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μ-Sulfido-bis[tricyclohexyltin(IV)]

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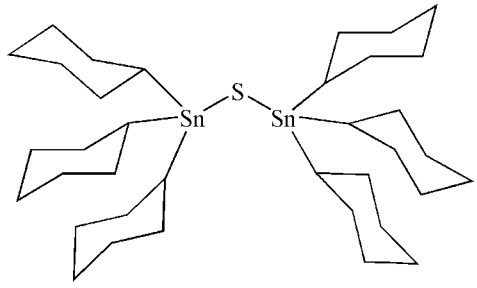
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.009 Å; R factor = 0.043; wR factor = 0.111; data-to-parameter ratio = 21.7.

The Sn atoms of the monomeric title compound, $[Sn_2(C_6H_{11})_6S]$, display slightly distorted $SnSC_3$ tetrahedral geometries, with mean Sn—C and Sn—S distances of 2.163 (6) and 2.4089 (14) Å, respectively. The bridging Sn—S—Sn angle is 113.43 (5)°.

Related literature

For related structures, see Glidewell & Liles (1982) and Batchelor *et al.* (1988).

For related literature, see: Steliou & Mrani (1982).



Experimental

Crystal data

$[Sn_2(C_6H_{11})_6S]$
M_r = 768.33
Monoclinic, $P2_1/n$
a = 10.3799 (15) Å
b = 14.418 (2) Å
c = 24.862 (4) Å
β = 96.558 (2)°
V = 3696.4 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.43 mm^{-1}
T = 295 (2) K
0.44 × 0.11 × 0.11 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.572, T_{max} = 0.859
29484 measured reflections
7651 independent reflections
6079 reflections with $I > 2\sigma(I)$
R_{int} = 0.041

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.111
S = 1.05
7651 reflections
352 parameters
42 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C13	2.141 (6)	Sn2—C25	2.160 (5)
Sn1—C1	2.164 (4)	Sn2—C19	2.163 (5)
Sn1—C7	2.176 (5)	Sn2—C31	2.173 (4)
Sn1—S1	2.4034 (13)	Sn2—S1	2.4143 (14)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2416).

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supplementary materials

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μ-Sulfido-bis[tricyclohexyltin(IV)]

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Comment

Bis(triorganotin) sulfides, $(R_3Sn)_2S$, show little tendency towards self-association. Bis(triphenyltin) sulfide, $(Ph_3Sn)_2S$ (Glidewell & Liles, 1982), and bis(tri-*tert*-butyltin) sulfide, $(^tBu_3Sn)_2S$ (Batchelor *et al.*, 1988), are both monomers with distorted tetrahedral tin atoms.

In the title compound, (I), which was synthesized by Steliou & Mrani in 1982, each Sn atom is also four-coordinate and possess a distorted $SnSC_3$ tetrahedral geometry (Fig. 1 & Table 1). The mean Sn—S distance is 2.4089 (14) Å, which is very similar to that [2.411 (8) Å] found in $(Ph_3Sn)_2S$ (Glidewell & Liles, 1982) and slightly shorter than that [2.427 (2) Å] of $(^tBu_3Sn)_2S$ (Batchelor *et al.*, 1988). For steric reasons, the angle Sn—S—Sn [113.43 (5)°] and the seperation of Sn···Sn [4.027 (3) Å] in (I) are slightly larger than the corresponding values in $(Ph_3Sn)_2S$ [107.3 (3)° and 3.883 (3) Å] and much smaller than in $(^tBu_3Sn)_2S$ [134.2 (2)° and 4.473 (1) Å].

Experimental

The title compound was synthesized according to the literature method (Steliou & Mrani, 1982). The crystals of (I) were obtained from chloroform–methanol (1:1, *v*/*v*) by slow evaporation at 298 K (yield 85%, m.p. 405–406 K).

Refinement

The C—C distances of the C13–C18 cyclohexyl ring were restrained to 1.53 (1) Å and 1,3-related distances to 2.50 (2) Å. The vibration of C14–C18 atoms were made approximately isotropic. The H atoms were placed at calculated positions (C—H = 0.97–0.98 Å) and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C)$.

Figures

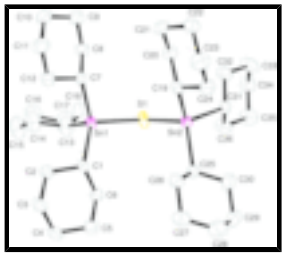


Fig. 1. The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

μ-Sulfido-bis[tricyclohexyltin(IV)]

Crystal data

$[Sn_2(C_6H_{11})_6S]$	F_{000} = 1592
M_r = 768.33	D_x = 1.381 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 7158 reflections
a = 10.3799 (15) Å	θ = 2.2–24.7º
b = 14.418 (2) Å	μ = 1.43 mm^{-1}
c = 24.862 (4) Å	T = 295 (2) K
β = 96.558 (2)º	Prism, colourless
V = 3696.4 (9) Å^3	0.44 × 0.11 × 0.11 mm
Z = 4	

Data collection

Bruker APEX CCD area-detector diffractometer	7651 independent reflections
Radiation source: fine-focus sealed tube	6079 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.041
T = 295(2) K	θ_{max} = 26.5º
ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	h = −13→13
T_{min} = 0.572, T_{max} = 0.859	k = −18→17
29484 measured reflections	l = −31→31

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.043	H-atom parameters constrained
$wR(F^2)$ = 0.111	$w = 1/[\sigma^2(F_o^2) + (0.051P)^2 + 3.1168P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
7651 reflections	$\Delta\rho_{max}$ = 0.87 e Å^{-3}
352 parameters	$\Delta\rho_{min}$ = −0.38 e Å^{-3}
42 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.51770 (3)	0.27799 (2)	0.103632 (12)	0.04466 (11)
Sn2	0.61299 (3)	0.45430 (2)	0.227440 (12)	0.04517 (11)
S1	0.52413 (15)	0.30496 (10)	0.19930 (5)	0.0642 (4)
C1	0.4037 (4)	0.3830 (3)	0.05779 (17)	0.0443 (10)
H1	0.4538	0.4407	0.0611	0.053*
C2	0.3788 (5)	0.3599 (4)	−0.00249 (19)	0.0611 (13)
H2A	0.4614	0.3544	−0.0170	0.073*
H2B	0.3355	0.3003	−0.0068	0.073*
C3	0.2973 (5)	0.4317 (4)	−0.0349 (2)	0.0682 (15)
H3A	0.3462	0.4889	−0.0356	0.082*
H3B	0.2776	0.4101	−0.0718	0.082*
C4	0.1734 (5)	0.4503 (4)	−0.0114 (2)	0.0693 (16)
H4A	0.1185	0.3958	−0.0158	0.083*
H4B	0.1279	0.5010	−0.0310	0.083*
C5	0.1975 (6)	0.4749 (5)	0.0477 (2)	0.0749 (17)
H5A	0.1149	0.4824	0.0620	0.090*
H5B	0.2430	0.5337	0.0517	0.090*
C6	0.2769 (5)	0.4013 (4)	0.0805 (2)	0.0634 (14)
H6A	0.2946	0.4216	0.1178	0.076*
H6B	0.2273	0.3442	0.0801	0.076*
C7	0.7155 (5)	0.2691 (3)	0.08308 (19)	0.0510 (11)
H7	0.7607	0.3250	0.0974	0.061*
C8	0.7873 (5)	0.1873 (4)	0.1099 (2)	0.0638 (14)
H8A	0.7431	0.1305	0.0976	0.077*
H8B	0.7862	0.1915	0.1487	0.077*
C9	0.9271 (6)	0.1830 (5)	0.0972 (2)	0.0804 (18)
H9A	0.9741	0.2360	0.1135	0.096*
H9B	0.9677	0.1273	0.1131	0.096*
C10	0.9365 (6)	0.1829 (5)	0.0376 (3)	0.0836 (19)
H10A	0.9009	0.1253	0.0221	0.100*
H10B	1.0270	0.1859	0.0314	0.100*
C11	0.8644 (6)	0.2637 (5)	0.0095 (2)	0.0784 (17)
H11A	0.8657	0.2580	−0.0293	0.094*

H11B	0.9079	0.3211	0.0211	0.094*
C12	0.7244 (5)	0.2675 (4)	0.0222 (2)	0.0643 (14)
H12A	0.6780	0.2139	0.0064	0.077*
H12B	0.6830	0.3226	0.0059	0.077*
C13	0.4104 (8)	0.1509 (4)	0.0966 (2)	0.096 (2)
H13	0.3213	0.1743	0.0938	0.115*
C14	0.4086 (8)	0.1009 (5)	0.0450 (2)	0.105 (2)
H14A	0.4964	0.0818	0.0407	0.125*
H14B	0.3805	0.1434	0.0158	0.125*
C15	0.3211 (10)	0.0156 (5)	0.0396 (3)	0.130 (3)
H15A	0.2323	0.0360	0.0304	0.156*
H15B	0.3444	−0.0217	0.0097	0.156*
C16	0.3271 (11)	−0.0426 (5)	0.0876 (3)	0.136 (3)
H16A	0.4076	−0.0774	0.0910	0.164*
H16B	0.2562	−0.0868	0.0831	0.164*
C17	0.3193 (10)	0.0111 (6)	0.1379 (3)	0.134 (3)
H17A	0.3380	−0.0298	0.1688	0.161*
H17B	0.2315	0.0340	0.1382	0.161*
C18	0.4133 (10)	0.0930 (5)	0.1438 (3)	0.137 (3)
H18A	0.3935	0.1308	0.1740	0.164*
H18B	0.5006	0.0692	0.1525	0.164*
C19	0.7906 (4)	0.4806 (3)	0.19223 (18)	0.0473 (11)
H19	0.7673	0.4849	0.1530	0.057*
C20	0.8900 (5)	0.4042 (4)	0.2019 (2)	0.0576 (12)
H20A	0.8517	0.3460	0.1885	0.069*
H20B	0.9152	0.3976	0.2404	0.069*
C21	1.0096 (5)	0.4240 (4)	0.1738 (2)	0.0664 (15)
H21A	1.0730	0.3750	0.1820	0.080*
H21B	0.9861	0.4252	0.1349	0.080*
C22	1.0683 (5)	0.5165 (4)	0.1925 (3)	0.0745 (17)
H22A	1.0994	0.5128	0.2307	0.089*
H22B	1.1420	0.5296	0.1730	0.089*
C23	0.9721 (6)	0.5938 (4)	0.1834 (3)	0.0817 (18)
H23A	0.9485	0.6023	0.1448	0.098*
H23B	1.0113	0.6509	0.1979	0.098*
C24	0.8494 (6)	0.5734 (4)	0.2106 (3)	0.0722 (16)
H24A	0.8711	0.5727	0.2496	0.087*
H24B	0.7863	0.6222	0.2017	0.087*
C25	0.4696 (5)	0.5609 (4)	0.2068 (2)	0.0589 (13)
H25	0.3863	0.5285	0.2009	0.071*
C26	0.4829 (6)	0.6117 (4)	0.1544 (2)	0.0660 (14)
H26A	0.4797	0.5670	0.1251	0.079*
H26B	0.5668	0.6420	0.1571	0.079*
C27	0.3775 (8)	0.6836 (5)	0.1409 (3)	0.095 (2)
H27A	0.3962	0.7187	0.1094	0.114*
H27B	0.2951	0.6524	0.1319	0.114*
C28	0.3671 (8)	0.7479 (5)	0.1862 (3)	0.105 (3)
H28A	0.2934	0.7886	0.1770	0.126*
H28B	0.4444	0.7861	0.1914	0.126*

C29	0.3510 (7)	0.6991 (5)	0.2379 (3)	0.094 (2)
H29A	0.2672	0.6687	0.2347	0.113*
H29B	0.3533	0.7442	0.2669	0.113*
C30	0.4570 (7)	0.6274 (5)	0.2519 (3)	0.090 (2)
H30A	0.5391	0.6590	0.2609	0.108*
H30B	0.4382	0.5930	0.2836	0.108*
C31	0.6426 (5)	0.4330 (4)	0.31450 (18)	0.0532 (12)
H31	0.6595	0.4939	0.3314	0.064*
C32	0.7556 (6)	0.3722 (5)	0.3327 (2)	0.0826 (19)
H32A	0.8340	0.4006	0.3225	0.099*
H32B	0.7444	0.3130	0.3143	0.099*
C33	0.7715 (7)	0.3559 (6)	0.3937 (2)	0.104 (3)
H33A	0.8413	0.3120	0.4030	0.124*
H33B	0.7951	0.4138	0.4122	0.124*
C34	0.6512 (7)	0.3198 (5)	0.4124 (2)	0.0847 (19)
H34A	0.6341	0.2581	0.3978	0.102*
H34B	0.6627	0.3150	0.4516	0.102*
C35	0.5390 (7)	0.3800 (6)	0.3956 (2)	0.097 (2)
H35A	0.5514	0.4395	0.4137	0.116*
H35B	0.4612	0.3520	0.4067	0.116*
C36	0.5210 (6)	0.3950 (5)	0.3345 (2)	0.0794 (18)
H36A	0.4985	0.3365	0.3165	0.095*
H36B	0.4500	0.4379	0.3252	0.095*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0527 (2)	0.04650 (19)	0.03447 (17)	−0.00494 (14)	0.00339 (13)	0.00176 (13)
Sn2	0.0506 (2)	0.0497 (2)	0.03501 (17)	0.00293 (14)	0.00387 (13)	0.00495 (13)
S1	0.0901 (10)	0.0663 (8)	0.0361 (6)	−0.0237 (7)	0.0074 (6)	0.0007 (6)
C1	0.042 (2)	0.051 (3)	0.040 (2)	−0.006 (2)	0.0018 (19)	0.003 (2)
C2	0.065 (3)	0.075 (4)	0.043 (3)	0.013 (3)	0.007 (2)	0.005 (2)
C3	0.061 (3)	0.097 (4)	0.045 (3)	0.002 (3)	−0.002 (2)	0.012 (3)
C4	0.052 (3)	0.090 (4)	0.063 (3)	0.007 (3)	−0.006 (3)	0.018 (3)
C5	0.059 (3)	0.101 (5)	0.065 (4)	0.023 (3)	0.011 (3)	0.006 (3)
C6	0.053 (3)	0.093 (4)	0.045 (3)	0.008 (3)	0.009 (2)	0.006 (3)
C7	0.056 (3)	0.051 (3)	0.045 (3)	0.007 (2)	0.003 (2)	−0.003 (2)
C8	0.069 (3)	0.068 (3)	0.055 (3)	0.016 (3)	0.007 (3)	0.009 (3)
C9	0.079 (4)	0.086 (4)	0.074 (4)	0.028 (3)	0.002 (3)	0.004 (3)
C10	0.079 (4)	0.095 (5)	0.080 (4)	0.025 (4)	0.022 (3)	−0.006 (4)
C11	0.079 (4)	0.096 (5)	0.064 (4)	0.011 (4)	0.026 (3)	0.011 (3)
C12	0.063 (3)	0.081 (4)	0.050 (3)	0.007 (3)	0.009 (3)	0.011 (3)
C13	0.151 (7)	0.065 (4)	0.072 (4)	−0.043 (4)	0.015 (4)	−0.005 (3)
C14	0.148 (6)	0.091 (5)	0.073 (4)	−0.037 (4)	0.009 (4)	−0.003 (4)
C15	0.182 (7)	0.090 (5)	0.113 (6)	−0.051 (5)	−0.013 (5)	−0.016 (4)
C16	0.195 (8)	0.087 (5)	0.124 (6)	−0.048 (5)	0.004 (6)	−0.001 (5)
C17	0.183 (7)	0.103 (5)	0.122 (6)	−0.062 (5)	0.039 (6)	0.008 (5)
C18	0.211 (8)	0.105 (5)	0.091 (5)	−0.076 (5)	0.001 (5)	0.006 (4)

C19	0.050 (3)	0.052 (3)	0.039 (2)	−0.005 (2)	0.002 (2)	0.003 (2)
C20	0.058 (3)	0.057 (3)	0.059 (3)	0.002 (2)	0.012 (2)	0.005 (2)
C21	0.055 (3)	0.076 (4)	0.071 (4)	0.008 (3)	0.021 (3)	0.001 (3)
C22	0.054 (3)	0.089 (4)	0.081 (4)	−0.009 (3)	0.010 (3)	−0.014 (3)
C23	0.067 (4)	0.062 (4)	0.118 (5)	−0.021 (3)	0.019 (4)	−0.003 (4)
C24	0.067 (4)	0.056 (3)	0.092 (4)	−0.003 (3)	0.004 (3)	−0.009 (3)
C25	0.067 (3)	0.054 (3)	0.055 (3)	0.014 (2)	0.006 (3)	0.001 (2)
C26	0.076 (4)	0.068 (3)	0.053 (3)	0.012 (3)	0.002 (3)	0.007 (3)
C27	0.126 (6)	0.076 (4)	0.076 (4)	0.029 (4)	−0.017 (4)	0.019 (4)
C28	0.124 (7)	0.064 (4)	0.120 (7)	0.020 (4)	−0.011 (5)	0.011 (4)
C29	0.111 (6)	0.072 (4)	0.100 (5)	0.022 (4)	0.017 (4)	−0.020 (4)
C30	0.121 (6)	0.081 (4)	0.065 (4)	0.025 (4)	0.003 (4)	−0.004 (3)
C31	0.068 (3)	0.057 (3)	0.035 (2)	0.001 (2)	0.004 (2)	0.002 (2)
C32	0.072 (4)	0.129 (6)	0.046 (3)	0.024 (4)	0.006 (3)	0.024 (3)
C33	0.085 (5)	0.176 (8)	0.048 (3)	0.020 (5)	0.000 (3)	0.037 (4)
C34	0.116 (5)	0.090 (5)	0.048 (3)	0.008 (4)	0.009 (3)	0.023 (3)
C35	0.090 (5)	0.139 (7)	0.065 (4)	0.014 (5)	0.027 (3)	0.034 (4)
C36	0.067 (4)	0.117 (5)	0.056 (3)	0.006 (4)	0.015 (3)	0.027 (3)

Geometric parameters (Å, °)

Sn1—C13	2.141 (6)	C17—H17A	0.9700
Sn1—C1	2.164 (4)	C17—H17B	0.9700
Sn1—C7	2.176 (5)	C18—H18A	0.9700
Sn1—S1	2.4034 (13)	C18—H18B	0.9700
Sn2—C25	2.160 (5)	C19—C20	1.510 (7)
Sn2—C19	2.163 (5)	C19—C24	1.519 (7)
Sn2—C31	2.173 (4)	C19—H19	0.9800
Sn2—S1	2.4143 (14)	C20—C21	1.519 (7)
C1—C6	1.513 (6)	C20—H20A	0.9700
C1—C2	1.528 (6)	C20—H20B	0.9700
C1—H1	0.9800	C21—C22	1.517 (8)
C2—C3	1.509 (7)	C21—H21A	0.9700
C2—H2A	0.9700	C21—H21B	0.9700
C2—H2B	0.9700	C22—C23	1.497 (8)
C3—C4	1.496 (7)	C22—H22A	0.9700
C3—H3A	0.9700	C22—H22B	0.9700
C3—H3B	0.9700	C23—C24	1.538 (8)
C4—C5	1.505 (8)	C23—H23A	0.9700
C4—H4A	0.9700	C23—H23B	0.9700
C4—H4B	0.9700	C24—H24A	0.9700
C5—C6	1.522 (7)	C24—H24B	0.9700
C5—H5A	0.9700	C25—C30	1.491 (7)
C5—H5B	0.9700	C25—C26	1.516 (7)
C6—H6A	0.9700	C25—H25	0.9800
C6—H6B	0.9700	C26—C27	1.517 (8)
C7—C8	1.508 (7)	C26—H26A	0.9700
C7—C12	1.527 (7)	C26—H26B	0.9700
C7—H7	0.9800	C27—C28	1.472 (10)

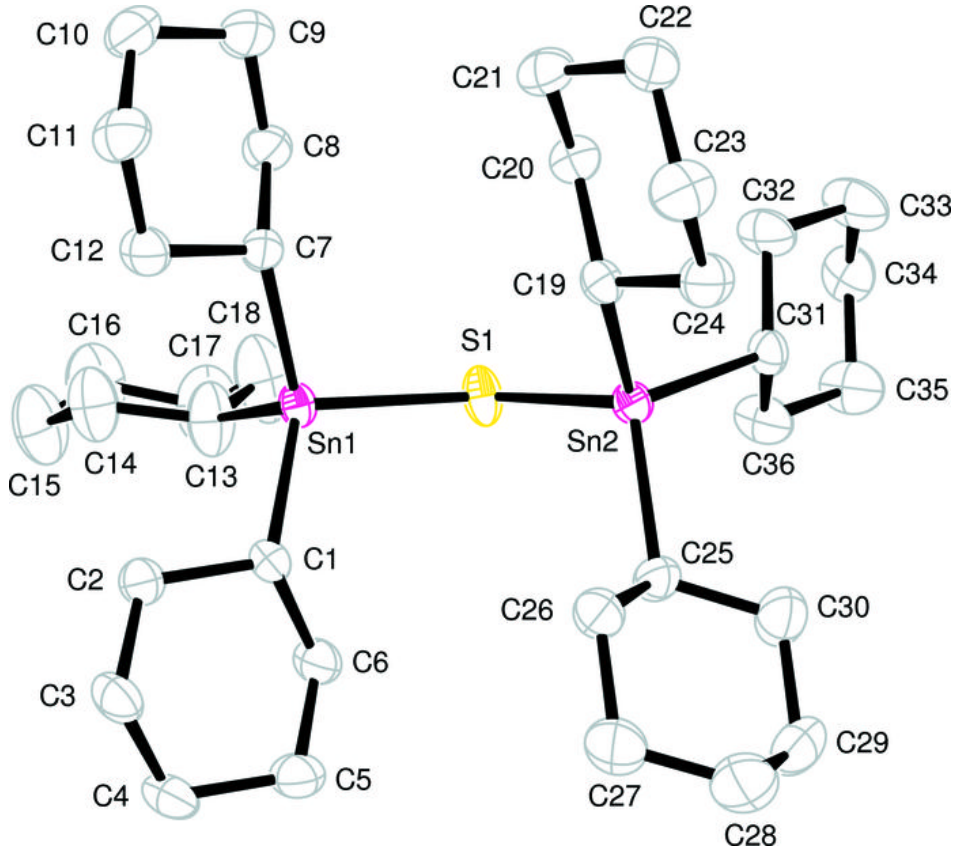
C8—C9	1.521 (8)	C27—H27A	0.9700
C8—H8A	0.9700	C27—H27B	0.9700
C8—H8B	0.9700	C28—C29	1.491 (10)
C9—C10	1.496 (8)	C28—H28A	0.9700
C9—H9A	0.9700	C28—H28B	0.9700
C9—H9B	0.9700	C29—C30	1.521 (9)
C10—C11	1.512 (8)	C29—H29A	0.9700
C10—H10A	0.9700	C29—H29B	0.9700
C10—H10B	0.9700	C30—H30A	0.9700
C11—C12	1.523 (8)	C30—H30B	0.9700
C11—H11A	0.9700	C31—C32	1.493 (7)
C11—H11B	0.9700	C31—C36	1.511 (7)
C12—H12A	0.9700	C31—H31	0.9800
C12—H12B	0.9700	C32—C33	1.526 (7)
C13—C18	1.437 (7)	C32—H32A	0.9700
C13—C14	1.469 (7)	C32—H32B	0.9700
C13—H13	0.9800	C33—C34	1.476 (9)
C14—C15	1.525 (7)	C33—H33A	0.9700
C14—H14A	0.9700	C33—H33B	0.9700
C14—H14B	0.9700	C34—C35	1.474 (9)
C15—C16	1.454 (7)	C34—H34A	0.9700
C15—H15A	0.9700	C34—H34B	0.9700
C15—H15B	0.9700	C35—C36	1.526 (8)
C16—C17	1.482 (7)	C35—H35A	0.9700
C16—H16A	0.9700	C35—H35B	0.9700
C16—H16B	0.9700	C36—H36A	0.9700
C17—C18	1.528 (7)	C36—H36B	0.9700
C13—Sn1—C1	107.9 (2)	C13—C18—C17	114.7 (6)
C13—Sn1—C7	115.2 (3)	C13—C18—H18A	108.6
C1—Sn1—C7	113.06 (17)	C17—C18—H18A	108.6
C13—Sn1—S1	100.05 (16)	C13—C18—H18B	108.6
C1—Sn1—S1	111.08 (12)	C17—C18—H18B	108.6
C7—Sn1—S1	108.76 (13)	H18A—C18—H18B	107.6
C25—Sn2—C19	112.03 (19)	C20—C19—C24	110.6 (4)
C25—Sn2—C31	110.60 (19)	C20—C19—Sn2	114.0 (3)
C19—Sn2—C31	113.45 (18)	C24—C19—Sn2	111.4 (3)
C25—Sn2—S1	109.63 (16)	C20—C19—H19	106.8
C19—Sn2—S1	110.75 (13)	C24—C19—H19	106.8
C31—Sn2—S1	99.71 (14)	Sn2—C19—H19	106.8
Sn1—S1—Sn2	113.43 (5)	C19—C20—C21	111.7 (4)
C6—C1—C2	110.3 (4)	C19—C20—H20A	109.3
C6—C1—Sn1	111.8 (3)	C21—C20—H20A	109.3
C2—C1—Sn1	112.7 (3)	C19—C20—H20B	109.3
C6—C1—H1	107.2	C21—C20—H20B	109.3
C2—C1—H1	107.2	H20A—C20—H20B	107.9
Sn1—C1—H1	107.2	C22—C21—C20	110.2 (5)
C3—C2—C1	113.3 (4)	C22—C21—H21A	109.6
C3—C2—H2A	108.9	C20—C21—H21A	109.6
C1—C2—H2A	108.9	C22—C21—H21B	109.6

C3—C2—H2B	108.9	C20—C21—H21B	109.6
C1—C2—H2B	108.9	H21A—C21—H21B	108.1
H2A—C2—H2B	107.7	C23—C22—C21	111.8 (5)
C4—C3—C2	111.7 (4)	C23—C22—H22A	109.3
C4—C3—H3A	109.3	C21—C22—H22A	109.3
C2—C3—H3A	109.3	C23—C22—H22B	109.3
C4—C3—H3B	109.3	C21—C22—H22B	109.3
C2—C3—H3B	109.3	H22A—C22—H22B	107.9
H3A—C3—H3B	107.9	C22—C23—C24	111.3 (5)
C3—C4—C5	111.7 (4)	C22—C23—H23A	109.4
C3—C4—H4A	109.3	C24—C23—H23A	109.4
C5—C4—H4A	109.3	C22—C23—H23B	109.4
C3—C4—H4B	109.3	C24—C23—H23B	109.4
C5—C4—H4B	109.3	H23A—C23—H23B	108.0
H4A—C4—H4B	107.9	C19—C24—C23	111.1 (5)
C4—C5—C6	112.2 (5)	C19—C24—H24A	109.4
C4—C5—H5A	109.2	C23—C24—H24A	109.4
C6—C5—H5A	109.2	C19—C24—H24B	109.4
C4—C5—H5B	109.2	C23—C24—H24B	109.4
C6—C5—H5B	109.2	H24A—C24—H24B	108.0
H5A—C5—H5B	107.9	C30—C25—C26	111.2 (5)
C1—C6—C5	111.3 (4)	C30—C25—Sn2	113.3 (4)
C1—C6—H6A	109.4	C26—C25—Sn2	114.8 (4)
C5—C6—H6A	109.4	C30—C25—H25	105.5
C1—C6—H6B	109.4	C26—C25—H25	105.5
C5—C6—H6B	109.4	Sn2—C25—H25	105.5
H6A—C6—H6B	108.0	C25—C26—C27	112.7 (5)
C8—C7—C12	110.1 (4)	C25—C26—H26A	109.1
C8—C7—Sn1	112.0 (3)	C27—C26—H26A	109.1
C12—C7—Sn1	113.5 (3)	C25—C26—H26B	109.1
C8—C7—H7	107.0	C27—C26—H26B	109.1
C12—C7—H7	107.0	H26A—C26—H26B	107.8
Sn1—C7—H7	107.0	C28—C27—C26	112.1 (5)
C7—C8—C9	112.0 (5)	C28—C27—H27A	109.2
C7—C8—H8A	109.2	C26—C27—H27A	109.2
C9—C8—H8A	109.2	C28—C27—H27B	109.2
C7—C8—H8B	109.2	C26—C27—H27B	109.2
C9—C8—H8B	109.2	H27A—C27—H27B	107.9
H8A—C8—H8B	107.9	C27—C28—C29	112.8 (6)
C10—C9—C8	112.1 (5)	C27—C28—H28A	109.0
C10—C9—H9A	109.2	C29—C28—H28A	109.0
C8—C9—H9A	109.2	C27—C28—H28B	109.0
C10—C9—H9B	109.2	C29—C28—H28B	109.0
C8—C9—H9B	109.2	H28A—C28—H28B	107.8
H9A—C9—H9B	107.9	C28—C29—C30	111.7 (6)
C9—C10—C11	111.8 (5)	C28—C29—H29A	109.3
C9—C10—H10A	109.3	C30—C29—H29A	109.3
C11—C10—H10A	109.3	C28—C29—H29B	109.3
C9—C10—H10B	109.3	C30—C29—H29B	109.3

C11—C10—H10B	109.3	H29A—C29—H29B	107.9
H10A—C10—H10B	107.9	C25—C30—C29	112.8 (5)
C10—C11—C12	111.5 (5)	C25—C30—H30A	109.0
C10—C11—H11A	109.3	C29—C30—H30A	109.0
C12—C11—H11A	109.3	C25—C30—H30B	109.0
C10—C11—H11B	109.3	C29—C30—H30B	109.0
C12—C11—H11B	109.3	H30A—C30—H30B	107.8
H11A—C11—H11B	108.0	C32—C31—C36	110.1 (5)
C11—C12—C7	111.9 (5)	C32—C31—Sn2	113.7 (3)
C11—C12—H12A	109.2	C36—C31—Sn2	110.5 (3)
C7—C12—H12A	109.2	C32—C31—H31	107.4
C11—C12—H12B	109.2	C36—C31—H31	107.4
C7—C12—H12B	109.2	Sn2—C31—H31	107.4
H12A—C12—H12B	107.9	C31—C32—C33	112.6 (5)
C18—C13—C14	115.1 (6)	C31—C32—H32A	109.1
C18—C13—Sn1	118.0 (4)	C33—C32—H32A	109.1
C14—C13—Sn1	116.5 (4)	C31—C32—H32B	109.1
C18—C13—H13	100.9	C33—C32—H32B	109.1
C14—C13—H13	100.9	H32A—C32—H32B	107.8
Sn1—C13—H13	100.9	C34—C33—C32	111.6 (6)
C13—C14—C15	114.9 (6)	C34—C33—H33A	109.3
C13—C14—H14A	108.5	C32—C33—H33A	109.3
C15—C14—H14A	108.5	C34—C33—H33B	109.3
C13—C14—H14B	108.5	C32—C33—H33B	109.3
C15—C14—H14B	108.5	H33A—C33—H33B	108.0
H14A—C14—H14B	107.5	C35—C34—C33	111.9 (6)
C16—C15—C14	115.1 (6)	C35—C34—H34A	109.2
C16—C15—H15A	108.5	C33—C34—H34A	109.2
C14—C15—H15A	108.5	C35—C34—H34B	109.2
C16—C15—H15B	108.5	C33—C34—H34B	109.2
C14—C15—H15B	108.5	H34A—C34—H34B	107.9
H15A—C15—H15B	107.5	C34—C35—C36	111.6 (6)
C15—C16—C17	112.9 (7)	C34—C35—H35A	109.3
C15—C16—H16A	109.0	C36—C35—H35A	109.3
C17—C16—H16A	109.0	C34—C35—H35B	109.3
C15—C16—H16B	109.0	C36—C35—H35B	109.3
C17—C16—H16B	109.0	H35A—C35—H35B	108.0
H16A—C16—H16B	107.8	C31—C36—C35	111.5 (5)
C16—C17—C18	112.8 (6)	C31—C36—H36A	109.3
C16—C17—H17A	109.0	C35—C36—H36A	109.3
C18—C17—H17A	109.0	C31—C36—H36B	109.3
C16—C17—H17B	109.0	C35—C36—H36B	109.3
C18—C17—H17B	109.0	H36A—C36—H36B	108.0
H17A—C17—H17B	107.8		
C13—Sn1—S1—Sn2	−172.4 (2)	C14—C13—C18—C17	−44.8 (12)
C1—Sn1—S1—Sn2	−58.56 (14)	Sn1—C13—C18—C17	171.5 (7)
C7—Sn1—S1—Sn2	66.48 (15)	C16—C17—C18—C13	49.0 (13)
C25—Sn2—S1—Sn1	77.05 (16)	C25—Sn2—C19—C20	−175.5 (3)
C19—Sn2—S1—Sn1	−47.07 (15)	C31—Sn2—C19—C20	58.4 (4)

C31—Sn2—S1—Sn1	−166.84 (15)	S1—Sn2—C19—C20	−52.7 (4)
C13—Sn1—C1—C6	62.9 (4)	C25—Sn2—C19—C24	58.6 (4)
C7—Sn1—C1—C6	−168.4 (3)	C31—Sn2—C19—C24	−67.5 (4)
S1—Sn1—C1—C6	−45.8 (4)	S1—Sn2—C19—C24	−178.6 (3)
C13—Sn1—C1—C2	−62.0 (4)	C24—C19—C20—C21	−56.7 (6)
C7—Sn1—C1—C2	66.7 (4)	Sn2—C19—C20—C21	177.0 (4)
S1—Sn1—C1—C2	−170.7 (3)	C19—C20—C21—C22	56.8 (6)
C6—C1—C2—C3	53.2 (6)	C20—C21—C22—C23	−56.2 (7)
Sn1—C1—C2—C3	178.9 (4)	C21—C22—C23—C24	55.4 (7)
C1—C2—C3—C4	−53.2 (7)	C20—C19—C24—C23	54.9 (6)
C2—C3—C4—C5	53.3 (7)	Sn2—C19—C24—C23	−177.3 (4)
C3—C4—C5—C6	−55.0 (7)	C22—C23—C24—C19	−54.7 (7)
C2—C1—C6—C5	−53.6 (6)	C19—Sn2—C25—C30	−103.2 (5)
Sn1—C1—C6—C5	−179.8 (4)	C31—Sn2—C25—C30	24.4 (5)
C4—C5—C6—C1	55.6 (7)	S1—Sn2—C25—C30	133.4 (4)
C13—Sn1—C7—C8	−47.5 (4)	C19—Sn2—C25—C26	26.0 (5)
C1—Sn1—C7—C8	−172.3 (3)	C31—Sn2—C25—C26	153.7 (4)
S1—Sn1—C7—C8	63.8 (4)	S1—Sn2—C25—C26	−97.3 (4)
C13—Sn1—C7—C12	77.9 (4)	C30—C25—C26—C27	−51.5 (7)
C1—Sn1—C7—C12	−46.9 (4)	Sn2—C25—C26—C27	178.2 (4)
S1—Sn1—C7—C12	−170.8 (3)	C25—C26—C27—C28	52.4 (8)
C12—C7—C8—C9	54.8 (6)	C26—C27—C28—C29	−53.3 (10)
Sn1—C7—C8—C9	−177.9 (4)	C27—C28—C29—C30	53.4 (9)
C7—C8—C9—C10	−55.0 (7)	C26—C25—C30—C29	51.9 (8)
C8—C9—C10—C11	53.7 (8)	Sn2—C25—C30—C29	−177.0 (5)
C9—C10—C11—C12	−53.6 (8)	C28—C29—C30—C25	−53.0 (9)
C10—C11—C12—C7	54.7 (7)	C25—Sn2—C31—C32	−170.2 (4)
C8—C7—C12—C11	−55.1 (6)	C19—Sn2—C31—C32	−43.4 (5)
Sn1—C7—C12—C11	178.5 (4)	S1—Sn2—C31—C32	74.4 (4)
C1—Sn1—C13—C18	−140.8 (7)	C25—Sn2—C31—C36	65.4 (4)
C7—Sn1—C13—C18	91.8 (7)	C19—Sn2—C31—C36	−167.8 (4)
S1—Sn1—C13—C18	−24.6 (8)	S1—Sn2—C31—C36	−50.0 (4)
C1—Sn1—C13—C14	76.0 (7)	C36—C31—C32—C33	−53.5 (8)
C7—Sn1—C13—C14	−51.4 (7)	Sn2—C31—C32—C33	−178.1 (5)
S1—Sn1—C13—C14	−167.8 (6)	C31—C32—C33—C34	54.1 (9)
C18—C13—C14—C15	41.2 (11)	C32—C33—C34—C35	−54.4 (9)
Sn1—C13—C14—C15	−174.6 (6)	C33—C34—C35—C36	55.4 (9)
C13—C14—C15—C16	−42.4 (12)	C32—C31—C36—C35	54.0 (7)
C14—C15—C16—C17	46.7 (13)	Sn2—C31—C36—C35	−179.6 (5)
C15—C16—C17—C18	−49.4 (13)	C34—C35—C36—C31	−55.4 (8)

Fig. 1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