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Dimethyl(2-oxido-1-naphthaldehyde isonicotinoylhydrazonato)tin(IV) methanol solvate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.059
wR factor = 0.163
Data-to-parameter ratio = 14.3

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

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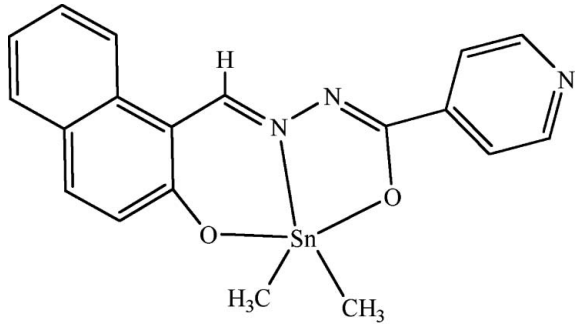
In the molecular structure of the title complex, $[Sn(CH_3)_2(C_{17}H_{11}N_3O_2)]\cdot CH_3OH$, the Sn atom is in a distorted trigonal–bipyramidal coodination, with Sn—O distances of 2.099 (6) and 2.128 (6) Å. A methanol solvent molecule is O—H···N hydrogen bonded to the complex molecule.

Comment

The molecular structure of the title mononuclear complex, (I), is shown in Fig. 1. The Sn atom is five-coordinated by two O atoms, two C atoms and one N atom in a disorted trigonal–bipyramidal coodination. The Schiff base ligand acts as a tridentate ligand *via* the azomethine N atom and two O atoms. The C11—N1—N2—C12 sequence of atoms shows π-electron delocalization, as evidenced by the values for the bond lengths (Table 1). The Sn—O and Sn—C bond lengths are all equivalent within experimental error. The methanol solvent molecule is O—H···N hydrogen bonded to the complex molecule through the pyridyl N atom (Table 2 and Fig. 2).



(I)

Experimental

The reaction was carried out under a nitrogen atmosphere using standard Schlenk techniques. The Schiff base ligand 2-hydroxy-1-naphthaldehyde isonicotinylhydrazone (0.1165 g, 0.4 mmol) was added to a mixture of methanol and benzene (1:3 *v*/*v*, 30 ml) with sodium ethoxide (0.272 g, 0.4 mmol). The mixture was stirred for 30 min, $(CH_3)_2SnCl_2$ (0.088 g, 0.4 mmol) was added, and stirring continued for 10 h under reflux. After cooling to room temperature, filtration and evaporation to dryness, the solid was then recrystallized from dichloromethane–methanol (3:1 *v*/*v*; m.p. 498–499 K). Analysis calculated for $C_{20}H_{21}N_3O_3Sn$: C 51.09, H 4.50, N 8.94%; found: C 50.91, N 4.43, N 8.81%.

Crystal data

$[Sn(CH_3)_2(C_{17}H_{11}N_3O_2)]\cdot CH_4O$	D_x = 1.576 Mg m^{-3}
M_r = 470.09	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 3830 reflections
a = 10.969 (2) Å	θ = 4.4–25.7°
b = 7.208 (2) Å	μ = 1.32 mm^{-1}
c = 25.269 (3) Å	T = 298 (2) K
β = 97.557 (3)°	Block, orange
V = 1980.7 (7) Å^3	0.35 × 0.22 × 0.19 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3481 independent reflections
	2647 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.076
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -13 \rightarrow 13$
T_{min} = 0.656, T_{max} = 0.788	$k = -8 \rightarrow 7$
7804 measured reflections	$l = -30 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.059	$w = 1/[\sigma^2(F_o^2) + (0.102P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.163	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.00	$\Delta\rho_{max}$ = 1.73 e Å^{-3}
3481 reflections	$\Delta\rho_{min}$ = −1.35 e Å^{-3}
244 parameters	

Table 1
Selected geometric parameters (Å, °).

Sn1—C18	2.083 (8)	Sn1—N1	2.202 (6)
Sn1—O1	2.099 (6)	N1—C11	1.294 (8)
Sn1—C19	2.123 (8)	N2—C12	1.305 (9)
Sn1—O2	2.128 (6)		
C18—Sn1—O1	96.8 (3)	C19—Sn1—O2	94.5 (3)
C18—Sn1—C19	134.9 (3)	C18—Sn1—N1	108.9 (3)
O1—Sn1—C19	93.0 (3)	O1—Sn1—N1	80.8 (2)
C18—Sn1—O2	95.7 (3)	C19—Sn1—N1	116.1 (3)
O1—Sn1—O2	153.54 (19)	O2—Sn1—N1	73.1 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···N3^{i}	0.82	2.33	2.787 (10)	116

Symmetry code: (i) $x+1, y, z$.

All H atoms were positioned geometrically and refined 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 C-bound H atoms. The largest peak in the final difference map is located 0.97 Å from atom Sn1 and the deepest hole 0.91 Å from atom Sn1.

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*.

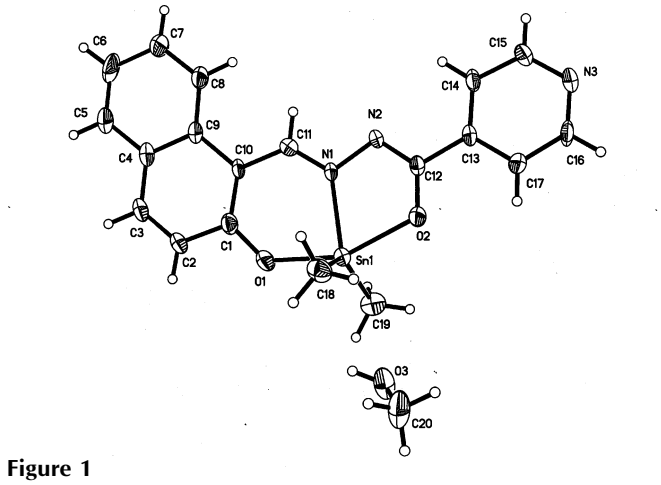


Figure 1
The molecular structure (I), showing 30% probability displacement ellipsoids.

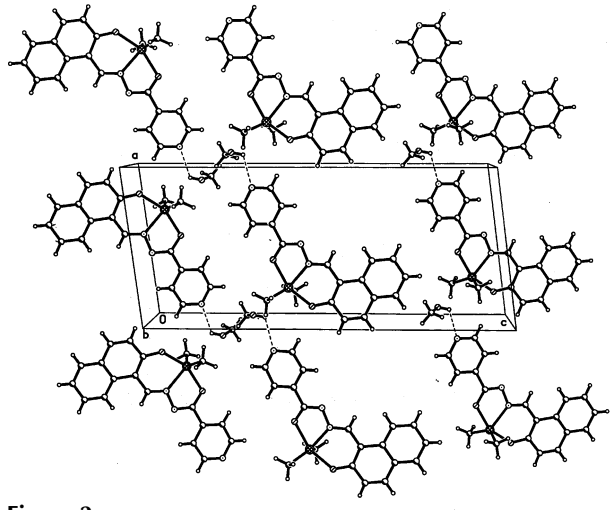


Figure 2
The packing of the title complex, showing hydrogen bonds as dashed lines.

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