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Dibenzylbis(naphthalene-2-thiolato-κS)-tin(IV)

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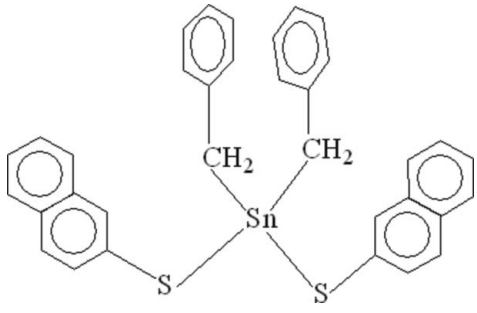
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.044; wR factor = 0.083; data-to-parameter ratio = 10.2.

In the crystal structure of the title compound, $[Sn(C_7H_7)_2(C_{10}H_7S)_2]$, the distorted tetrahedral coordination around the Sn atom consists of two benzyl C atoms and two S atoms of naphthalenethiolate groups. The bond angles in the coordination environment are in the range 102.27 (5)–116.63 (19)°. The average Sn—C and Sn—S bond lengths are 2.151 (4) and 2.4172 (13) Å, respectively. One of the naphthalenethiolate groups is disordered, with a relative occupancy ratio of 0.726 (8):0.274 (8).

Related literature

For related literature, see: Clarke *et al.* (1973); Mohamed-Ibrahim *et al.* (1996); Kalsoom *et al.* (1997); Speziali *et al.* (1994).



Experimental

Crystal data

$[Sn(C_7H_7)_2(C_{10}H_7S)_2]$
M_r = 619.44
Monoclinic, $P2_1/c$
a = 10.732 (2) Å
b = 27.497 (3) Å
c = 9.789 (2) Å
β = 94.033 (3)°
V = 2881.6 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.05 mm^{-1}
T = 295 K
0.20 × 0.15 × 0.12 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (*MolEN*; fair, 1990)
T_{min} = 0.909, T_{max} = 0.999 (expected range = 0.802–0.882)
5873 measured reflections
5435 independent reflections
3312 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
3 standard reflections
frequency: 120 min
intensity decay: −4.2%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.083
S = 1.03
3312 reflections
325 parameters
25 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn—C8	2.149 (4)	Sn—S1	2.4103 (14)
Sn—C1	2.153 (5)	Sn—S2	2.4241 (12)
C8—Sn—C1	116.63 (19)	C8—Sn—S2	107.09 (12)
C8—Sn—S1	110.09 (14)	C1—Sn—S2	110.03 (14)
C1—Sn—S1	109.73 (16)	S1—Sn—S2	102.27 (5)

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1992); cell refinement: *CAD-4 EXPRESS*; data reduction: *MolEN* (Fair, 1990); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2013).

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supplementary materials

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Dibenzylbis(naphthalene-2-thiolato-κ*S*)tin(IV)

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Comment

Relatively few crystal structures have been reported containing only Sn—S and Sn—C bonds such as triphenyltin *p-tert*-butylphenylsulfide (Clarke *et al.*, 1973), (benzenethiolato-κ*S*)triphenyltin(IV) and bis(benzenethiolato- κ*S*)diphenylltin(IV) (Speziali *et al.*, 1994), bis(*O*-cyclohexyl dithiocarbanato)dimethyltin(IV) (Mohamed-Ibrahim *et al.*, 1996). The crystal structures of (naphthalenethiolato-S) triphenyltin(IV) and bis(naphthalenethiolato-*S*)dimethyltin(IV) (Kalsoom *et al.*, 1997), have been published. The crystal structure of the title compound is determined to study the effect on coordination of Sn in the presence of two benzyl and two thionaphthyl groups simultaneously, which might help to understand the properties of such complexes. The coordination around Sn atom is distorted tetrahedral containing two benzyl C-atoms and two S-atoms of the thionaphthyl groups. The angles around Sn vary between 102.27 (5) and 116.63 (19)°. This distortion from the ideal value of 109.5° exists in related compounds mentioned above also, but the variation ranges are different. The Sn environment in the present compound resembles with bis(benzenethiolato-κ*S*)diphenylltin(IV) and that of bis (naphthalen-ethiolato-*S*)dimethyltin(IV). It is observed that C—Sn—C bond angle is always larger than the S—Sn—S or C—Sn—S bond angles, however, in the present case it is smaller than the reported structures. The average Sn—C [2.151 (4) Å] and Sn—S [2.4172 (13) Å] bond lengths in the title compound are slightly larger than the corresponding values observed in the related compounds; 2.119 (7)Å and 2.414 (3)Å (Clarke *et al.*, 1973), 2.127 (5)Å and 2.409 (2)Å (Speziali *et al.*, 1994). The dihedral angle between the phenyl groups (C2—C7) and (C9—C14) is 48.5 (2)°. All the nephthyl groups are planar. The distance of S1 atom from the least square plane of C15—C24 is 0.237 (6) Å. The dihedral angle between the two nephthyl groups is 87.3 (3)°. One of the thionapthalene group is disordered with a percentage relative occupancy ratio of 72.6 (8) and 27.4 (8). The possible cause of disorder is the closest intra-molecular C8···C25*a* [3.49 (1) Å], C8···C25*b*[3.40 (2) Å] and inter-molecular S2···S2(−*x*, −*y*, 1 − *z*)[3.404 (2) Å] interactions. However, no possible hydrogen bond exists.

Experimental

0.04 mole (6.4 g) of 2-thionaphthalene in 60 ml THF was added to 0.04 mole (4.4 ml) of triethylamine in a three necked flask fitted with reflux condenser under inert atmosphere. 0.02 mole (7.44 g) of dibenzyltin dichloride in 40 ml of THF was added dropwise with stirring. The reaction mixture was left for overnight stirring. The mixture was filtered and solvent was removed by rotary evaporator and crystallized in light petroleum ether (40–60°C).

Refinement

Early stages of the refinement indicated that the C—C bond distances in one of the thionaphthyl group are extremly larger and hence a disorder exists. The disorder could be resolved by assuming that all C-atoms of the thionaphthyl group are splitted over two sites. The opening of the two groups with respect to S atom [C25A—S2—C25B] is 13.3 (5)°. The two groups seem to be rotated over S-atom but are coplaner. The occupancy factor of two groups is 72.6 (8) and 27.4 (8)%. The *R* and ωR values became smaller drastically when disorder was removed rather than refining thionapthyl group using

constraints. However, disordered group of low occupancy factor was treated as similar to the non-disordered group. All the disordered atoms were treated isotropically. H-atoms were attached geometrically including the C-atoms of each fragment.

H atoms to the carbon atoms were bonded geometrically 0.930Å from the corresponding atoms of the rings, while the H-atoms of CH_2 groups were fixed geometrically at a distance of 0.970Å from the respective C-atom. Thermal parameter of all H atoms was taken 1.2 times of the corresponding atoms and treated fixed. Riding model was used for all hydrogen atoms.

Figures

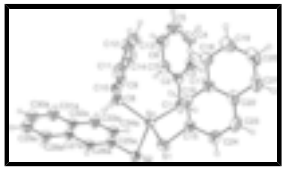


Fig. 1. *ORTEP* drawing of the title compound, $(C_6H_5CH_2)_2Sn(C_{10}H_7S)_2$, with the atom numbering scheme. The thermal ellipsoids are drawn at the 30% probability level. H-atoms are shown by small circles of arbitrary radii.

Dibenzylbis(naphthalene-2-thiolato-κ*S*)tin(IV)

Crystal data

$[Sn(C_7H_7)_2(C_{10}H_7S)_2]$	F_{000} = 1256
M_r = 619.44	D_x = 1.428 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 22 reflections
a = 10.732 (2) Å	θ = 9.9–18.0º
b = 27.497 (3) Å	μ = 1.05 mm^{-1}
c = 9.789 (2) Å	T = 295 K
β = 94.033 (3)º	Prismatic, colourless
V = 2881.6 (9) Å^3	0.20 × 0.15 × 0.12 mm
Z = 4	

Data collection

Enraf–Nonius CAD-4 diffractometer	θ_{max} = 25.7º
ω/2θ scans	θ_{min} = 2.2º
Absorption correction: ψ scan (MolEN; Fair, 1990)	h = −13→13
T_{min} = 0.909, T_{max} = 0.999	k = 0→33
5873 measured reflections	l = 0→11
5435 independent reflections	3 standard reflections
3312 reflections with $I > 2\sigma(I)$	every 120 min
R_{int} = 0.024	intensity decay: −4.2%

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map

$R[F^2 > 2\sigma(F^2)] = 0.044$

$wR(F^2) = 0.083$

$S = 1.03$

3312 reflections

325 parameters

25 restraints

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.45$ e Å^{-3}

$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn	0.35025 (3)	−0.023520 (11)	0.26320 (3)	0.04872 (12)	
S1	0.52595 (13)	−0.06857 (5)	0.18903 (16)	0.0709 (4)	
S2	0.45085 (13)	0.04396 (5)	0.38622 (14)	0.0659 (4)	
C1	0.2498 (5)	−0.0673 (2)	0.4009 (5)	0.0689 (14)	
H1A	0.2966	−0.0970	0.4209	0.083*	
H1B	0.2448	−0.0498	0.4863	0.083*	
C2	0.1209 (5)	−0.08051 (18)	0.3464 (5)	0.0555 (12)	
C3	0.0950 (6)	−0.1254 (2)	0.2871 (6)	0.0745 (15)	
H3	0.1585	−0.1481	0.2824	0.089*	
C4	−0.0240 (8)	−0.1366 (3)	0.2351 (7)	0.105 (2)	
H4	−0.0408	−0.1672	0.1977	0.126*	
C5	−0.1158 (7)	−0.1036 (4)	0.2382 (8)	0.117 (3)	
H5	−0.1951	−0.1117	0.2006	0.140*	
C6	−0.0969 (7)	−0.0596 (4)	0.2934 (8)	0.107 (2)	
H6	−0.1621	−0.0374	0.2957	0.129*	
C7	0.0231 (6)	−0.0478 (2)	0.3478 (6)	0.0808 (16)	
H7	0.0376	−0.0172	0.3859	0.097*	
C8	0.2434 (5)	0.00648 (16)	0.0893 (5)	0.0573 (13)	
H8A	0.1690	0.0218	0.1203	0.069*	
H8B	0.2925	0.0315	0.0485	0.069*	
C9	0.2054 (4)	−0.03060 (15)	−0.0178 (4)	0.0507 (11)	
C10	0.2851 (5)	−0.04268 (17)	−0.1192 (5)	0.0571 (12)	
H10	0.3626	−0.0277	−0.1201	0.069*	
C11	0.2499 (6)	−0.0767 (2)	−0.2180 (5)	0.0725 (15)	
H11	0.3038	−0.0845	−0.2850	0.087*	
C12	0.1348 (6)	−0.0990 (2)	−0.2175 (6)	0.0769 (16)	
H12	0.1098	−0.1213	−0.2857	0.092*	
C13	0.0583 (5)	−0.08846 (19)	−0.1170 (6)	0.0714 (15)	
H13	−0.0181	−0.1043	−0.1149	0.086*	

C14	0.0927 (4)	−0.05428 (17)	−0.0177 (5)	0.0579 (12)	
H14	0.0388	−0.0472	0.0500	0.070*	
C15	0.4715 (4)	−0.12983 (16)	0.1911 (5)	0.0562 (12)	
C16	0.3779 (4)	−0.14643 (17)	0.1036 (5)	0.0593 (12)	
H16	0.3346	−0.1246	0.0454	0.071*	
C17	0.3442 (5)	−0.19616 (17)	0.0983 (5)	0.0602 (13)	
C18	0.2485 (6)	−0.2143 (2)	0.0077 (6)	0.0906 (19)	
H18	0.2020	−0.1927	−0.0486	0.109*	
C19	0.2218 (7)	−0.2622 (2)	−0.0001 (8)	0.110 (2)	
H19	0.1585	−0.2733	−0.0620	0.132*	
C20	0.2888 (8)	−0.2948 (2)	0.0840 (8)	0.110 (2)	
H20	0.2700	−0.3278	0.0785	0.132*	
C21	0.3810 (8)	−0.2791 (2)	0.1739 (8)	0.107 (2)	
H21	0.4258	−0.3014	0.2293	0.129*	
C22	0.4108 (6)	−0.22853 (19)	0.1851 (6)	0.0776 (16)	
C23	0.5061 (7)	−0.2104 (2)	0.2758 (7)	0.106 (2)	
H23	0.5508	−0.2317	0.3345	0.128*	
C24	0.5346 (6)	−0.1626 (2)	0.2799 (6)	0.0889 (18)	
H24	0.5971	−0.1514	0.3427	0.107*	
C25A	0.3499 (8)	0.0918 (3)	0.3350 (9)	0.053 (2)*	0.726 (8)
C26A	0.3698 (7)	0.1177 (3)	0.2183 (8)	0.051 (2)*	0.726 (8)
H26A	0.4360	0.1093	0.1667	0.061*	0.726 (8)
C27A	0.2909 (7)	0.1571 (3)	0.1751 (7)	0.0528 (18)*	0.726 (8)
C28A	0.3107 (7)	0.1835 (3)	0.0545 (7)	0.069 (2)*	0.726 (8)
H28A	0.3754	0.1748	0.0010	0.083*	0.726 (8)
C29A	0.2342 (8)	0.2221 (3)	0.0164 (9)	0.084 (3)*	0.726 (8)
H29A	0.2455	0.2392	−0.0637	0.100*	0.726 (8)
C30A	0.1432 (11)	0.2346 (4)	0.0968 (10)	0.089 (3)*	0.726 (8)
H30A	0.0944	0.2615	0.0714	0.107*	0.726 (8)
C31A	0.1177 (9)	0.2106 (3)	0.2127 (9)	0.084 (3)*	0.726 (8)
H31A	0.0516	0.2199	0.2634	0.101*	0.726 (8)
C32A	0.1972 (7)	0.1701 (3)	0.2543 (8)	0.056 (2)*	0.726 (8)
C33A	0.1786 (7)	0.1432 (3)	0.3744 (8)	0.074 (2)*	0.726 (8)
H33A	0.1136	0.1516	0.4278	0.089*	0.726 (8)
C34A	0.2553 (7)	0.1050 (3)	0.4129 (9)	0.065 (2)*	0.726 (8)
H34A	0.2426	0.0880	0.4928	0.078*	0.726 (8)
C25B	0.3670 (14)	0.0957 (6)	0.2982 (17)	0.030 (5)*	0.274 (8)
C26B	0.2631 (17)	0.1157 (6)	0.352 (2)	0.066 (6)*	0.274 (8)
H26B	0.2339	0.1020	0.4307	0.079*	0.274 (8)
C27B	0.1990 (14)	0.1567 (6)	0.2912 (17)	0.043 (5)*	0.274 (8)
C28B	0.0987 (17)	0.1801 (7)	0.335 (2)	0.091 (8)*	0.274 (8)
H28B	0.0654	0.1695	0.4153	0.109*	0.274 (8)
C29B	0.046 (2)	0.2174 (7)	0.269 (2)	0.094 (7)*	0.274 (8)
H29B	−0.0232	0.2324	0.3025	0.112*	0.274 (8)
C30B	0.0929 (16)	0.2346 (6)	0.1485 (17)	0.050 (5)*	0.274 (8)
H30B	0.0530	0.2610	0.1050	0.060*	0.274 (8)
C31B	0.191 (2)	0.2156 (8)	0.093 (2)	0.102 (10)*	0.274 (8)
H31B	0.2216	0.2274	0.0124	0.122*	0.274 (8)
C32B	0.2464 (16)	0.1745 (6)	0.1690 (16)	0.055 (5)*	0.274 (8)

C33B	0.3470 (17)	0.1525 (6)	0.1171 (19)	0.072 (6)*	0.274 (8)
H33B	0.3766	0.1645	0.0366	0.087*	0.274 (8)
C34B	0.4037 (17)	0.1146 (6)	0.1775 (17)	0.048 (5)*	0.274 (8)
H34B	0.4706	0.1004	0.1370	0.057*	0.274 (8)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.05049 (19)	0.04538 (17)	0.04885 (18)	−0.00717 (17)	−0.00680 (12)	0.00091 (16)
S1	0.0569 (8)	0.0546 (8)	0.1018 (11)	−0.0056 (7)	0.0095 (7)	−0.0058 (7)
S2	0.0769 (9)	0.0522 (7)	0.0644 (8)	−0.0066 (6)	−0.0255 (7)	−0.0037 (6)
C1	0.069 (4)	0.084 (4)	0.053 (3)	−0.018 (3)	0.000 (3)	0.014 (3)
C2	0.053 (3)	0.061 (3)	0.053 (3)	−0.006 (3)	0.008 (2)	0.008 (2)
C3	0.071 (4)	0.066 (4)	0.087 (4)	−0.010 (3)	0.009 (3)	0.011 (3)
C4	0.109 (6)	0.097 (5)	0.108 (5)	−0.050 (5)	0.004 (5)	0.006 (4)
C5	0.064 (5)	0.159 (9)	0.126 (7)	−0.026 (5)	0.000 (4)	0.023 (6)
C6	0.068 (5)	0.151 (7)	0.107 (6)	0.036 (5)	0.029 (4)	0.043 (5)
C7	0.088 (5)	0.088 (4)	0.068 (4)	0.008 (4)	0.015 (3)	0.001 (3)
C8	0.073 (3)	0.042 (3)	0.054 (3)	−0.005 (2)	−0.015 (2)	0.002 (2)
C9	0.058 (3)	0.046 (3)	0.046 (2)	0.002 (2)	−0.011 (2)	0.009 (2)
C10	0.056 (3)	0.062 (3)	0.052 (3)	−0.012 (2)	−0.006 (2)	0.009 (2)
C11	0.083 (4)	0.083 (4)	0.051 (3)	0.006 (3)	0.004 (3)	0.005 (3)
C12	0.088 (4)	0.076 (4)	0.064 (3)	−0.003 (3)	−0.017 (3)	−0.023 (3)
C13	0.063 (4)	0.069 (3)	0.080 (4)	−0.011 (3)	−0.011 (3)	−0.015 (3)
C14	0.051 (3)	0.062 (3)	0.059 (3)	0.002 (2)	−0.001 (2)	−0.005 (2)
C15	0.059 (3)	0.045 (3)	0.064 (3)	0.000 (2)	0.003 (2)	−0.001 (2)
C16	0.058 (3)	0.050 (3)	0.069 (3)	0.005 (2)	−0.002 (3)	0.008 (2)
C17	0.066 (3)	0.052 (3)	0.063 (3)	0.001 (3)	0.003 (3)	−0.002 (2)
C18	0.098 (5)	0.058 (4)	0.111 (5)	−0.006 (3)	−0.023 (4)	−0.005 (3)
C19	0.126 (6)	0.068 (4)	0.133 (6)	−0.023 (4)	−0.022 (5)	−0.019 (4)
C20	0.148 (7)	0.054 (4)	0.130 (6)	−0.021 (4)	0.021 (5)	−0.010 (4)
C21	0.152 (7)	0.054 (4)	0.114 (6)	0.008 (4)	−0.001 (5)	0.021 (4)
C22	0.098 (5)	0.053 (3)	0.082 (4)	0.006 (3)	0.006 (3)	0.009 (3)
C23	0.140 (6)	0.066 (4)	0.106 (5)	0.016 (4)	−0.040 (5)	0.021 (4)
C24	0.092 (5)	0.076 (4)	0.094 (4)	0.000 (3)	−0.031 (3)	0.005 (3)

Geometric parameters (Å, °)

Sn—C8	2.149 (4)	C20—C21	1.349 (9)
Sn—C1	2.153 (5)	C20—H20	0.9300
Sn—S1	2.4103 (14)	C21—C22	1.429 (8)
Sn—S2	2.4241 (12)	C21—H21	0.9300
S1—C15	1.783 (5)	C22—C23	1.398 (8)
S2—C25A	1.754 (8)	C23—C24	1.349 (7)
S2—C25B	1.863 (15)	C23—H23	0.9300
C1—C2	1.492 (6)	C24—H24	0.9300
C1—H1A	0.9700	C25A—C34A	1.362 (11)
C1—H1B	0.9700	C25A—C26A	1.376 (11)
C2—C3	1.382 (7)	C26A—C27A	1.421 (10)

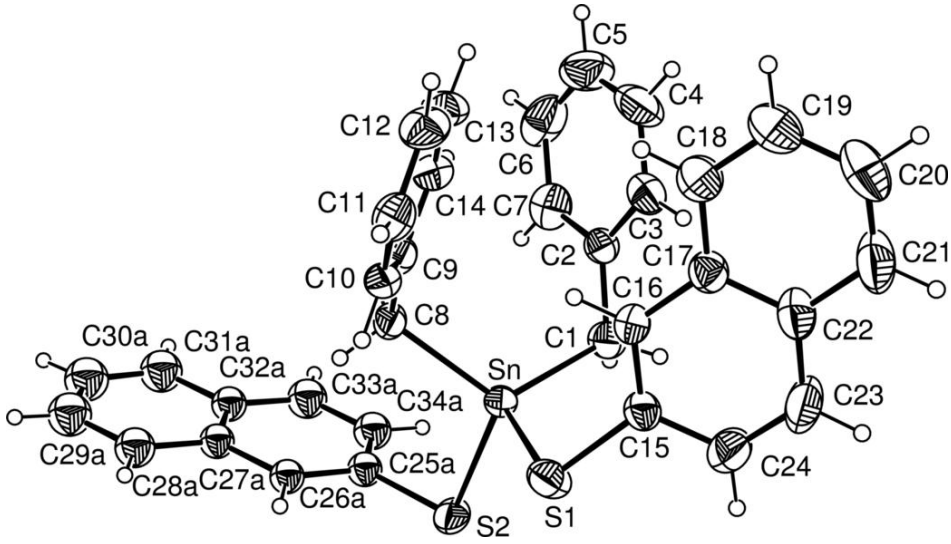
C2—C7	1.382 (7)	C26A—H26A	0.9300
C3—C4	1.376 (8)	C27A—C32A	1.361 (10)
C3—H3	0.9300	C27A—C28A	1.414 (9)
C4—C5	1.341 (10)	C28A—C29A	1.377 (10)
C4—H4	0.9300	C28A—H28A	0.9300
C5—C6	1.335 (11)	C29A—C30A	1.341 (13)
C5—H5	0.9300	C29A—H29A	0.9300
C6—C7	1.397 (9)	C30A—C31A	1.357 (12)
C6—H6	0.9300	C30A—H30A	0.9300
C7—H7	0.9300	C31A—C32A	1.444 (11)
C8—C9	1.499 (6)	C31A—H31A	0.9300
C8—H8A	0.9700	C32A—C33A	1.414 (11)
C8—H8B	0.9700	C33A—C34A	1.370 (10)
C9—C14	1.374 (6)	C33A—H33A	0.9300
C9—C10	1.394 (6)	C34A—H34A	0.9300
C10—C11	1.378 (7)	C25B—C34B	1.374 (17)
C10—H10	0.9300	C25B—C26B	1.380 (16)
C11—C12	1.381 (7)	C26B—C27B	1.429 (16)
C11—H11	0.9300	C26B—H26B	0.9300
C12—C13	1.356 (7)	C27B—C28B	1.351 (16)
C12—H12	0.9300	C27B—C32B	1.419 (16)
C13—C14	1.384 (6)	C28B—C29B	1.321 (17)
C13—H13	0.9300	C28B—H28B	0.9300
C14—H14	0.9300	C29B—C30B	1.395 (18)
C15—C16	1.353 (6)	C29B—H29B	0.9300
C15—C24	1.395 (6)	C30B—C31B	1.329 (18)
C16—C17	1.414 (6)	C30B—H30B	0.9300
C16—H16	0.9300	C31B—C32B	1.458 (17)
C17—C22	1.392 (7)	C31B—H31B	0.9300
C17—C18	1.401 (7)	C32B—C33B	1.367 (17)
C18—C19	1.350 (7)	C33B—C34B	1.323 (16)
C18—H18	0.9300	C33B—H33B	0.9300
C19—C20	1.383 (9)	C34B—H34B	0.9300
C19—H19	0.9300		
C8—Sn—C1	116.63 (19)	C21—C20—H20	119.7
C8—Sn—S1	110.09 (14)	C19—C20—H20	119.7
C1—Sn—S1	109.73 (16)	C20—C21—C22	120.8 (6)
C8—Sn—S2	107.09 (12)	C20—C21—H21	119.6
C1—Sn—S2	110.03 (14)	C22—C21—H21	119.6
S1—Sn—S2	102.27 (5)	C17—C22—C23	118.7 (5)
C15—S1—Sn	102.60 (16)	C17—C22—C21	118.2 (6)
C25A—S2—C25B	13.2 (5)	C23—C22—C21	123.0 (6)
C25A—S2—Sn	100.8 (3)	C24—C23—C22	121.4 (5)
C25B—S2—Sn	99.9 (5)	C24—C23—H23	119.3
C2—C1—Sn	113.8 (3)	C22—C23—H23	119.3
C2—C1—H1A	108.8	C23—C24—C15	120.8 (5)
Sn—C1—H1A	108.8	C23—C24—H24	119.6
C2—C1—H1B	108.8	C15—C24—H24	119.6
Sn—C1—H1B	108.8	C34A—C25A—C26A	119.4 (7)

H1A—C1—H1B	107.7	C34A—C25A—S2	120.7 (7)
C3—C2—C7	116.9 (5)	C26A—C25A—S2	119.8 (6)
C3—C2—C1	121.4 (5)	C25A—C26A—C27A	121.2 (7)
C7—C2—C1	121.6 (5)	C25A—C26A—H26A	119.4
C4—C3—C2	120.7 (6)	C27A—C26A—H26A	119.4
C4—C3—H3	119.7	C32A—C27A—C28A	120.1 (8)
C2—C3—H3	119.7	C32A—C27A—C26A	118.6 (7)
C5—C4—C3	120.2 (7)	C28A—C27A—C26A	121.3 (7)
C5—C4—H4	119.9	C29A—C28A—C27A	120.0 (8)
C3—C4—H4	119.9	C29A—C28A—H28A	120.0
C6—C5—C4	122.1 (7)	C27A—C28A—H28A	120.0
C6—C5—H5	118.9	C30A—C29A—C28A	118.9 (9)
C4—C5—H5	118.9	C30A—C29A—H29A	120.5
C5—C6—C7	118.3 (7)	C28A—C29A—H29A	120.5
C5—C6—H6	120.9	C29A—C30A—C31A	124.3 (11)
C7—C6—H6	120.9	C29A—C30A—H30A	117.8
C2—C7—C6	121.7 (6)	C31A—C30A—H30A	117.8
C2—C7—H7	119.1	C30A—C31A—C32A	117.4 (9)
C6—C7—H7	119.1	C30A—C31A—H31A	121.3
C9—C8—Sn	113.4 (3)	C32A—C31A—H31A	121.3
C9—C8—H8A	108.9	C27A—C32A—C33A	119.3 (8)
Sn—C8—H8A	108.9	C27A—C32A—C31A	119.2 (8)
C9—C8—H8B	108.9	C33A—C32A—C31A	121.5 (7)
Sn—C8—H8B	108.9	C34A—C33A—C32A	120.8 (8)
H8A—C8—H8B	107.7	C34A—C33A—H33A	119.6
C14—C9—C10	118.2 (4)	C32A—C33A—H33A	119.6
C14—C9—C8	121.2 (4)	C25A—C34A—C33A	120.5 (8)
C10—C9—C8	120.6 (4)	C25A—C34A—H34A	119.7
C11—C10—C9	120.6 (5)	C33A—C34A—H34A	119.7
C11—C10—H10	119.7	C34B—C25B—C26B	117.8 (15)
C9—C10—H10	119.7	C34B—C25B—S2	121.9 (11)
C10—C11—C12	120.0 (5)	C26B—C25B—S2	120.2 (12)
C10—C11—H11	120.0	C25B—C26B—C27B	122.1 (15)
C12—C11—H11	120.0	C25B—C26B—H26B	118.9
C13—C12—C11	119.6 (5)	C27B—C26B—H26B	118.9
C13—C12—H12	120.2	C28B—C27B—C32B	116.5 (14)
C11—C12—H12	120.2	C28B—C27B—C26B	127.8 (15)
C12—C13—C14	120.7 (5)	C32B—C27B—C26B	115.7 (13)
C12—C13—H13	119.7	C29B—C28B—C27B	122.4 (17)
C14—C13—H13	119.7	C29B—C28B—H28B	118.8
C9—C14—C13	120.8 (5)	C27B—C28B—H28B	118.8
C9—C14—H14	119.6	C28B—C29B—C30B	120.9 (18)
C13—C14—H14	119.6	C28B—C29B—H29B	119.6
C16—C15—C24	118.9 (4)	C30B—C29B—H29B	119.6
C16—C15—S1	122.7 (4)	C31B—C30B—C29B	123.8 (17)
C24—C15—S1	118.2 (4)	C31B—C30B—H30B	118.1
C15—C16—C17	121.7 (4)	C29B—C30B—H30B	118.1
C15—C16—H16	119.1	C30B—C31B—C32B	113.6 (17)
C17—C16—H16	119.1	C30B—C31B—H31B	123.2

C22—C17—C18	118.8 (5)	C32B—C31B—H31B	123.2
C22—C17—C16	118.5 (5)	C33B—C32B—C27B	120.0 (14)
C18—C17—C16	122.7 (5)	C33B—C32B—C31B	117.2 (15)
C19—C18—C17	121.7 (6)	C27B—C32B—C31B	122.9 (15)
C19—C18—H18	119.1	C34B—C33B—C32B	122.2 (17)
C17—C18—H18	119.1	C34B—C33B—H33B	118.9
C18—C19—C20	120.0 (6)	C32B—C33B—H33B	118.9
C18—C19—H19	120.0	C33B—C34B—C25B	122.1 (16)
C20—C19—H19	120.0	C33B—C34B—H34B	119.0
C21—C20—C19	120.5 (6)	C25B—C34B—H34B	119.0
C8—Sn—S1—C15	−98.8 (2)	C21—C22—C23—C24	177.5 (7)
C1—Sn—S1—C15	30.9 (2)	C22—C23—C24—C15	−1.5 (11)
S2—Sn—S1—C15	147.67 (17)	C16—C15—C24—C23	2.3 (9)
C8—Sn—S2—C25A	24.6 (3)	S1—C15—C24—C23	−173.0 (6)
C1—Sn—S2—C25A	−103.0 (3)	C25B—S2—C25A—C34A	−178 (3)
S1—Sn—S2—C25A	140.4 (3)	Sn—S2—C25A—C34A	94.4 (7)
C8—Sn—S2—C25B	11.3 (5)	C25B—S2—C25A—C26A	−1(3)
C1—Sn—S2—C25B	−116.4 (5)	Sn—S2—C25A—C26A	−88.7 (6)
S1—Sn—S2—C25B	127.0 (5)	C34A—C25A—C26A—C27A	−2.1 (11)
C8—Sn—C1—C2	11.6 (5)	S2—C25A—C26A—C27A	−179.0 (6)
S1—Sn—C1—C2	−114.4 (4)	C25A—C26A—C27A—C32A	2.4 (11)
S2—Sn—C1—C2	133.8 (4)	C25A—C26A—C27A—C28A	−179.5 (7)
Sn—C1—C2—C3	98.9 (5)	C32A—C27A—C28A—C29A	−0.7 (11)
Sn—C1—C2—C7	−78.5 (5)	C26A—C27A—C28A—C29A	−178.8 (7)
C7—C2—C3—C4	−1.3 (8)	C27A—C28A—C29A—C30A	1.4 (12)
C1—C2—C3—C4	−178.8 (5)	C28A—C29A—C30A—C31A	−2.3 (14)
C2—C3—C4—C5	1.7 (10)	C29A—C30A—C31A—C32A	2.4 (14)
C3—C4—C5—C6	−1.5 (12)	C28A—C27A—C32A—C33A	179.9 (7)
C4—C5—C6—C7	0.9 (12)	C26A—C27A—C32A—C33A	−2.0 (10)
C3—C2—C7—C6	0.7 (8)	C28A—C27A—C32A—C31A	0.8 (11)
C1—C2—C7—C6	178.2 (5)	C26A—C27A—C32A—C31A	179.0 (7)
C5—C6—C7—C2	−0.5 (10)	C30A—C31A—C32A—C27A	−1.6 (12)
C1—Sn—C8—C9	−72.7 (4)	C30A—C31A—C32A—C33A	179.4 (8)
S1—Sn—C8—C9	53.2 (4)	C27A—C32A—C33A—C34A	1.3 (11)
S2—Sn—C8—C9	163.6 (3)	C31A—C32A—C33A—C34A	−179.7 (7)
Sn—C8—C9—C14	92.3 (5)	C26A—C25A—C34A—C33A	1.3 (12)
Sn—C8—C9—C10	−86.4 (4)	S2—C25A—C34A—C33A	178.2 (6)
C14—C9—C10—C11	1.4 (7)	C32A—C33A—C34A—C25A	−1.0 (11)
C8—C9—C10—C11	−179.8 (4)	C25A—S2—C25B—C34B	−179 (4)
C9—C10—C11—C12	0.1 (7)	Sn—S2—C25B—C34B	−84.3 (14)
C10—C11—C12—C13	−2.0 (8)	C25A—S2—C25B—C26B	−1(2)
C11—C12—C13—C14	2.2 (8)	Sn—S2—C25B—C26B	94.3 (14)
C10—C9—C14—C13	−1.2 (7)	C34B—C25B—C26B—C27B	−4(3)
C8—C9—C14—C13	180.0 (4)	S2—C25B—C26B—C27B	177.4 (15)
C12—C13—C14—C9	−0.6 (8)	C25B—C26B—C27B—C28B	−178 (2)
Sn—S1—C15—C16	67.4 (4)	C25B—C26B—C27B—C32B	2(3)
Sn—S1—C15—C24	−117.5 (4)	C32B—C27B—C28B—C29B	0(3)
C24—C15—C16—C17	−1.2 (8)	C26B—C27B—C28B—C29B	−179 (2)
S1—C15—C16—C17	173.9 (4)	C27B—C28B—C29B—C30B	0(4)

C15—C16—C17—C22	−0.6 (8)	C28B—C29B—C30B—C31B	0(3)
C15—C16—C17—C18	−179.4 (5)	C29B—C30B—C31B—C32B	0(3)
C22—C17—C18—C19	−1.9 (9)	C28B—C27B—C32B—C33B	−179.4 (19)
C16—C17—C18—C19	176.8 (6)	C26B—C27B—C32B—C33B	0(2)
C17—C18—C19—C20	0.9 (12)	C28B—C27B—C32B—C31B	0(3)
C18—C19—C20—C21	−0.2 (12)	C26B—C27B—C32B—C31B	179 (2)
C19—C20—C21—C22	0.6 (12)	C30B—C31B—C32B—C33B	179.2 (19)
C18—C17—C22—C23	−179.8 (6)	C30B—C31B—C32B—C27B	0(3)
C16—C17—C22—C23	1.4 (8)	C27B—C32B—C33B—C34B	0(3)
C18—C17—C22—C21	2.3 (8)	C31B—C32B—C33B—C34B	−179 (2)
C16—C17—C22—C21	−176.5 (5)	C32B—C33B—C34B—C25B	−2(3)
C20—C21—C22—C17	−1.6 (10)	C26B—C25B—C34B—C33B	4(3)
C20—C21—C22—C23	−179.5 (7)	S2—C25B—C34B—C33B	−177.7 (15)
C17—C22—C23—C24	−0.3 (11)		

Fig. 1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