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(3-Methoxy-2-oxidobenzaldehyde benzoylhydrazonato)dimethyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.031
wR factor = 0.083
Data-to-parameter ratio = 14.1

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

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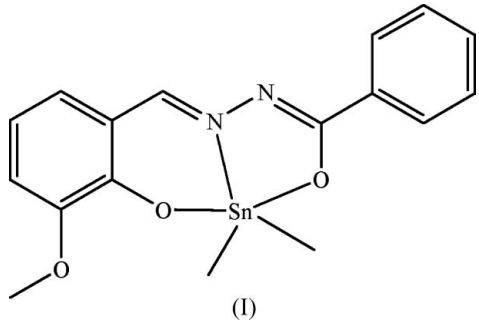
In the title complex, $[Sn(CH_3)_2(C_{15}H_{12}N_2O_3)]$, the Sn atom is found in a distorted trigonal–bipyramidal geometry with Sn—O distances of 2.131 (3) and 2.178 (3) Å. Intermolecular Sn···O contacts stabilize the crystal packing.

Comment

The title molecule, (I) (Fig. 1), is a monomer in which the Sn atom is five-coordinated by two O atoms, two C atoms and one N atom (Table 1). The Schiff base is coordinated to the Sn atom and the two deprotonated O atoms. The Sn1—N2 distance is 2.188 (3) Å, which is close to the sum of the non-polar covalent radii (2.15 Å; Sanderson, 1967), indicating a strong tin–nitrogen interaction. The distorted trigonal–bipyramidal geometry around the Sn atom is the result of the strain imposed by the tridentate Schiff base ligand, and from the constraints imposed by the five- and six-membered rings Sn—N—N—C—O and Sn—N—C—C—C—O. The dihedral angle between these two rings is 0.7 (2)°, indicating their coplanarity. The distorted geometry can be seen from departures of bonding angles from the values characteristic for trigonal–bipyramidal coordination (Table 1); the C16—Sn1—C17 angle should be 180°, but its value is 140.97 (16)°. The structure of the title compound is very similar to that of a compound already reported (Camacho-Camacho *et al.*, 1998).



(I)

The crystal packing of the title complex displays a weak Sn···O(1 − *x*, 2 − *y*, 1 − *z*) interaction [3.095 (2) Å] which stabilizes the crystal structure.

Experimental

The reaction was carried out under a nitrogen atmosphere with use of the standed Schlenk technique. The Schiff base (0.2692 g, 1.0 mmol) was added to a mixture of ethanol and benzene (1:3, 30 ml) with sodium ethoxide (0.068 g, 1.0 mmol); the mixture was stirred for 0.5 h and $(CH_3)_2SnCl_2$ (0.2196 g, 1.0 mmol) was added; the mixture was stirred for 7 h under reflux. After cooling to room temperature, the

solution was filtered and evaporated to dryness. The title solid was recrystallized from dichloromethane–hexane (1:1 *v*/*v*; m. p. 486–487 K). Analysis $C_{17}H_{18}N_2O_3Sn$: C 48.95, H 4.35, N 6.71%; found: C 48.65, N 4.12, N 6.54%.

Crystal data

$[Sn(CH_3)_2(C_{15}H_{12}N_2O_3)]$	$Z = 8$
$M_r = 417.02$	$D_x = 1.658$ Mg m^{-3}
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 26.477$ (4) Å	$\mu = 1.55$ mm^{-1}
$b = 9.5444$ (16) Å	$T = 298$ (2) K
$c = 13.594$ (2) Å	Block, orange
$\beta = 103.475$ (2)°	0.49 × 0.43 × 0.30 mm
$V = 3340.8$ (9) Å^3	

Data collection

Siemens SMART CCD area-detector diffractometer	8516 measured reflections
	2947 independent reflections
φ and ω scans	2381 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.040$
	$\theta_{max} = 25.0°$
$T_{min} = 0.518$, $T_{max} = 0.654$	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.042P)^2 + 2.9384P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.031$	
$wR(F^2) = 0.083$	
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.002$
2947 reflections	$\Delta\rho_{max} = 0.48$ e Å^{-3}
209 parameters	$\Delta\rho_{min} = -0.50$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—C16	2.099 (4)	Sn1—N2	2.188 (3)
Sn1—C17	2.102 (4)	N1—C7	1.306 (5)
Sn1—O2	2.131 (3)	N1—N2	1.405 (4)
Sn1—O1	2.178 (3)	N2—C8	1.285 (5)
C16—Sn1—C17	140.97 (16)	O2—Sn1—N2	83.39 (11)
C17—Sn1—O2	97.46 (14)	O1—Sn1—N2	72.01 (11)
O2—Sn1—O1	154.34 (11)		

All H atoms were placed 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*.

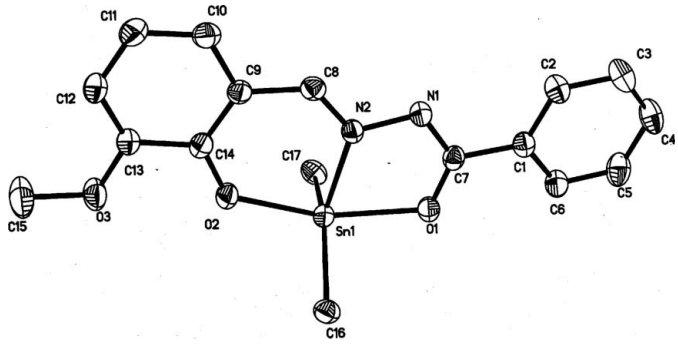


Figure 1
The structure of the title complex and the atom-numbering, with displacement ellipsoids shown at the 30% probability level. H atoms have been omitted.

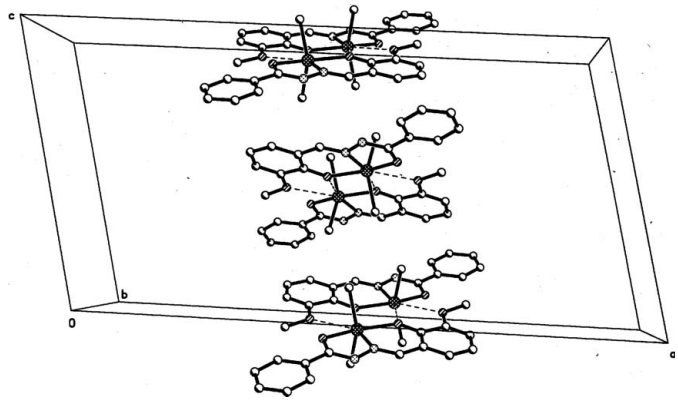


Figure 2
Partial crystal packing of the title complex, with the intermolecular Sn···O interactions (dashed lines). H atoms have been omitted.

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