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[2-Oxido-1-naphthaldehyde oxido(4-pyridyl)methylhydrazone]diphenyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.033
wR factor = 0.083
Data-to-parameter ratio = 13.3

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

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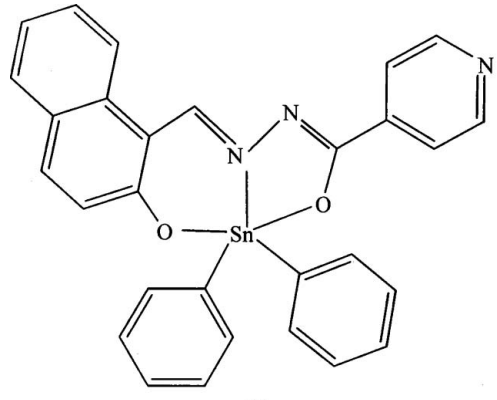
In the title complex, $[Sn(C_6H_5)_2(C_{17}H_{11}N_3O_2)]$, the Sn atom is in a distorted trigonal–bipyramidal geometry, with Sn—O distances in the range 2.074 (3)–2.141 (3) Å. The dihedral angles between the two chelated benzene rings and the O(naphthyl oxide)—Sn—N group are 75.8 (1) and 50.6 (3)°.

Comment

The structure of the title molecule, (I), in Fig. 1 shows that the complex is a monomer in which the Sn atom adopts a five-coordinate geometry, being coordinated by two O atoms, two C atoms and one N atom. The Schiff base is coordinated to the Sn atom as a tridentate ligand *via* the azomethine N atom, the hydroxyl O atom and the carbonyl O atom. The dihedral angles between the two chelated benzene rings and the O(naphthyl oxide)—Sn—N group are 75.8 (1) and 50.6 (3)°. The C—N—N—C chain shows conjugation, as evidenced by the intermediate values for the bond lengths (Table 1). The Sn1—N3 distance is 2.141 (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 bond. These lengths are similar to those of the Sn—C bonds. Very similar structural parameters were observed in the compound studied by Yearwood *et al.* (2002). The angles at Sn1 confirm that the complex has a distorted trigonal–bipyramidal configuration.



(I)

Experimental

The synthesis of (I) was carried out under a nitrogen atmosphere using standard Schlenk techniques. The Schiff base (0.1165 g, 4 mmol) was added to a mixture of ethanol and benzene (1:3 *v*/*v*, 30 ml) with sodium ethoxide (0.272 g, 4 mmol). The mixture was stirred for 0.5 h and then Ph_2SnCl_2 (0.1376 g, 4 mmol) was added and

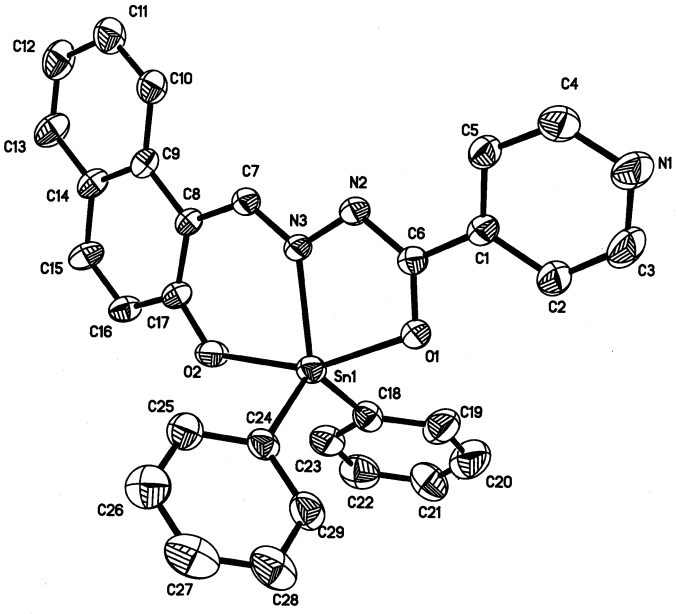


Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

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. 515–516 K). Analysis, calculated for $C_{29}H_{21}N_3O_2Sn$: C 61.95, H 3.76, N 7.47%; found: C 61.73, N 3.65, N 7.58%.

Crystal data

$[Sn(C_6H_5)_2(C_{17}H_{11}N_3O_2)]$	D_x = 1.556 Mg m^{-3}
M_r = 562.18	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4361 reflections
a = 10.283 (4) Å	θ = 2.4–24.7°
b = 21.060 (8) Å	μ = 1.10 mm^{-1}
c = 11.984 (5) Å	T = 298 (2) K
β = 112.380 (5)°	Block, orange
V = 2399.9 (15) Å^3	0.49 × 0.47 × 0.43 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	4205 independent reflections
φ and ω scans	3087 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.042
T_{min} = 0.616, T_{max} = 0.650	θ_{max} = 25.0°
12415 measured reflections	$h = -12 \rightarrow 12$
	$k = -25 \rightarrow 23$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 1.5741P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.033	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.083	$\Delta\rho_{max}$ = 0.63 e Å^{-3}
S = 1.03	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
4205 reflections	
316 parameters	
H-atom parameters constrained	

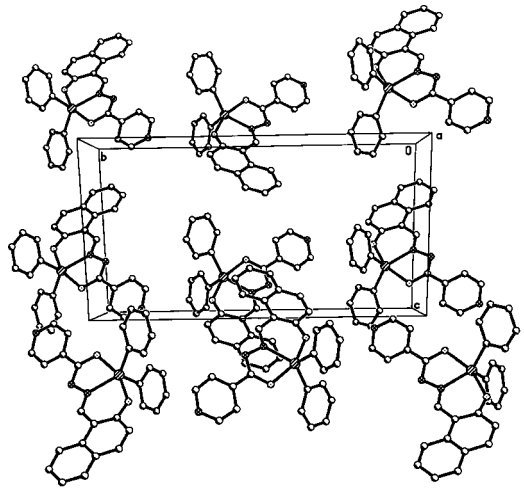


Figure 2
The crystal packing of the title complex. H atoms have been omitted.

Table 1
Selected geometric parameters (Å, °).

Sn1—O2	2.074 (3)	Sn1—N3	2.141 (3)
Sn1—C24	2.109 (4)	N2—C6	1.297 (4)
Sn1—C18	2.112 (4)	N2—N3	1.403 (4)
Sn1—O1	2.117 (2)	N3—C7	1.308 (4)
O2—Sn1—C24	96.74 (14)	C18—Sn1—O1	95.33 (14)
O2—Sn1—C18	95.03 (14)	O2 —Sn1—N3	82.36 (10)
C24—Sn1—C18	120.33 (15)	C24—Sn1—N3	112.95 (13)
O2—Sn1—O1	155.90 (10)	C18—Sn1—N3	126.55 (13)
C24—Sn1—O1	96.68 (13)	O1—Sn1—N3	74.00 (10)

All H atoms were positioned geometrically and treated as riding on their parent atoms, with C—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

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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