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[4-(2-Hydroxybenzylideneamino)-benzenethiolato]triphenyltin(IV)

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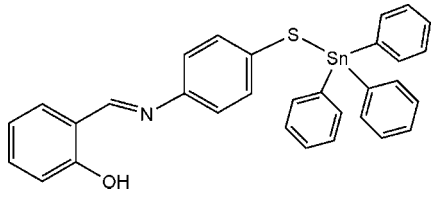
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.013 Å; R factor = 0.064; wR factor = 0.142; data-to-parameter ratio = 14.6.

The title mononuclear Schiff base compound, $[Sn(C_6H_5)_3\{SC_6H_4\text{-}4\text{-}N{=}C(H)C_6H_4{-}OH\text{-}2\}]$, contains two essentially identical molecules in the asymmetric unit, each of which features a slightly distorted C_3S tetrahedral geometry for the Sn atom.

Related literature

For related literature, see: Anderson *et al.* (1997); Li *et al.* (2007); Garnovski *et al.* (1993); Nath *et al.* (1997).



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_{13}H_{10}NOS)]$
M_r = 578.27
Triclinic, $P\overline{1}$
a = 9.5561 (10) Å
b = 9.6073 (11) Å
c = 30.110 (3) Å
α = 92.064 (2)°
β = 95.430 (2)°
γ = 104.936 (3)°
V = 2653.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.07 mm^{-1}
T = 298 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.857, T_{max} = 0.901
13756 measured reflections
9194 independent reflections
6702 reflections with $I > 2\sigma(I)$
R_{int} = 0.046

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.142
S = 1.00
9194 reflections
631 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.58 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—S1	2.421 (2)	Sn2—S2	2.423 (2)
Sn1—C14	2.124 (6)	Sn2—C45	2.127 (7)
Sn1—C20	2.113 (7)	Sn2—C51	2.120 (7)
Sn1—C26	2.120 (7)	Sn2—C57	2.129 (7)
S1—Sn1—C14	107.92 (18)	S2—Sn2—C45	107.0 (2)
S1—Sn1—C20	103.24 (19)	S2—Sn2—C51	102.5 (2)
S1—Sn1—C26	109.69 (18)	S2—Sn2—C57	109.46 (18)
Sn1—S1—C1	101.2 (2)	Sn2—S2—C32	101.1 (2)

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2196).

References

Anderson, O. P., Cour, A. L., Findeisen, M., Hennig, L., Simonsen, O., Taylor, L. & Toflund, H. (1997). *J. Chem. Soc. Dalton Trans.* pp. 111–120.
Garnovski, A. D., Nivorozhkin, A. L. & Minki, V. I. (1993). *Coord. Chem. Rev.* **126**, 1–69.
Li, J. K., Wei, C. P., Qiu, L. L. & Ma, C. L. (2007). *Anal. Sci.* **23**, 69–70.
Nath, M., Yadav, R., Gielen, M., Dalil, H., De Vos, D. & Eng, G. (1997). *Appl. Organomet. Chem.* **11**, 727–736.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

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supplementary materials

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[4-(2-Hydroxybenzylideneamino)benzenethiolato]triphenyltin(IV)

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Comment

Recently, a number of Schiff-bases have been investigated in terms of their crystallography and coordination chemistry (Garnovski *et al.*, 1993). During the last decade, Schiff-base complexes have been applied in catalytic reactions and biological systems (Anderson *et al.*, 1997). Organotin complexes containing Schiff-bases have attracted much attention owing to their potential biological activities (Nath *et al.*, 1997). The title compound (I) was synthesized and its crystal structure determined (Fig. 1 and Table 1). Two independent molecules comprise the crystallographic asymmetric unit. In each of these, the central tin atom exists in a distorted tetrahedron defined by a C_3S donor set. The geometric parameters are in good agreement with those found in (4,5-diphenyl-4-oxazoline-2-thiolato)triphenyltin (Li *et al.*, 2007). The mean planes of the two benzene rings in (I) make a dihedral angle of 31.0 (5)° (molecule 1) and 31.3 (6)° (molecule 2) showing that the Schiff-base ligand adopts a non-planar conformation in each case.

Experimental

The Schiff-base ligand was synthesized by the reaction of salicylaldehyde and 4-aminothiophenol in ethanol solution. Under an N_2 atmosphere, the Schiff-base (0.229 g, 1 mmol) and $(C_6H_5)_3SnCl$ (0.385 g, 1 mmol) were added to a solution of dry benzene (30 ml) in a Schlenk flask and stirred under reflux conditions (353 K) for 12 h. The solution was filtered and after a week yellow crystals suitable for X-ray diffraction study were obtained. Yield, 0.503 g, 82%. m.p. 430–432 K.

Analysis found: C 64.32, H 4.45, N 2.38, O 2.75, S 5.50%; $C_{19}H_{19}NOSSn$ requires: C 64.38, H 4.36, N 2.42, O 2.77, S 5.54%.

Refinement

The H-atoms were included in the riding-model approximation with C—H = 0.93 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C-aromatic) and U_{iso}(H) = 1.5U_{eq}(O). The maximum and minimum residual electron denisty peaks were located 1.68 and 1.20 Å, respectively, from the O2 and Sn2 atoms.

Figures

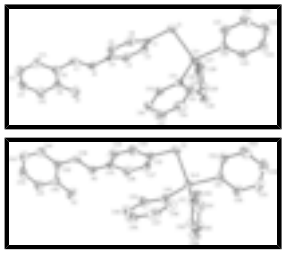

Figure 1. The molecular structures of the two independent molecules in (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.

[4-(2-Hydroxybenzylideneamino)benzenethiolato]triphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_{13}H_{10}NOS)]$	$Z = 4$
$M_r = 578.27$	$F_{000} = 1168$
Triclinic, $P\overline{1}$	$D_x = 1.447$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.5561$ (10) Å	Cell parameters from 4515 reflections
$b = 9.6073$ (11) Å	$\theta = 2.3$–24.1º
$c = 30.110$ (3) Å	$\mu = 1.07$ mm^{-1}
$\alpha = 92.064$ (2)º	$T = 298$ (2) K
$\beta = 95.430$ (2)º	Block, yellow
$\gamma = 104.936$ (3)º	0.15 × 0.12 × 0.10 mm
$V = 2653.8$ (5) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	9194 independent reflections
Radiation source: sealed tube	6702 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.046$
$T = 298$(2) K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.2$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.857$, $T_{max} = 0.901$	$k = -11 \rightarrow 11$
13756 measured reflections	$l = -35 \rightarrow 24$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.142$	$w = 1/[\sigma^2(F_o^2) + 13.8664P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
9194 reflections	$\Delta\rho_{max} = 0.58$ e Å^{-3}
631 parameters	$\Delta\rho_{min} = -1.26$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.83590 (5)	0.29973 (5)	0.379460 (17)	0.04023 (15)
Sn2	0.18962 (6)	0.14815 (6)	0.123781 (17)	0.04579 (17)
N1	0.8033 (7)	0.2038 (6)	0.6046 (2)	0.0445 (15)
N2	0.3049 (7)	0.2040 (7)	−0.0979 (2)	0.0497 (16)
O1	0.9884 (6)	0.3102 (7)	0.6745 (2)	0.0760 (18)
H1	0.9593	0.2891	0.6480	0.114*
O2	0.2069 (8)	0.0204 (6)	−0.1663 (2)	0.082 (2)
H2	0.2270	0.0490	−0.1399	0.123*
S1	0.6851 (2)	0.0845 (2)	0.40714 (7)	0.0572 (6)
S2	0.4112 (2)	0.3014 (3)	0.10086 (7)	0.0626 (6)
C1	0.7213 (8)	0.1246 (7)	0.4656 (2)	0.0429 (18)
C2	0.8510 (9)	0.1208 (8)	0.4893 (3)	0.053 (2)
H2A	0.9235	0.0990	0.4740	0.063*
C3	0.8760 (8)	0.1484 (8)	0.5349 (3)	0.051 (2)
H3	0.9654	0.1475	0.5498	0.061*
C4	0.7693 (8)	0.1772 (7)	0.5583 (3)	0.0419 (17)
C5	0.6407 (8)	0.1816 (8)	0.5353 (3)	0.051 (2)
H5	0.5679	0.2018	0.5508	0.062*
C6	0.6166 (8)	0.1569 (8)	0.4900 (3)	0.051 (2)
H6	0.5283	0.1618	0.4752	0.061*
C7	0.7035 (9)	0.1796 (8)	0.6311 (3)	0.051 (2)
H7	0.6075	0.1399	0.6191	0.061*
C8	0.7341 (9)	0.2112 (8)	0.6789 (3)	0.0480 (19)
C9	0.8756 (9)	0.2730 (8)	0.6991 (3)	0.052 (2)
C10	0.9019 (11)	0.2999 (10)	0.7448 (3)	0.068 (2)
H10	0.9959	0.3420	0.7582	0.081*
C11	0.7879 (11)	0.2639 (10)	0.7704 (3)	0.066 (2)
H11	0.8063	0.2830	0.8012	0.080*
C12	0.6478 (12)	0.2006 (10)	0.7521 (3)	0.070 (3)
H12	0.5721	0.1762	0.7701	0.085*
C13	0.6225 (10)	0.1743 (9)	0.7064 (3)	0.062 (2)
H13	0.5282	0.1308	0.6935	0.075*
C14	0.7899 (7)	0.4815 (7)	0.4112 (2)	0.0368 (16)

C15	0.8120 (9)	0.5105 (8)	0.4571 (2)	0.055 (2)
H15	0.8518	0.4512	0.4753	0.066*
C16	0.7750 (10)	0.6266 (9)	0.4756 (3)	0.071 (3)
H16	0.7861	0.6433	0.5065	0.085*
C17	0.7216 (10)	0.7190 (9)	0.4491 (4)	0.070 (3)
H17	0.6991	0.7992	0.4618	0.084*
C18	0.7028 (10)	0.6922 (9)	0.4055 (3)	0.070 (3)
H18	0.6670	0.7549	0.3876	0.084*
C19	0.7343 (9)	0.5744 (7)	0.3855 (3)	0.053 (2)
H19	0.7181	0.5576	0.3546	0.063*
C20	0.7698 (7)	0.2763 (7)	0.3100 (2)	0.0404 (17)
C21	0.6255 (8)	0.2188 (9)	0.2936 (3)	0.057 (2)
H21	0.5558	0.1919	0.3134	0.068*
C22	0.5833 (10)	0.2009 (10)	0.2481 (3)	0.069 (3)
H22	0.4864	0.1602	0.2373	0.083*
C23	0.6877 (11)	0.2443 (10)	0.2189 (3)	0.070 (3)
H23	0.6606	0.2330	0.1882	0.084*
C24	0.8268 (12)	0.3024 (11)	0.2345 (3)	0.075 (3)
H24	0.8961	0.3317	0.2146	0.090*
C25	0.8690 (9)	0.3195 (9)	0.2807 (3)	0.056 (2)
H25	0.9660	0.3610	0.2913	0.067*
C26	1.0586 (7)	0.3039 (7)	0.3935 (2)	0.0353 (15)
C27	1.1091 (9)	0.1821 (8)	0.3947 (3)	0.0479 (19)
H27	1.0430	0.0916	0.3905	0.058*
C28	1.2557 (9)	0.1921 (9)	0.4023 (3)	0.060 (2)
H28	1.2873	0.1083	0.4030	0.072*
C29	1.3557 (9)	0.3235 (10)	0.4086 (3)	0.058 (2)
H29	1.4545	0.3298	0.4146	0.070*
C30	1.3080 (9)	0.4440 (9)	0.4061 (3)	0.064 (2)
H30	1.3748	0.5341	0.4087	0.077*
C31	1.1602 (9)	0.4342 (8)	0.3998 (3)	0.054 (2)
H31	1.1293	0.5185	0.3999	0.065*
C32	0.3776 (8)	0.2722 (8)	0.0419 (3)	0.0488 (19)
C33	0.3434 (10)	0.3769 (10)	0.0168 (3)	0.064 (2)
H33	0.3351	0.4618	0.0309	0.077*
C34	0.3212 (10)	0.3583 (9)	−0.0289 (3)	0.065 (2)
H34	0.3004	0.4320	−0.0454	0.078*
C35	0.3290 (8)	0.2332 (8)	−0.0509 (3)	0.0444 (18)
C36	0.3589 (9)	0.1266 (8)	−0.0257 (3)	0.055 (2)
H36	0.3618	0.0397	−0.0397	0.066*
C37	0.3850 (9)	0.1462 (9)	0.0206 (3)	0.057 (2)
H37	0.4076	0.0736	0.0372	0.068*
C38	0.3319 (7)	0.3032 (8)	−0.1252 (3)	0.049 (2)
H38	0.3701	0.3981	−0.1137	0.058*
C39	0.3061 (8)	0.2756 (9)	−0.1726 (3)	0.053 (2)
C40	0.2437 (9)	0.1339 (9)	−0.1923 (3)	0.058 (2)
C41	0.2205 (11)	0.1116 (10)	−0.2381 (3)	0.071 (3)
H41	0.1795	0.0190	−0.2512	0.085*
C42	0.2583 (10)	0.2268 (12)	−0.2648 (3)	0.073 (3)

H42	0.2435	0.2116	−0.2957	0.087*
C43	0.3175 (11)	0.3630 (12)	−0.2456 (4)	0.079 (3)
H43	0.3429	0.4402	−0.2636	0.095*
C44	0.3394 (10)	0.3865 (9)	−0.2005 (3)	0.067 (2)
H44	0.3781	0.4803	−0.1882	0.080*
C45	0.0125 (8)	0.1969 (7)	0.0849 (3)	0.0459 (18)
C46	−0.0866 (10)	0.2497 (9)	0.1066 (3)	0.070 (3)
H46	−0.0772	0.2590	0.1377	0.084*
C47	−0.1986 (10)	0.2886 (9)	0.0826 (3)	0.071 (3)
H47	−0.2627	0.3270	0.0974	0.085*
C48	−0.2159 (10)	0.2708 (10)	0.0366 (3)	0.072 (3)
H48	−0.2930	0.2950	0.0204	0.086*
C49	−0.1210 (9)	0.2182 (11)	0.0153 (3)	0.074 (3)
H49	−0.1319	0.2067	−0.0157	0.089*
C50	−0.0074 (9)	0.1813 (10)	0.0397 (3)	0.060 (2)
H50	0.0572	0.1447	0.0246	0.072*
C51	0.2063 (8)	0.2095 (8)	0.1928 (2)	0.0425 (17)
C52	0.2661 (9)	0.3513 (9)	0.2087 (3)	0.053 (2)
H52	0.2955	0.4224	0.1888	0.064*
C53	0.2822 (10)	0.3874 (10)	0.2542 (3)	0.070 (3)
H53	0.3217	0.4831	0.2646	0.084*
C54	0.2416 (11)	0.2861 (12)	0.2837 (3)	0.071 (3)
H54	0.2522	0.3116	0.3141	0.086*
C55	0.1846 (11)	0.1458 (11)	0.2682 (3)	0.074 (3)
H55	0.1579	0.0755	0.2885	0.088*
C56	0.1659 (9)	0.1061 (9)	0.2231 (3)	0.058 (2)
H56	0.1263	0.0099	0.2131	0.070*
C57	0.1900 (7)	−0.0722 (7)	0.1137 (2)	0.0440 (17)
C58	0.0583 (8)	−0.1736 (8)	0.1075 (3)	0.062 (2)
H58	−0.0271	−0.1440	0.1074	0.074*
C59	0.0497 (10)	−0.3186 (10)	0.1016 (3)	0.077 (3)
H59	−0.0410	−0.3853	0.0968	0.093*
C60	0.1745 (10)	−0.3652 (10)	0.1027 (3)	0.069 (3)
H60	0.1690	−0.4632	0.0997	0.083*
C61	0.3038 (11)	−0.2672 (10)	0.1081 (4)	0.082 (3)
H61	0.3886	−0.2975	0.1077	0.098*
C62	0.3137 (8)	−0.1205 (9)	0.1143 (3)	0.069 (2)
H62	0.4047	−0.0546	0.1190	0.082*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0453 (3)	0.0343 (3)	0.0401 (3)	0.0108 (2)	−0.0004 (2)	−0.0004 (2)
Sn2	0.0435 (3)	0.0486 (3)	0.0428 (3)	0.0098 (3)	0.0006 (2)	−0.0022 (2)
N1	0.051 (4)	0.034 (3)	0.049 (4)	0.012 (3)	0.003 (3)	0.010 (3)
N2	0.044 (4)	0.046 (4)	0.060 (4)	0.011 (3)	0.010 (3)	0.005 (3)
O1	0.049 (4)	0.112 (5)	0.056 (4)	0.005 (3)	0.000 (3)	0.004 (4)
O2	0.136 (6)	0.050 (4)	0.058 (4)	0.015 (4)	0.024 (4)	0.008 (3)

S1	0.0698 (14)	0.0401 (11)	0.0488 (12)	−0.0052 (10)	−0.0032 (10)	0.0021 (9)
S2	0.0473 (12)	0.0721 (15)	0.0532 (13)	−0.0083 (11)	−0.0003 (10)	−0.0045 (11)
C1	0.052 (5)	0.026 (3)	0.044 (4)	−0.001 (3)	0.000 (4)	0.004 (3)
C2	0.053 (5)	0.057 (5)	0.052 (5)	0.020 (4)	0.009 (4)	0.011 (4)
C3	0.041 (4)	0.055 (5)	0.054 (5)	0.009 (4)	−0.002 (4)	0.009 (4)
C4	0.046 (4)	0.026 (4)	0.051 (5)	0.004 (3)	0.004 (4)	0.002 (3)
C5	0.041 (5)	0.059 (5)	0.050 (5)	0.008 (4)	0.002 (4)	−0.003 (4)
C6	0.041 (5)	0.050 (5)	0.060 (5)	0.011 (4)	−0.002 (4)	0.009 (4)
C7	0.054 (5)	0.033 (4)	0.061 (5)	0.005 (4)	0.000 (4)	−0.002 (4)
C8	0.053 (5)	0.039 (4)	0.054 (5)	0.015 (4)	0.005 (4)	0.002 (4)
C9	0.053 (5)	0.049 (5)	0.051 (5)	0.012 (4)	0.003 (4)	0.004 (4)
C10	0.068 (6)	0.085 (7)	0.053 (6)	0.028 (5)	−0.003 (5)	0.005 (5)
C11	0.088 (7)	0.065 (6)	0.050 (5)	0.027 (5)	0.004 (5)	0.002 (4)
C12	0.083 (7)	0.069 (6)	0.064 (6)	0.021 (5)	0.027 (5)	0.013 (5)
C13	0.055 (5)	0.065 (6)	0.067 (6)	0.013 (4)	0.014 (5)	0.014 (5)
C14	0.031 (4)	0.032 (4)	0.049 (4)	0.009 (3)	0.006 (3)	0.006 (3)
C15	0.080 (6)	0.037 (4)	0.046 (5)	0.015 (4)	0.002 (4)	−0.001 (4)
C16	0.084 (7)	0.062 (6)	0.059 (6)	0.008 (5)	0.015 (5)	−0.020 (5)
C17	0.064 (6)	0.047 (5)	0.102 (8)	0.019 (5)	0.019 (6)	−0.025 (5)
C18	0.073 (6)	0.053 (5)	0.089 (8)	0.029 (5)	0.004 (5)	0.003 (5)
C19	0.059 (5)	0.041 (4)	0.059 (5)	0.015 (4)	0.002 (4)	0.005 (4)
C20	0.050 (5)	0.033 (4)	0.042 (4)	0.018 (3)	0.006 (4)	0.004 (3)
C21	0.049 (5)	0.067 (5)	0.053 (5)	0.012 (4)	0.002 (4)	0.000 (4)
C22	0.063 (6)	0.076 (6)	0.062 (6)	0.016 (5)	−0.019 (5)	−0.007 (5)
C23	0.099 (8)	0.076 (6)	0.038 (5)	0.035 (6)	−0.009 (5)	−0.003 (5)
C24	0.088 (8)	0.087 (7)	0.053 (6)	0.023 (6)	0.019 (5)	−0.003 (5)
C25	0.048 (5)	0.059 (5)	0.055 (5)	0.006 (4)	0.004 (4)	−0.005 (4)
C26	0.043 (4)	0.029 (3)	0.035 (4)	0.013 (3)	0.000 (3)	−0.002 (3)
C27	0.056 (5)	0.033 (4)	0.055 (5)	0.011 (4)	0.008 (4)	0.008 (3)
C28	0.060 (6)	0.051 (5)	0.080 (6)	0.035 (5)	0.009 (5)	0.021 (5)
C29	0.050 (5)	0.077 (6)	0.054 (5)	0.028 (5)	0.002 (4)	0.012 (5)
C30	0.054 (5)	0.046 (5)	0.081 (7)	−0.004 (4)	−0.002 (5)	−0.002 (4)
C31	0.052 (5)	0.030 (4)	0.080 (6)	0.017 (4)	−0.005 (4)	−0.003 (4)
C32	0.038 (4)	0.053 (5)	0.053 (5)	0.006 (4)	0.012 (4)	0.004 (4)
C33	0.081 (7)	0.058 (5)	0.051 (5)	0.014 (5)	0.006 (5)	−0.004 (4)
C34	0.087 (7)	0.048 (5)	0.066 (6)	0.026 (5)	0.007 (5)	0.005 (4)
C35	0.034 (4)	0.047 (4)	0.049 (5)	0.005 (3)	0.004 (3)	−0.001 (4)
C36	0.065 (6)	0.044 (4)	0.061 (6)	0.021 (4)	0.018 (4)	0.007 (4)
C37	0.062 (5)	0.062 (5)	0.057 (5)	0.029 (4)	0.018 (4)	0.018 (4)
C38	0.032 (4)	0.039 (4)	0.070 (6)	0.002 (3)	0.003 (4)	−0.002 (4)
C39	0.041 (5)	0.051 (5)	0.068 (6)	0.011 (4)	0.004 (4)	0.008 (4)
C40	0.060 (5)	0.061 (5)	0.054 (5)	0.017 (4)	0.008 (4)	0.010 (4)
C41	0.088 (7)	0.064 (6)	0.057 (6)	0.016 (5)	0.008 (5)	−0.004 (5)
C42	0.072 (7)	0.111 (9)	0.048 (5)	0.043 (6)	0.008 (5)	0.009 (6)
C43	0.073 (7)	0.082 (7)	0.075 (7)	0.008 (6)	−0.004 (6)	0.026 (6)
C44	0.073 (6)	0.051 (5)	0.070 (7)	0.007 (5)	0.000 (5)	0.010 (5)
C45	0.045 (4)	0.040 (4)	0.054 (5)	0.009 (3)	0.010 (4)	0.008 (4)
C46	0.071 (6)	0.063 (6)	0.079 (7)	0.022 (5)	0.020 (5)	0.003 (5)
C47	0.055 (6)	0.054 (5)	0.107 (9)	0.018 (5)	0.022 (6)	0.005 (5)

C48	0.055 (6)	0.064 (6)	0.100 (8)	0.026 (5)	−0.013 (6)	0.012 (6)
C49	0.063 (6)	0.090 (7)	0.059 (6)	0.010 (5)	−0.012 (5)	0.000 (5)
C50	0.053 (5)	0.082 (6)	0.046 (5)	0.025 (5)	−0.001 (4)	−0.012 (4)
C51	0.041 (4)	0.044 (4)	0.044 (4)	0.014 (3)	0.002 (3)	0.003 (3)
C52	0.065 (5)	0.054 (5)	0.041 (5)	0.019 (4)	0.003 (4)	0.001 (4)
C53	0.081 (7)	0.065 (6)	0.065 (6)	0.023 (5)	0.004 (5)	−0.021 (5)
C54	0.076 (7)	0.097 (8)	0.050 (6)	0.035 (6)	0.018 (5)	0.002 (6)
C55	0.097 (8)	0.084 (7)	0.052 (6)	0.037 (6)	0.025 (5)	0.023 (5)
C56	0.071 (6)	0.055 (5)	0.051 (5)	0.020 (4)	0.009 (4)	0.010 (4)
C57	0.037 (4)	0.052 (4)	0.043 (4)	0.010 (3)	0.007 (3)	0.001 (3)
C58	0.043 (4)	0.049 (5)	0.095 (6)	0.017 (4)	0.003 (4)	−0.005 (4)
C59	0.067 (6)	0.064 (6)	0.092 (8)	0.009 (5)	−0.003 (5)	−0.011 (5)
C60	0.082 (7)	0.054 (5)	0.076 (7)	0.022 (5)	0.017 (5)	0.006 (5)
C61	0.075 (7)	0.081 (7)	0.119 (9)	0.059 (6)	0.036 (6)	0.033 (6)
C62	0.044 (5)	0.078 (6)	0.085 (6)	0.017 (4)	0.007 (4)	0.016 (5)

Geometric parameters (Å, °)

Sn1—S1	2.421 (2)	C27—C28	1.376 (11)
Sn1—C14	2.124 (6)	C27—H27	0.9300
Sn1—C20	2.113 (7)	C28—C29	1.367 (12)
Sn1—C26	2.120 (7)	C28—H28	0.9300
Sn2—S2	2.423 (2)	C29—C30	1.351 (11)
Sn2—C45	2.127 (7)	C29—H29	0.9300
Sn2—C51	2.120 (7)	C30—C31	1.385 (11)
Sn2—C57	2.129 (7)	C30—H30	0.9300
N1—C7	1.281 (9)	C31—H31	0.9300
N1—C4	1.401 (9)	C32—C33	1.366 (11)
N2—C38	1.273 (9)	C32—C37	1.370 (11)
N2—C35	1.417 (10)	C33—C34	1.370 (12)
O1—C9	1.345 (9)	C33—H33	0.9300
O1—H1	0.8200	C34—C35	1.375 (11)
O2—C40	1.358 (9)	C34—H34	0.9300
O2—H2	0.8200	C35—C36	1.369 (10)
S1—C1	1.771 (7)	C36—C37	1.391 (11)
S2—C32	1.774 (8)	C36—H36	0.9300
C1—C2	1.379 (10)	C37—H37	0.9300
C1—C6	1.385 (10)	C38—C39	1.429 (11)
C2—C3	1.374 (11)	C38—H38	0.9300
C2—H2A	0.9300	C39—C44	1.372 (11)
C3—C4	1.372 (10)	C39—C40	1.420 (11)
C3—H3	0.9300	C40—C41	1.376 (12)
C4—C5	1.365 (10)	C41—C42	1.383 (13)
C5—C6	1.363 (11)	C41—H41	0.9300
C5—H5	0.9300	C42—C43	1.367 (13)
C6—H6	0.9300	C42—H42	0.9300
C7—C8	1.445 (11)	C43—C44	1.355 (13)
C7—H7	0.9300	C43—H43	0.9300
C8—C13	1.394 (11)	C44—H44	0.9300

C8—C9	1.398 (11)	C45—C50	1.356 (10)
C9—C10	1.379 (11)	C45—C46	1.386 (8)
C10—C11	1.373 (12)	C46—C47	1.374 (12)
C10—H10	0.9300	C46—H46	0.9300
C11—C12	1.372 (13)	C47—C48	1.377 (8)
C11—H11	0.9300	C47—H47	0.9300
C12—C13	1.378 (12)	C48—C49	1.346 (12)
C12—H12	0.9300	C48—H48	0.9300
C13—H13	0.9300	C49—C50	1.381 (8)
C14—C19	1.376 (9)	C49—H49	0.9300
C14—C15	1.386 (7)	C50—H50	0.9300
C15—C16	1.370 (11)	C51—C56	1.378 (10)
C15—H15	0.9300	C51—C52	1.383 (10)
C16—C17	1.376 (8)	C52—C53	1.385 (11)
C16—H16	0.9300	C52—H52	0.9300
C17—C18	1.314 (12)	C53—C54	1.348 (13)
C17—H17	0.9300	C53—H53	0.9300
C18—C19	1.377 (8)	C54—C55	1.363 (13)
C18—H18	0.9300	C54—H54	0.9300
C19—H19	0.9300	C55—C56	1.380 (12)
C20—C25	1.353 (10)	C55—H55	0.9300
C20—C21	1.382 (7)	C56—H56	0.9300
C21—C22	1.382 (11)	C57—C58	1.371 (7)
C21—H21	0.9300	C57—C62	1.375 (7)
C22—C23	1.386 (8)	C58—C59	1.378 (11)
C22—H22	0.9300	C58—H58	0.9300
C23—C24	1.334 (13)	C59—C60	1.376 (8)
C23—H23	0.9300	C59—H59	0.9300
C24—C25	1.404 (8)	C60—C61	1.339 (12)
C24—H24	0.9300	C60—H60	0.9300
C25—H25	0.9300	C61—C62	1.392 (8)
C26—C31	1.367 (10)	C61—H61	0.9300
C26—C27	1.376 (9)	C62—H62	0.9300
C20—Sn1—C26	111.6 (3)	C30—C29—C28	118.6 (8)
C20—Sn1—C14	112.9 (2)	C30—C29—H29	120.7
C26—Sn1—C14	111.1 (2)	C28—C29—H29	120.7
S1—Sn1—C14	107.92 (18)	C29—C30—C31	120.5 (8)
S1—Sn1—C20	103.24 (19)	C29—C30—H30	119.8
S1—Sn1—C26	109.69 (18)	C31—C30—H30	119.8
Sn1—S1—C1	101.2 (2)	C26—C31—C30	121.6 (7)
C51—Sn2—C45	114.2 (3)	C26—C31—H31	119.2
C51—Sn2—C57	111.1 (3)	C30—C31—H31	119.2
C45—Sn2—C57	112.0 (3)	C33—C32—C37	118.8 (8)
S2—Sn2—C45	107.0 (2)	C33—C32—S2	119.8 (6)
S2—Sn2—C51	102.5 (2)	C37—C32—S2	121.4 (6)
S2—Sn2—C57	109.46 (18)	C32—C33—C34	120.7 (8)
Sn2—S2—C32	101.1 (2)	C32—C33—H33	119.6
C7—N1—C4	121.3 (7)	C34—C33—H33	119.6
C38—N2—C35	122.5 (7)	C33—C34—C35	121.4 (8)

C9—O1—H1	109.5	C33—C34—H34	119.3
C40—O2—H2	109.5	C35—C34—H34	119.3
C2—C1—C6	116.8 (7)	C36—C35—C34	117.8 (8)
C2—C1—S1	122.5 (6)	C36—C35—N2	117.1 (7)
C6—C1—S1	120.6 (6)	C34—C35—N2	125.1 (7)
C3—C2—C1	121.9 (8)	C35—C36—C37	121.0 (8)
C3—C2—H2A	119.1	C35—C36—H36	119.5
C1—C2—H2A	119.1	C37—C36—H36	119.5
C4—C3—C2	120.2 (7)	C32—C37—C36	120.2 (8)
C4—C3—H3	119.9	C32—C37—H37	119.9
C2—C3—H3	119.9	C36—C37—H37	119.9
C5—C4—C3	118.5 (7)	N2—C38—C39	123.0 (7)
C5—C4—N1	124.8 (7)	N2—C38—H38	118.5
C3—C4—N1	116.7 (7)	C39—C38—H38	118.5
C6—C5—C4	121.4 (8)	C44—C39—C40	118.0 (8)
C6—C5—H5	119.3	C44—C39—C38	120.6 (8)
C4—C5—H5	119.3	C40—C39—C38	121.4 (7)
C5—C6—C1	121.2 (7)	O2—C40—C41	119.8 (8)
C5—C6—H6	119.4	O2—C40—C39	120.4 (8)
C1—C6—H6	119.4	C41—C40—C39	119.7 (8)
N1—C7—C8	122.7 (8)	C40—C41—C42	120.0 (9)
N1—C7—H7	118.6	C40—C41—H41	120.0
C8—C7—H7	118.6	C42—C41—H41	120.0
C13—C8—C9	118.0 (8)	C43—C42—C41	120.0 (9)
C13—C8—C7	120.2 (8)	C43—C42—H42	120.0
C9—C8—C7	121.7 (7)	C41—C42—H42	120.0
O1—C9—C10	118.5 (8)	C44—C43—C42	120.5 (9)
O1—C9—C8	121.0 (7)	C44—C43—H43	119.7
C10—C9—C8	120.4 (8)	C42—C43—H43	119.7
C11—C10—C9	119.3 (9)	C43—C44—C39	121.7 (9)
C11—C10—H10	120.3	C43—C44—H44	119.1
C9—C10—H10	120.3	C39—C44—H44	119.1
C12—C11—C10	122.3 (9)	C50—C45—C46	117.9 (8)
C12—C11—H11	118.9	C50—C45—Sn2	123.3 (5)
C10—C11—H11	118.9	C46—C45—Sn2	118.9 (6)
C11—C12—C13	118.0 (9)	C47—C46—C45	120.6 (9)
C11—C12—H12	121.0	C47—C46—H46	119.7
C13—C12—H12	121.0	C45—C46—H46	119.7
C12—C13—C8	121.9 (9)	C46—C47—C48	120.0 (8)
C12—C13—H13	119.1	C46—C47—H47	120.0
C8—C13—H13	119.1	C48—C47—H47	120.0
C19—C14—C15	118.0 (7)	C49—C48—C47	119.8 (8)
C19—C14—Sn1	119.2 (5)	C49—C48—H48	120.1
C15—C14—Sn1	122.8 (5)	C47—C48—H48	120.1
C16—C15—C14	119.9 (7)	C48—C49—C50	119.8 (9)
C16—C15—H15	120.1	C48—C49—H49	120.1
C14—C15—H15	120.1	C50—C49—H49	120.1
C15—C16—C17	120.9 (8)	C45—C50—C49	121.9 (8)
C15—C16—H16	119.6	C45—C50—H50	119.1

C17—C16—H16	119.6	C49—C50—H50	119.1
C18—C17—C16	119.0 (8)	C56—C51—C52	118.8 (7)
C18—C17—H17	120.5	C56—C51—Sn2	120.1 (6)
C16—C17—H17	120.5	C52—C51—Sn2	121.0 (5)
C17—C18—C19	122.1 (9)	C51—C52—C53	119.9 (8)
C17—C18—H18	118.9	C51—C52—H52	120.1
C19—C18—H18	118.9	C53—C52—H52	120.1
C14—C19—C18	120.1 (8)	C54—C53—C52	121.2 (9)
C14—C19—H19	120.0	C54—C53—H53	119.4
C18—C19—H19	120.0	C52—C53—H53	119.4
C25—C20—C21	118.7 (7)	C53—C54—C55	119.1 (9)
C25—C20—Sn1	120.1 (5)	C53—C54—H54	120.5
C21—C20—Sn1	121.2 (6)	C55—C54—H54	120.5
C20—C21—C22	120.9 (8)	C54—C55—C56	121.3 (9)
C20—C21—H21	119.5	C54—C55—H55	119.3
C22—C21—H21	119.5	C56—C55—H55	119.3
C21—C22—C23	119.0 (8)	C51—C56—C55	119.7 (8)
C21—C22—H22	120.5	C51—C56—H56	120.1
C23—C22—H22	120.5	C55—C56—H56	120.1
C24—C23—C22	120.4 (8)	C58—C57—C62	117.6 (7)
C24—C23—H23	119.8	C58—C57—Sn2	117.9 (5)
C22—C23—H23	119.8	C62—C57—Sn2	124.5 (5)
C23—C24—C25	120.3 (9)	C57—C58—C59	121.4 (7)
C23—C24—H24	119.9	C57—C58—H58	119.3
C25—C24—H24	119.9	C59—C58—H58	119.3
C20—C25—C24	120.6 (8)	C60—C59—C58	120.4 (9)
C20—C25—H25	119.7	C60—C59—H59	119.8
C24—C25—H25	119.7	C58—C59—H59	119.8
C31—C26—C27	117.2 (7)	C61—C60—C59	118.9 (9)
C31—C26—Sn1	119.0 (5)	C61—C60—H60	120.6
C27—C26—Sn1	123.8 (5)	C59—C60—H60	120.6
C28—C27—C26	121.0 (7)	C60—C61—C62	121.1 (8)
C28—C27—H27	119.5	C60—C61—H61	119.4
C26—C27—H27	119.5	C62—C61—H61	119.4
C29—C28—C27	121.0 (7)	C57—C62—C61	120.7 (8)
C29—C28—H28	119.5	C57—C62—H62	119.7
C27—C28—H28	119.5	C61—C62—H62	119.7
C20—Sn1—S1—C1	−170.2 (3)	C27—C26—C31—C30	1.7 (12)
C26—Sn1—S1—C1	70.7 (3)	Sn1—C26—C31—C30	−175.7 (7)
C14—Sn1—S1—C1	−50.5 (3)	C29—C30—C31—C26	−3.7 (14)
C51—Sn2—S2—C32	−169.5 (3)	Sn2—S2—C32—C33	105.7 (7)
C45—Sn2—S2—C32	−49.1 (4)	Sn2—S2—C32—C37	−74.3 (7)
C57—Sn2—S2—C32	72.4 (4)	C37—C32—C33—C34	−1.9 (13)
Sn1—S1—C1—C2	−73.9 (6)	S2—C32—C33—C34	178.1 (7)
Sn1—S1—C1—C6	108.2 (6)	C32—C33—C34—C35	1.6 (14)
C6—C1—C2—C3	−0.3 (11)	C33—C34—C35—C36	0.4 (13)
S1—C1—C2—C3	−178.2 (6)	C33—C34—C35—N2	178.8 (8)
C1—C2—C3—C4	1.7 (12)	C38—N2—C35—C36	−152.0 (7)
C2—C3—C4—C5	−1.8 (11)	C38—N2—C35—C34	29.6 (12)

C2—C3—C4—N1	179.8 (7)	C34—C35—C36—C37	−2.0 (12)
C7—N1—C4—C5	27.7 (11)	N2—C35—C36—C37	179.5 (7)
C7—N1—C4—C3	−154.0 (7)	C33—C32—C37—C36	0.4 (12)
C3—C4—C5—C6	0.5 (11)	S2—C32—C37—C36	−179.6 (6)
N1—C4—C5—C6	178.8 (7)	C35—C36—C37—C32	1.6 (12)
C4—C5—C6—C1	0.8 (12)	C35—N2—C38—C39	−179.1 (7)
C2—C1—C6—C5	−0.9 (11)	N2—C38—C39—C44	−179.0 (8)
S1—C1—C6—C5	177.0 (6)	N2—C38—C39—C40	2.0 (12)
C4—N1—C7—C8	−177.4 (6)	C44—C39—C40—O2	−179.1 (8)
N1—C7—C8—C13	−176.0 (7)	C38—C39—C40—O2	−0.1 (12)
N1—C7—C8—C9	1.1 (12)	C44—C39—C40—C41	1.0 (13)
C13—C8—C9—O1	179.6 (7)	C38—C39—C40—C41	180.0 (8)
C7—C8—C9—O1	2.4 (12)	O2—C40—C41—C42	−179.8 (8)
C13—C8—C9—C10	−1.8 (12)	C39—C40—C41—C42	0.1 (14)
C7—C8—C9—C10	−178.9 (8)	C40—C41—C42—C43	−0.6 (15)
O1—C9—C10—C11	179.4 (8)	C41—C42—C43—C44	−0.1 (15)
C8—C9—C10—C11	0.7 (13)	C42—C43—C44—C39	1.2 (16)
C9—C10—C11—C12	0.5 (14)	C40—C39—C44—C43	−1.7 (14)
C10—C11—C12—C13	−0.6 (14)	C38—C39—C44—C43	179.3 (9)
C11—C12—C13—C8	−0.6 (14)	C51—Sn2—C45—C50	172.4 (7)
C9—C8—C13—C12	1.7 (12)	C57—Sn2—C45—C50	−60.2 (7)
C7—C8—C13—C12	178.9 (8)	S2—Sn2—C45—C50	59.7 (7)
C20—Sn1—C14—C19	−5.1 (6)	C51—Sn2—C45—C46	−6.4 (7)
C26—Sn1—C14—C19	121.1 (6)	C57—Sn2—C45—C46	121.0 (6)
S1—Sn1—C14—C19	−118.6 (5)	S2—Sn2—C45—C46	−119.1 (6)
C20—Sn1—C14—C15	174.1 (6)	C50—C45—C46—C47	−1.8 (13)
C26—Sn1—C14—C15	−59.6 (7)	Sn2—C45—C46—C47	177.0 (7)
S1—Sn1—C14—C15	60.7 (6)	C45—C46—C47—C48	2.1 (14)
C19—C14—C15—C16	1.7 (12)	C46—C47—C48—C49	−1.5 (14)
Sn1—C14—C15—C16	−177.6 (6)	C47—C48—C49—C50	0.5 (15)
C14—C15—C16—C17	−2.7 (14)	C46—C45—C50—C49	0.9 (13)
C15—C16—C17—C18	1.8 (15)	Sn2—C45—C50—C49	−177.9 (7)
C16—C17—C18—C19	0.2 (15)	C48—C49—C50—C45	−0.2 (15)
C15—C14—C19—C18	0.2 (11)	C45—Sn2—C51—C56	105.5 (6)
Sn1—C14—C19—C18	179.5 (6)	C57—Sn2—C51—C56	−22.4 (7)
C17—C18—C19—C14	−1.2 (14)	S2—Sn2—C51—C56	−139.2 (6)
C26—Sn1—C20—C25	−25.1 (7)	C45—Sn2—C51—C52	−78.8 (7)
C14—Sn1—C20—C25	100.9 (6)	C57—Sn2—C51—C52	153.4 (6)
S1—Sn1—C20—C25	−142.8 (6)	S2—Sn2—C51—C52	36.5 (6)
C26—Sn1—C20—C21	155.8 (6)	C56—C51—C52—C53	−1.1 (12)
C14—Sn1—C20—C21	−78.2 (6)	Sn2—C51—C52—C53	−176.9 (6)
S1—Sn1—C20—C21	38.1 (6)	C51—C52—C53—C54	0.6 (14)
C25—C20—C21—C22	2.3 (12)	C52—C53—C54—C55	0.5 (15)
Sn1—C20—C21—C22	−178.6 (6)	C53—C54—C55—C56	−1.0 (15)
C20—C21—C22—C23	−1.4 (13)	C52—C51—C56—C55	0.6 (12)
C21—C22—C23—C24	0.1 (14)	Sn2—C51—C56—C55	176.4 (7)
C22—C23—C24—C25	0.3 (15)	C54—C55—C56—C51	0.5 (14)
C21—C20—C25—C24	−1.9 (12)	C51—Sn2—C57—C58	92.6 (7)
Sn1—C20—C25—C24	179.0 (7)	C45—Sn2—C57—C58	−36.4 (7)

C23—C24—C25—C20	0.6 (14)	S2—Sn2—C57—C58	−154.9 (6)
C20—Sn1—C26—C31	95.4 (6)	C51—Sn2—C57—C62	−85.1 (7)
C14—Sn1—C26—C31	−31.6 (7)	C45—Sn2—C57—C62	145.9 (7)
S1—Sn1—C26—C31	−150.8 (6)	S2—Sn2—C57—C62	27.4 (8)
C20—Sn1—C26—C27	−81.8 (6)	C62—C57—C58—C59	−1.0 (14)
C14—Sn1—C26—C27	151.3 (6)	Sn2—C57—C58—C59	−178.8 (7)
S1—Sn1—C26—C27	32.0 (6)	C57—C58—C59—C60	1.4 (15)
C31—C26—C27—C28	0.1 (11)	C58—C59—C60—C61	−2.2 (16)
Sn1—C26—C27—C28	177.4 (6)	C59—C60—C61—C62	2.5 (16)
C26—C27—C28—C29	0.0 (13)	C58—C57—C62—C61	1.3 (13)
C27—C28—C29—C30	−1.9 (13)	Sn2—C57—C62—C61	178.9 (7)
C28—C29—C30—C31	3.7 (14)	C60—C61—C62—C57	−2.1 (16)

Fig. 1

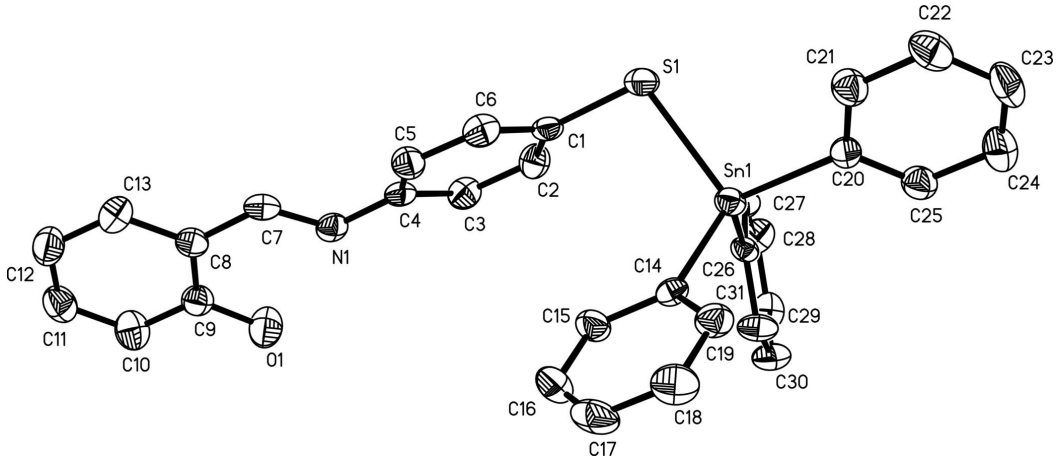
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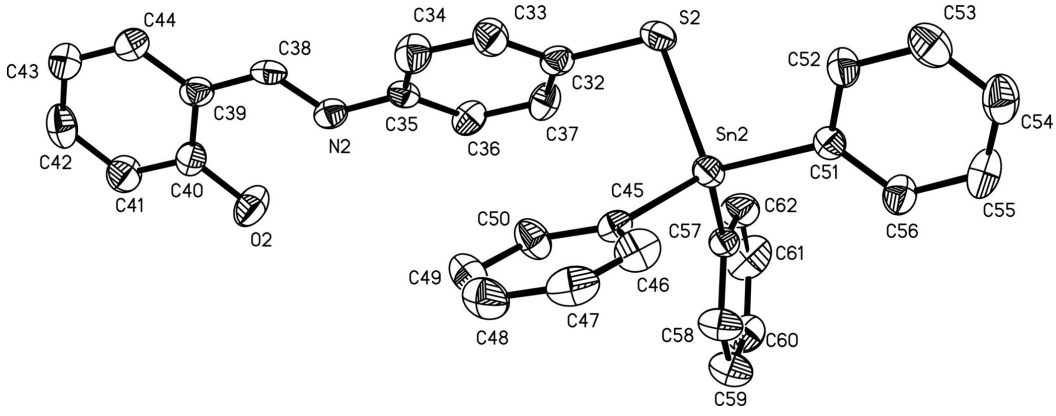
Fig. 2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