'2	0.9900
Sn1—S1 <sup>iii</sup>	2.5211 (19)	C7'—H7'1	0.9800
S1—C5	1.718 (9)	C7'—H7'2	0.9800
S2—C5	1.707 (8)	C7'—H7'3	0.9800
N1—C5	1.350 (11)	C8—C9	1.4998
N1—C8	1.499 (14)	C8—H8A	0.9900
N1—C8'	1.508 (15)	C8—H8B	0.9900
N1—C8 <sup>iii</sup>	1.508 (15)	C9—C10	1.527 (9)
N1—C6	1.528 (14)	C9—H9A	0.9900
N1—C6 <sup>ii</sup>	1.528 (14)	C9—H9B	0.9900
N1—C6 <sup>iii</sup>	1.534 (15)	C10—C11	1.536 (10)
N1—C6'	1.534 (15)	C10—H10A	0.9900
C1—C2	1.536 (9)	C10—H10B	0.9900
C1—H1A	0.9900	C11—H11A	0.9800
C1—H1B	0.9900	C11—H11B	0.9800
C2—C3	1.520 (9)	C11—H11C	0.9800
C2—H2A	0.9900	C8'—C9'	1.536 (10)
C2—H2B	0.9900	C8'—H8C	0.9900
C3—C4	1.540 (10)	C8'—H8D	0.9900
C3—H3A	0.9900	C9'—C10'	1.529 (10)
C3—H3B	0.9900	C9'—H9C	0.9900

C4—H4A	0.9800	C9'—H9D	0.9900
C4—H4B	0.9800	C10'—C11'	1.543 (10)
C4—H4C	0.9800	C10'—H10C	0.9900
C6—C7	1.4925	C10'—H10D	0.9900
C6—H6A	0.9900	C11'—H11D	0.9800
C6—H6B	0.9900	C11'—H11E	0.9800
C7—H7A	0.9800	C11'—H11F	0.9800
C1—Sn1—C1 <sup>ii</sup>	127.4 (9)	C6—C7—H7A	109.5
C1 <sup>i</sup> —Sn1—C1 <sup>ii</sup>	128.0 (6)	C6—C7—H7B	109.5
C1—Sn1—C1 <sup>iii</sup>	128.0 (6)	H7A—C7—H7B	109.5
C1 <sup>i</sup> —Sn1—C1 <sup>iii</sup>	127.4 (9)	C6—C7—H7C	109.5
C1—Sn1—S1	106.9 (14)	H7A—C7—H7C	109.5
C1 <sup>i</sup> —Sn1—S1	111.9 (15)	H7B—C7—H7C	109.5
C1 <sup>ii</sup> —Sn1—S1	106.9 (14)	N1—C6'—C7'	106.5 (19)
C1 <sup>iii</sup> —Sn1—S1	111.9 (15)	N1—C6'—H6'1	110.4
C1—Sn1—S1 <sup>iii</sup>	111.9 (15)	C7'—C6'—H6'1	110.4
C1 <sup>i</sup> —Sn1—S1 <sup>iii</sup>	106.9 (14)	N1—C6'—H6'2	110.4
C1 <sup>ii</sup> —Sn1—S1 <sup>iii</sup>	111.9 (15)	C7'—C6'—H6'2	110.4
C1 <sup>iii</sup> —Sn1—S1 <sup>iii</sup>	106.9 (14)	H6'1—C6'—H6'2	108.6
S1—Sn1—S1 <sup>iii</sup>	81.64 (10)	C6'—C7'—H7'1	109.5
C5—S1—Sn1	95.1 (3)	C6'—C7'—H7'2	109.5
C5—N1—C8	124.9 (12)	H7'1—C7'—H7'2	109.5
C5—N1—C8'	122.0 (17)	C6'—C7'—H7'3	109.5
C5—N1—C8 <sup>ii</sup>	122.0 (17)	H7'1—C7'—H7'3	109.5
C5—N1—C6	121.7 (12)	H7'2—C7'—H7'3	109.5
C8—N1—C6	113.3 (14)	N1—C8—C9	110.5 (8)
C8'—N1—C6	115.5 (18)	N1—C8—H8A	109.6
C8 <sup>iii</sup> —N1—C6	116.1 (19)	C9—C8—H8A	109.6
C5—N1—C6 <sup>ii</sup>	121.7 (12)	N1—C8—H8B	109.6
C8—N1—C6 <sup>ii</sup>	113.4 (14)	C9—C8—H8B	109.6
C8'—N1—C6 <sup>ii</sup>	116.1 (19)	H8A—C8—H8B	108.1
C8 <sup>iii</sup> —N1—C6 <sup>ii</sup>	115.5 (18)	C8—C9—C10	115.2 (9)
C5—N1—C6 <sup>iii</sup>	119.7 (16)	C8—C9—H9A	108.5
C8—N1—C6 <sup>iii</sup>	115.1 (18)	C10—C9—H9A	108.5
C8'—N1—C6 <sup>iii</sup>	118 (2)	C8—C9—H9B	108.5
C8 <sup>iii</sup> —N1—C6 <sup>iii</sup>	116 (2)	C10—C9—H9B	108.5
C5—N1—C6'	119.7 (16)	H9A—C9—H9B	107.5
C8—N1—C6'	114.8 (18)	C9—C10—C11	109.7 (12)
C8'—N1—C6'	116 (2)	C9—C10—H10A	109.7
C8 <sup>iii</sup> —N1—C6'	118 (2)	C11—C10—H10A	109.7
C2—C1—Sn1	112.7 (9)	C9—C10—H10B	109.7
C2—C1—H1A	109.1	C11—C10—H10B	109.7
Sn1—C1—H1A	109.1	H10A—C10—H10B	108.2
C2—C1—H1B	109.1	C10—C11—H11A	109.5

## supplementary materials

Sn1—C1—H1B	109.1	C10—C11—H11B	109.5
H1A—C1—H1B	107.8	H11A—C11—H11B	109.5
C3—C2—C1	114.1 (9)	C10—C11—H11C	109.5
C3—C2—H2A	108.7	H11A—C11—H11C	109.5
C1—C2—H2A	108.7	H11B—C11—H11C	109.5
C3—C2—H2B	108.7	N1—C8'—C9'	111.1 (17)
C1—C2—H2B	108.7	N1—C8'—H8C	109.4
H2A—C2—H2B	107.6	C9'—C8'—H8C	109.4
C2—C3—C4	109.4 (13)	N1—C8'—H8D	109.4
C2—C3—H3A	109.8	C9'—C8'—H8D	109.4
C4—C3—H3A	109.8	H8C—C8'—H8D	108.0
C2—C3—H3B	109.8	C10'—C9'—C8'	111.9 (11)
C4—C3—H3B	109.8	C10'—C9'—H9C	109.2
H3A—C3—H3B	108.2	C8'—C9'—H9C	109.2
C3—C4—H4A	109.5	C10'—C9'—H9D	109.2
C3—C4—H4B	109.5	C8'—C9'—H9D	109.2
H4A—C4—H4B	109.5	H9C—C9'—H9D	107.9
C3—C4—H4C	109.5	C9'—C10'—C11'	112.1 (12)
H4A—C4—H4C	109.5	C9'—C10'—H10C	109.2
H4B—C4—H4C	109.5	C11'—C10'—H10C	109.2
N1—C5—S2	121.3 (7)	C9'—C10'—H10D	109.2
N1—C5—S1	120.3 (6)	C11'—C10'—H10D	109.2
S2—C5—S1	118.4 (5)	H10C—C10'—H10D	107.9
C7—C6—N1	109.8 (11)	C10'—C11'—H11D	109.5
C7—C6—H6A	109.7	C10'—C11'—H11E	109.5
N1—C6—H6A	109.7	H11D—C11'—H11E	109.5
C7—C6—H6B	109.7	C10'—C11'—H11F	109.5
N1—C6—H6B	109.7	H11D—C11'—H11F	109.5
H6A—C6—H6B	108.2	H11E—C11'—H11F	109.5
C1—Sn1—S1—C5	-69.5 (16)	C6 <sup>iii</sup> —N1—C5—S1	8.7 (14)
C1 <sup>i</sup> —Sn1—S1—C5	-75.1 (16)	C6'—N1—C5—S1	-8.7 (14)
C1 <sup>ii</sup> —Sn1—S1—C5	69.5 (16)	Sn1—S1—C5—N1	180.000 (3)
C1 <sup>iii</sup> —Sn1—S1—C5	75.1 (16)	Sn1—S1—C5—S2	0.000 (2)
S1 <sup>iii</sup> —Sn1—S1—C5	180.000 (2)	C5—N1—C6—C7	78.1 (9)
C8—N1—C5—S2	1.1 (10)	C8—N1—C6—C7	-105.3 (10)
C8'—N1—C5—S2	8.2 (12)	C8'—N1—C6—C7	-112.2 (12)
C8 <sup>iii</sup> —N1—C5—S2	-8.2 (12)	C8 <sup>iii</sup> —N1—C6—C7	-96.8 (13)
C6—N1—C5—S2	177.2 (14)	C6 <sup>ii</sup> —N1—C6—C7	-13.4 (4)
C6 <sup>ii</sup> —N1—C5—S2	-177.2 (14)	C5—N1—C8—C9	-78.2 (8)
C6 <sup>iii</sup> —N1—C5—S2	-171.3 (14)	C8'—N1—C8—C9	-144 (19)
C6'—N1—C5—S2	171.3 (14)	C8 <sup>iii</sup> —N1—C8—C9	-6(15)
C8—N1—C5—S1	-178.9 (10)	C6—N1—C8—C9	105.4 (14)
C8'—N1—C5—S1	-171.8 (12)	C6 <sup>ii</sup> —N1—C8—C9	100.2 (14)
C8 <sup>iii</sup> —N1—C5—S1	171.8 (12)	C6 <sup>iii</sup> —N1—C8—C9	94.5 (15)
C6—N1—C5—S1	-2.8 (14)	C6'—N1—C8—C9	111.1 (14)
C6 <sup>ii</sup> —N1—C5—S1	2.8 (14)		



Symmetry codes: (i)  $x, -y+1/2, z$ ; (ii)  $-x+3/2, y, z$ ; (iii)  $-x+3/2, -y+1/2, z$ .

Fig. 1

