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The one-dimensional chain compound *n*-butyldichloro[2-oxido-1-naphthaldehyde (4-pyridylcarbonyl)hydrazonato]tin(IV) methanol disolvate

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.037
wR factor = 0.120
Data-to-parameter ratio = 15.2

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

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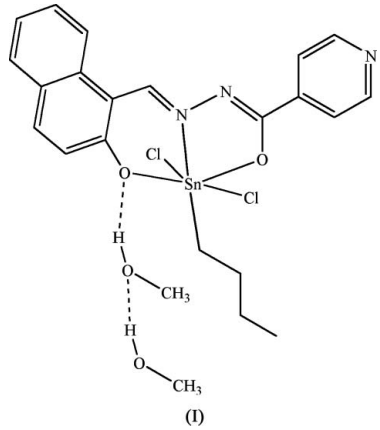
In the title complex, $[Sn(C_4H_9)(C_{17}H_{11}N_3O_2)Cl_2]\cdot 2CH_4O$, the Sn atom is in a distorted octahedral geometry, with Sn—O distances of 2.093 (3) and 2.125 (3) Å. The tridentate Schiff base coordinates to the Sn *via* the azomethine N atom, the hydroxyl O atom and the carbonyl O atom. The complex is stabilized by intramolecular O—H···O hydrogen bonds, forming a one-dimensional chain.

Comment

The structure of the title compound, (I) (Fig. 1), shows that the complex is a monomer in which the Sn atom adopts a distorted octahedral geometry, being coordinated by two O atoms, one C atom, two Cl atoms and one N atom. The tridentate Schiff base coordinates to the Sn atom *via* the azomethine N atom, the hydroxyl O atom and the carbonyl O atom. The distorted octahedral geometry around the Sn atom (Table 1) is the result of the strain imposed by the tridentate Schiff base ligand and of the constraints imposed by the five- and six-membered chelate rings. The dihedral angle between the two rings is 0.1 (2)°, indicating that they are coplanar. In the title molecule, the Sn1—N1 distance is 2.153 (4) Å, which is close to the sum of the non-polar covalent radii (2.15 Å; Sanderson, 1967), indicating a strong Sn—N interaction. The O atoms coordinate to the Sn atom with two shorter and one longer Sn—O bond (Table 1). A search of the Cambridge Structural Database (Version 5.27; Allen, 2002) showed only four previous structures containing an SnO_2Cl_2NC chromophore (Camacho-Camacho *et al.*, 1998; Jímenez-Pérez *et al.*, 2000; Vicente *et al.*, 1992).



(I)

The packing of the unit cell (Fig. 2) shows that the molecules form a one-dimensional chain connected by intermolecular O—H···O hydrogen bonds (Table 2).

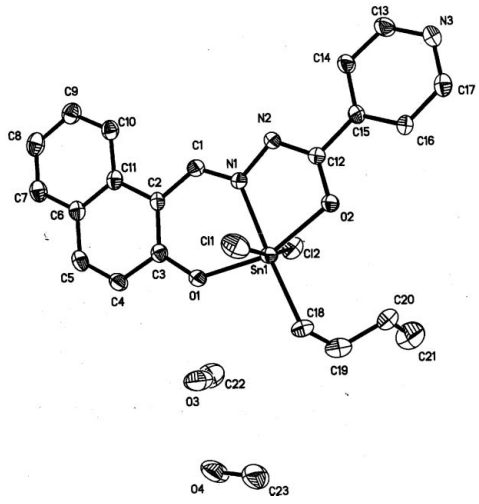


Figure 1
The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

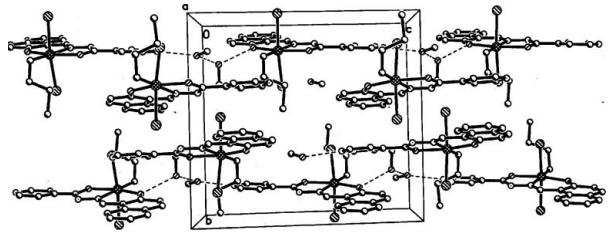


Figure 2
The crystal packing of the title complex. Dashed lines indicate hydrogen bonds. H atoms have been omitted.

Experimental

The reaction was carried out under a nitrogen atmosphere with the use of standard Schlenk techniques. The Schiff base (0.2913 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, $C_4H_9SnCl_3$ (0.2822 g, 1.0 mmol) was added, and the mixture was further stirred and refluxed for 10 h. After cooling to room temperature, the solution was filtered and evaporated to dryness. The resulting solid was then recrystallized from dichloromethane–hexane (3:1 *v*/*v*) (m.p. 523–524 K). Analysis calculated for $C_{23}H_{28}Cl_2N_3O_4Sn$: C 46.03, H 4.70, N 7.00%; found: C 45.95, H 4.52, N 6.91%.

Crystal data

$[Sn(C_4H_9)(C_{17}H_{11}N_3O_2)]\cdot Cl_2\cdot 2CH_4O$	V = 2588.7 (11) Å^3
M_r = 600.07	Z = 4
Monoclinic, $P2_1/n$	D_x = 1.540 Mg m^{-3}
a = 12.896 (3) Å	Mo $K\alpha$ radiation
b = 13.523 (3) Å	μ = 1.23 mm^{-1}
c = 15.000 (4) Å	T = 298 (2) K
β = 98.259 (3)°	Block, colourless
	0.43 × 0.42 × 0.37 mm

Data collection

Bruker SMART CCD area-detector diffractometer	13281 measured reflections
	4552 independent reflections
φ and ω scans	3298 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	R_{int} = 0.031
	θ_{max} = 25.0°
T_{min} = 0.621, T_{max} = 0.660	

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 3.6848P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.037	
$wR(F^2)$ = 0.120	
S = 1.01	$(\Delta/\sigma)_{max}$ = 0.001
4552 reflections	$\Delta\rho_{max}$ = 1.06 e Å^{-3}
300 parameters	$\Delta\rho_{min}$ = −0.48 e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.093 (3)	Sn1—N1	2.153 (4)
Sn1—C18	2.123 (5)	Sn1—Cl1	2.4810 (17)
Sn1—O2	2.125 (3)	Sn1—Cl2	2.5172 (15)
O1—Sn1—C18	100.3 (2)	O2—Sn1—Cl1	88.82 (10)
O1—Sn1—O2	157.85 (12)	N1—Sn1—Cl1	86.46 (11)
C18—Sn1—O2	101.8 (2)	O1—Sn1—Cl2	89.57 (11)
O1—Sn1—N1	83.08 (13)	C18—Sn1—Cl2	98.9 (2)
C18—Sn1—N1	176.1 (2)	O2—Sn1—Cl2	88.37 (10)
O2—Sn1—N1	74.78 (13)	N1—Sn1—Cl2	82.99 (11)
O1—Sn1—Cl1	89.20 (11)	Cl1—Sn1—Cl2	169.45 (5)
C18—Sn1—Cl1	91.6 (2)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O1	0.82	2.05	2.858 (1)	170
O4—H4···O3	0.82	1.88	2.686 (1)	166

All H atoms were placed geometrically and treated as riding on their parent atoms, with C—H distances of 0.93 Å (aromatic), 0.97 Å (CH_2) and 0.96 Å (methyl), and O—H distances of 0.82 Å. The U_{iso}(H) values were set at 1.5U_{eq}(C,O) for the methyl and hydroxy H atoms and at 1.2U_{eq}(C) for the other H atoms. The highest density peak is located 1.18 Å from atom C19.

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 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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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bruker (1996). *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.

Camacho-Camacho, C., Tlahuext, H., Nöth, H. & Contreras, R. (1998). *Heteroatom Chem*, **9**, 321–326.
Jímenez-Pérez, V. M., Camacho-Camacho, C., Güizado-Rodríguez, M., Nöth, H. & Contreras, R. (2000). *J. Organomet. Chem.* **614–615**, 283–293.
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*). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.10. Bruker AXS Inc., Madison, Wisconsin, USA.
Vicente, J., Chicote, M.-T., Ramírez-de-Arellano, M. C. & Jones, P. G. (1992). *J. Chem. Soc. Dalton Trans.* pp. 1839–1845.