Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-{[4-(Trimethylstannylthio)phenylimino]methyl}phenol

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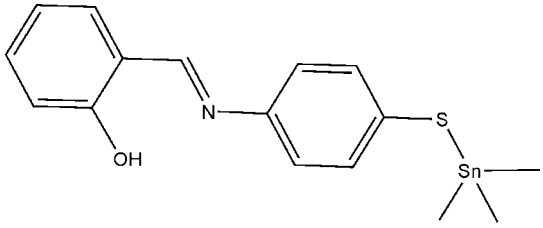
Received 1 September 2007; accepted 4 September 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.054; wR factor = 0.165; data-to-parameter ratio = 16.9.

The mononuclear Schiff base compound $C_{16}H_{19}NOSSn$ or $[(CH_3)_3Sn(SC_6H_4\text{-}4\text{-}N{=}C(H)C_6H_4\text{-}OH\text{-}2)]$ features a slightly distorted C_3S tetrahedral geometry for Sn. The mean planes of the two benzene rings make a dihedral angle of 41.8 (2)°, indicating nonplanarity of the molecule.

Related literature

For related literature, see: Anderson *et al.* (1997); Cea-Olivares *et al.* (1994); Garnovski *et al.* (1993); Nath *et al.* (1997).



Experimental

Crystal data

$C_{16}H_{19}NOSSn$
M_r = 392.07
Monoclinic, $P2_1/n$
a = 11.1385 (16) Å
b = 6.4148 (12) Å
c = 24.490 (2) Å
β = 96.254 (2)°
V = 1739.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 298 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.797, T_{max} = 0.858
8291 measured reflections
3104 independent reflections
2284 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.165
S = 1.01
3104 reflections
184 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—S1	2.425 (2)	Sn1—C16	2.138 (7)
Sn1—C14	2.117 (7)	N1—C7	1.277 (8)
Sn1—C15	2.137 (9)		
S1—Sn1—C14	105.6 (2)	C14—Sn1—C16	115.6 (3)
S1—Sn1—C15	106.4 (3)	C15—Sn1—C16	113.1 (4)
S1—Sn1—C16	105.0 (2)	Sn1—S1—C1	99.1 (2)
C14—Sn1—C15	110.3 (3)		

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*.

The authors thank the Postgraduate Foundation of Taishan University (No. Y06-2-12) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2193).

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  doi:10.1107/S1600536807043371

supplementary materials

Acta Cryst. (2007). E**63**, m2498 [**doi:10.1107/S1600536807043371**]

2-{[4-(Trimethylstannylthio)phenylimino]methyl}phenol

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Comment

Schiff-bases are well known chelating ligands in 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). In this contribution, the title compound (I) was synthesized and its crystal structure determined (Fig. 1 and Table 1). 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 (1-phenyl-1*H*-tetrazole-5-thiolato)trimethyltin (Cea-Olivares *et al.*, 1994). The mean planes of the two benzene rings in (I) make a dihedral angle of 41.8 (2)°.

Experimental

The Schiff-base ligand was synthesized by the reaction of salicylaldehyde and 4-aminothiophenol in ethanol solution. The syntheses of (I) was carried out under an N_2 atmosphere. The Schiff-base (0.229 g, 1 mmol) and $(CH_3)_3SnCl$ (0.199 g, 1 mmol) were added to a solution of dry benzene (30 ml) in a Schlenk flash and stirred under refux 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, 0.423 g, 85%. m.p. 412–414 K.

Analysis found: C 48.85, H 4.91, N 3.54, O 4.02, S 8.10%; $C_{19}H_{19}NOSSn$ requires: C 49.01, H 4.88, N 3.57, O 4.08, S 8.18%.

Refinement

The H-atoms were included in the riding-model approximation with C—H = 0.93 − 0.96 Å and O—H = 0.82 Å, and with U_{iso}(H) = 1.2U_{eq}(C-aromatic) and U_{iso}(H) = 1.5U_{eq}(*C*-methyl and O).

Figures

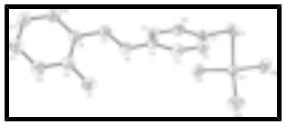

Fig. 1. The structure of (I) showing 30% probability displacement ellipsoids and the atom-numbering scheme. The H atoms are omitted for clarity.

2-{[4-(Trimethylstannylthio)phenylimino]methyl}phenol

Crystal data

$C_{16}H_{19}NOSSn$ F_{000} = 784

M_r = 392.07	D_x = 1.497 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2868 reflections
a = 11.1385 (16) Å	θ = 3.0–23.6°
b = 6.4148 (12) Å	μ = 1.58 mm^{-1}
c = 24.490 (2) Å	T = 298 (2) K
β = 96.254 (2)°	Block, yellow
V = 1739.5 (4) Å^3	0.15 × 0.12 × 0.10 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	3104 independent reflections
Radiation source: sealed tube	2284 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.051
T = 298(2) K	θ_{max} = 25.1°
φ and ω scans	θ_{min} = 1.7°
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→13
T_{min} = 0.797, T_{max} = 0.858	k = −7→7
8291 measured reflections	l = −22→29

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.054	H-atom parameters constrained
$wR(F^2)$ = 0.165	$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 2.8254P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.004
3104 reflections	$\Delta\rho_{max}$ = 0.38 e Å^{-3}
184 parameters	$\Delta\rho_{min}$ = −0.96 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 calculat-

ing *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	0.19708 (4)	0.26552 (7)	0.617154 (19)	0.0594 (2)
N1	0.1773 (4)	0.6301 (8)	0.3530 (2)	0.0482 (12)
O1	0.0779 (4)	0.9533 (7)	0.30112 (19)	0.0684 (14)
H1	0.1096	0.8859	0.3273	0.103*
S1	0.36707 (17)	0.2139 (3)	0.56463 (8)	0.0702 (6)
C1	0.3083 (5)	0.3377 (9)	0.5024 (2)	0.0501 (13)
C2	0.3372 (6)	0.5430 (10)	0.4916 (2)	0.0565 (14)
H2	0.3859	0.6194	0.5177	0.068*
C3	0.2936 (5)	0.6341 (11)	0.4421 (2)	0.0555 (14)
H3	0.3136	0.7717	0.4354	0.067*
C4	0.2206 (5)	0.5249 (9)	0.4022 (2)	0.0459 (12)
C5	0.1911 (6)	0.3221 (9)	0.4132 (2)	0.0518 (13)
H5	0.1416	0.2470	0.3872	0.062*
C6	0.2341 (6)	0.2275 (10)	0.4626 (2)	0.0561 (14)
H6	0.2134	0.0901	0.4693	0.067*
C7	0.1657 (5)	0.5321 (10)	0.3073 (2)	0.0479 (12)
H7	0.1893	0.3932	0.3066	0.057*
C8	0.1166 (5)	0.6320 (9)	0.2562 (2)	0.0476 (12)
C9	0.0727 (5)	0.8369 (10)	0.2554 (3)	0.0530 (13)
C10	0.0284 (6)	0.9290 (11)	0.2056 (2)	0.0595 (14)
H10	0.0018	1.0666	0.2049	0.071*
C11	0.0238 (6)	0.8166 (11)	0.1574 (3)	0.0631 (15)
H11	−0.0086	0.8776	0.1246	0.076*
C12	0.0668 (6)	0.6144 (10)	0.1571 (3)	0.0607 (14)
H12	0.0644	0.5403	0.1243	0.073*
C13	0.1135 (5)	0.5237 (11)	0.2063 (2)	0.0553 (14)
H13	0.1432	0.3883	0.2062	0.066*
C14	0.0469 (6)	0.1300 (14)	0.5697 (3)	0.0709 (19)
H14A	0.0054	0.0390	0.5924	0.085*
H14B	0.0743	0.0517	0.5400	0.085*
H14C	−0.0070	0.2380	0.5551	0.085*
C15	0.1731 (9)	0.5949 (15)	0.6232 (4)	0.109 (3)
H15A	0.1490	0.6512	0.5873	0.131*
H15B	0.2477	0.6580	0.6381	0.131*
H15C	0.1117	0.6236	0.6468	0.131*
C16	0.2493 (7)	0.1208 (15)	0.6947 (3)	0.077 (2)
H16A	0.1990	0.0016	0.6988	0.093*
H16B	0.2404	0.2184	0.7237	0.093*
H16C	0.3321	0.0772	0.6965	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0621 (3)	0.0607 (4)	0.0553 (3)	−0.0029 (2)	0.0070 (2)	−0.0069 (2)
N1	0.047 (3)	0.054 (3)	0.044 (3)	0.003 (2)	0.008 (2)	0.000 (3)
O1	0.087 (3)	0.061 (3)	0.057 (3)	0.020 (3)	0.005 (3)	−0.004 (2)
S1	0.0544 (10)	0.0942 (15)	0.0622 (11)	0.0173 (9)	0.0081 (8)	0.0232 (10)
C1	0.043 (3)	0.057 (3)	0.051 (3)	0.004 (2)	0.012 (2)	0.001 (3)
C2	0.058 (3)	0.062 (3)	0.048 (3)	−0.008 (3)	0.003 (3)	−0.004 (3)
C3	0.060 (3)	0.053 (3)	0.053 (3)	−0.005 (3)	0.007 (2)	0.001 (3)
C4	0.047 (2)	0.050 (3)	0.043 (3)	−0.001 (2)	0.013 (2)	−0.002 (2)
C5	0.056 (3)	0.056 (3)	0.046 (3)	−0.007 (2)	0.013 (2)	−0.007 (2)
C6	0.063 (3)	0.055 (3)	0.053 (3)	−0.002 (3)	0.015 (3)	0.000 (3)
C7	0.045 (2)	0.053 (3)	0.047 (3)	0.000 (2)	0.010 (2)	0.000 (2)
C8	0.038 (2)	0.058 (3)	0.048 (3)	−0.002 (2)	0.010 (2)	−0.001 (2)
C9	0.041 (3)	0.063 (3)	0.056 (3)	−0.006 (2)	0.009 (2)	−0.003 (3)
C10	0.053 (3)	0.065 (3)	0.060 (3)	0.000 (3)	0.006 (3)	0.010 (3)
C11	0.049 (3)	0.081 (4)	0.059 (3)	−0.007 (3)	0.005 (3)	0.010 (3)
C12	0.052 (3)	0.078 (3)	0.053 (3)	−0.009 (3)	0.008 (2)	−0.009 (3)
C13	0.052 (3)	0.063 (3)	0.052 (3)	−0.006 (3)	0.010 (2)	−0.003 (3)
C14	0.061 (4)	0.088 (5)	0.064 (4)	−0.009 (4)	0.010 (3)	−0.019 (4)
C15	0.114 (7)	0.071 (6)	0.141 (8)	0.011 (5)	0.005 (6)	−0.018 (6)
C16	0.085 (5)	0.093 (6)	0.055 (4)	−0.012 (4)	0.012 (4)	−0.001 (4)

Geometric parameters (Å, °)

Sn1—S1	2.425 (2)	C7—H7	0.9300
Sn1—C14	2.117 (7)	C8—C13	1.402 (7)
Sn1—C15	2.137 (9)	C8—C9	1.402 (7)
Sn1—C16	2.138 (7)	C9—C10	1.397 (7)
N1—C7	1.277 (8)	C10—C11	1.380 (7)
N1—C4	1.420 (7)	C10—H10	0.9300
O1—C9	1.342 (7)	C11—C12	1.382 (7)
O1—H1	0.8200	C11—H11	0.9300
S1—C1	1.779 (6)	C12—C13	1.388 (7)
C1—C2	1.388 (7)	C12—H12	0.9300
C1—C6	1.398 (7)	C13—H13	0.9300
C2—C3	1.385 (7)	C14—H14A	0.9600
C2—H2	0.9300	C14—H14B	0.9600
C3—C4	1.391 (6)	C14—H14C	0.9600
C3—H3	0.9300	C15—H15A	0.9600
C4—C5	1.376 (7)	C15—H15B	0.9600
C5—C6	1.392 (7)	C15—H15C	0.9600
C5—H5	0.9300	C16—H16A	0.9600
C6—H6	0.9300	C16—H16B	0.9600
C7—C8	1.459 (8)	C16—H16C	0.9600
S1—Sn1—C14	105.6 (2)	O1—C9—C10	118.2 (6)

S1—Sn1—C15	106.4 (3)	O1—C9—C8	121.8 (5)
S1—Sn1—C16	105.0 (2)	C10—C9—C8	119.9 (6)
C14—Sn1—C15	110.3 (3)	C11—C10—C9	120.2 (6)
C14—Sn1—C16	115.6 (3)	C11—C10—H10	119.9
C15—Sn1—C16	113.1 (4)	C9—C10—H10	119.9
C7—N1—C4	120.2 (5)	C10—C11—C12	121.0 (6)
C9—O1—H1	109.5	C10—C11—H11	119.5
Sn1—S1—C1	99.1 (2)	C12—C11—H11	119.5
C2—C1—C6	118.7 (6)	C11—C12—C13	119.1 (6)
C2—C1—S1	121.0 (5)	C11—C12—H12	120.5
C6—C1—S1	120.4 (5)	C13—C12—H12	120.5
C3—C2—C1	120.0 (6)	C12—C13—C8	121.4 (6)
C3—C2—H2	120.0	C12—C13—H13	119.3
C1—C2—H2	120.0	C8—C13—H13	119.3
C2—C3—C4	121.7 (6)	Sn1—C14—H14A	109.5
C2—C3—H3	119.1	Sn1—C14—H14B	109.5
C4—C3—H3	119.1	H14A—C14—H14B	109.5
C5—C4—C3	118.2 (6)	Sn1—C14—H14C	109.5
C5—C4—N1	123.3 (5)	H14A—C14—H14C	109.5
C3—C4—N1	118.5 (5)	H14B—C14—H14C	109.5
C4—C5—C6	121.0 (6)	Sn1—C15—H15A	109.5
C4—C5—H5	119.5	Sn1—C15—H15B	109.5
C6—C5—H5	119.5	H15A—C15—H15B	109.5
C5—C6—C1	120.4 (6)	Sn1—C15—H15C	109.5
C5—C6—H6	119.8	H15A—C15—H15C	109.5
C1—C6—H6	119.8	H15B—C15—H15C	109.5
N1—C7—C8	121.9 (6)	Sn1—C16—H16A	109.5
N1—C7—H7	119.1	Sn1—C16—H16B	109.5
C8—C7—H7	119.1	H16A—C16—H16B	109.5
C13—C8—C9	118.5 (6)	Sn1—C16—H16C	109.5
C13—C8—C7	120.1 (5)	H16A—C16—H16C	109.5
C9—C8—C7	121.4 (5)	H16B—C16—H16C	109.5

Fig. 1