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Dimethyl[2-oxido-1-benzaldehyde (2-thienylcarbonyl)hydrazonato]tin(IV)

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Key indicators

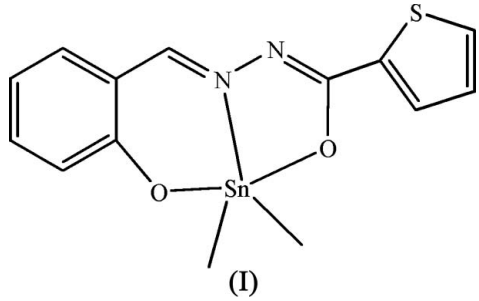
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.029
wR factor = 0.083
Data-to-parameter ratio = 14.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title complex, $[Sn(CH_3)_2(C_{12}H_8N_2O_2S)]$, the Sn atom is in a distorted trigonal–bipyramidal configuration, with Sn—O distances in the range 2.087 (3)–2.177 (3) Å. The Schiff base molecule is coordinated to the Sn atom in a tridentate fashion *via* the azomethine N atom, the hydroxy O atom and the carbonyl O atom.

Comment

The structure of the title molecule, (I), in Fig. 1 shows that the complex is a monomer in which the Schiff base is coordinated to the Sn atom as a tridentate ligand *via* the azomethine N atom, the hydroxy O atom and the carbonyl O atom. The angles at Sn1 confirm that the complex has a distorted trigonal–bipyramidal configuration (Table 1). The distortion around the Sn atom is a result of the constraints imposed by the Sn1/N1/N2/C1/O1 and Sn1/N1/C6/C7/C8/O2 rings. The Sn1—N1 distance is 2.175 (3) Å, close to the sum of the covalent radii (2.15 Å; Sanderson, 1967), indicating a strong Sn—N interaction. The O atoms coordinate to the Sn atom with one shorter and one longer Sn—O bonds. The C—N—N—C chain shows conjugation, as evidenced by the intermediate values for the bond lengths (Table 1). The dihedral angle between the benzene and thiophene rings is 9.3 (3)°. A view of the crystal packing is shown in Fig. 2.



(I)

Experimental

The synthesis of (I) was carried out under a nitrogen atmosphere using standard Schlenk techniques. The Schiff base (0.2216 g, 1.0 mmol) was added to a mixture of ethanol and benzene (1:3 *v*/*v*, 30 ml) with sodium ethoxide (0.068 g, 1.0 mmol). The mixture was stirred for 0.5 h then $(CH_3)_2SnCl_2$ (0.2197 g, 1.0 mmol) was added and the mixture stirred for 10 h under reflux. After cooling to room temperature, the mixture was filtered and evaporated to dryness. The resulting solid, (I), was then recrystallized from dichloromethane–hexane (3:1 *v*/*v*) (m.p. 509–510 K). Analysis calculated for

$C_{14}H_{14}N_2O_2SSn$: C 42.78, H 3.59, N 7.13%; found: C 42.67, N 3.50, N 7.04%.

Crystal data

$[Sn(CH_3)_2(C_{12}H_8N_2O_2S)]$	D_x = 1.735 Mg m^{-3}
M_r = 393.02	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4148 reflections
a = 25.644 (5) Å	θ = 2.3–28.1°
b = 9.701 (2) Å	μ = 1.84 mm^{-1}
c = 14.051 (3) Å	T = 298 (2) K
β = 120.594 (2)°	Block, colourless
V = 3009.1 (11) Å^3	0.28 × 0.26 × 0.25 mm
Z = 8	

Data collection

Siemens SMART CCD area-detector diffractometer	2656 independent reflections
	2151 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.046
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -30 \rightarrow 27$
T_{min} = 0.627, T_{max} = 0.656	$k = -11 \rightarrow 7$
7625 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.7212P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.029	
$wR(F^2)$ = 0.083	
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.002
2656 reflections	$\Delta\rho_{max}$ = 0.59 e Å^{-3}
182 parameters	$\Delta\rho_{min}$ = −0.68 e Å^{-3}
H-atom parameters constrained	Extinction correction: *SHELXL97*
	Extinction coefficient: 0.0043 (2)

Table 1
Selected geometric parameters (Å, °).

Sn1—O2	2.087 (3)	Sn1—O1	2.177 (3)
Sn1—C14	2.102 (4)	N1—C6	1.293 (4)
Sn1—C13	2.105 (4)	N1—N2	1.386 (4)
Sn1—N1	2.175 (3)	N2—C1	1.309 (4)
O2—Sn1—C14	97.69 (16)	C13—Sn1—N1	123.08 (14)
O2—Sn1—C13	94.77 (15)	O2—Sn1—O1	155.62 (10)
C14—Sn1—C13	127.60 (18)	C14—Sn1—O1	94.76 (16)
O2—Sn1—N1	83.86 (10)	C13—Sn1—O1	94.09 (14)
C14—Sn1—N1	108.79 (15)	N1—Sn1—O1	72.29 (10)

All H atoms were positioned geometrically and treated as riding on their parent atoms, with aromatic C—H distances of 0.93 Å and methyl C—H distances of 0.96 Å. The U_{iso}(H) values were set at 1.5U_{eq}(C) for the methyl H atoms and at 1.2U_{eq}(C) for the other H atoms.

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*.

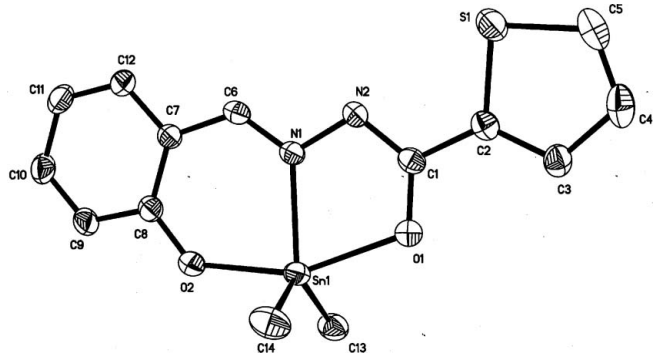


Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

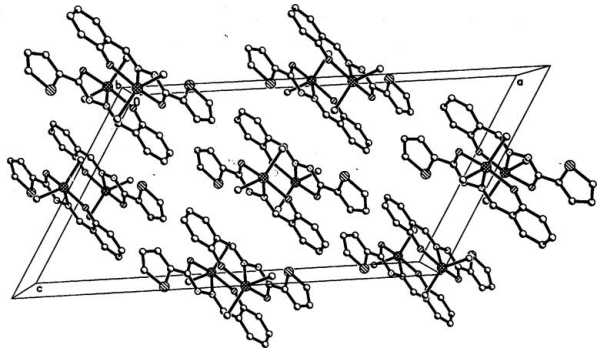


Figure 2
The crystal packing of the title complex. H atoms have been omitted.

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References

Sanderson, R. T. (1967). *Inorganic Chemistry*, p. 74. New York: Reinhold.
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.