

## *n*-Butyldichlorido(2-[(1*E*)-1-[2-(pyridin-2-yl)hydrazin-1-ylidene]ethyl]-phenolato)tin(IV)

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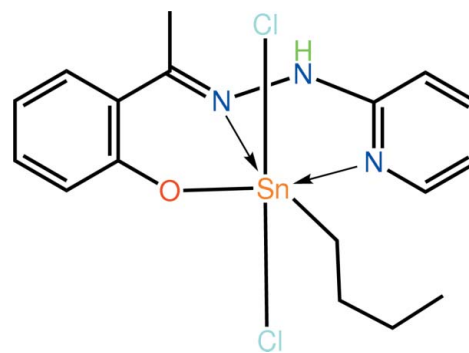
Received 9 October 2010; accepted 10 October 2010

Key indicators: single-crystal X-ray study;  $T = 100$  K; mean  $\sigma(\text{C}-\text{C}) = 0.012$  Å;  $R$  factor = 0.042;  $wR$  factor = 0.108; data-to-parameter ratio = 18.6.

Two independent molecules comprise the asymmetric unit of the title compound,  $[\text{Sn}(\text{C}_4\text{H}_9)(\text{C}_{13}\text{H}_{12}\text{N}_3\text{O})\text{Cl}_2]$ . The Sn atom in each is coordinated by the tridentate ligand *via* the phenoxide O, hydrazine N and pyridyl N atoms, forming five- and six-membered chelate rings. The approximately octahedral coordination geometry is completed by the  $\alpha$ -C atom of the *n*-butyl group (which is *trans* to the hydrazine N atom) and two mutually *trans* Cl atoms. Differences between the molecules are evident in the relative planarity of the chelate rings and in the conformations of the *n*-butyl groups [ $\text{C}-\text{C}-\text{C} = 177.2$  (5) and  $-64.4$  (11)°]. Significant differences in the Sn—Cl bond lengths are related to the formation of N—H...Cl hydrogen bonds, which link the molecules comprising the asymmetric unit into dimeric aggregates. These are consolidated in the crystal packing by C—H...Cl contacts. The structure was refined as an inversion twin; the minor twin component is 37 (3)%.

### Related literature

For background to related organotin compounds, see: Affan *et al.* (2009). For background to the varied biological activities of organotin compounds, see: Gielen & Tiekink (2005). For additional structure analysis, see: Spek (2009).



### Experimental

#### Crystal data

$[\text{Sn}(\text{C}_4\text{H}_9)(\text{C}_{13}\text{H}_{12}\text{N}_3\text{O})\text{Cl}_2]$

$M_r = 472.96$

Monoclinic,  $Pc$

$a = 8.9566$  (6) Å

$b = 21.0210$  (13) Å

$c = 10.3974$  (7) Å

$\beta = 110.567$  (1)°

$V = 1832.8$  (2) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 1.70$  mm<sup>-1</sup>

$T = 100$  K

$0.25 \times 0.15 \times 0.05$  mm

#### Data collection

Bruker SMART APEX CCD

diffractometer

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\text{min}} = 0.677$ ,  $T_{\text{max}} = 0.920$

17203 measured reflections

8239 independent reflections

7357 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.032$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.108$

$S = 1.02$

8239 reflections

442 parameters

4 restraints

H atoms treated by a mixture of independent and constrained refinement

$\Delta\rho_{\text{max}} = 2.28$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -1.21$  e Å<sup>-3</sup>

Absolute structure: Flack (1983),

4006 Friedel pairs

Flack parameter: 0.37 (3)

**Table 1**

Selected bond lengths (Å).

Sn1—Cl1	2.4504 (17)	Sn2—Cl3	2.456 (2)
Sn1—Cl2	2.5225 (16)	Sn2—Cl4	2.5116 (18)
Sn1—O1	2.004 (5)	Sn2—O2	2.017 (5)
Sn1—N1	2.266 (6)	Sn2—N4	2.248 (6)
Sn1—N3	2.198 (6)	Sn2—N6	2.212 (7)
Sn1—C4	2.169 (7)	Sn2—C21	2.142 (7)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2n...Cl4	0.86 (3)	2.47 (4)	3.283 (7)	159 (7)
N5—H5n...Cl2	0.86 (3)	2.48 (5)	3.235 (7)	147 (7)
C15—H15...Cl2 <sup>i</sup>	0.95	2.79	3.538 (9)	137
C17—H17...Cl1 <sup>ii</sup>	0.95	2.80	3.540 (9)	135
C34—H34...Cl3 <sup>iii</sup>	0.95	2.75	3.534 (9)	141

Symmetry codes: (i)  $x - 1, y, z$ ; (ii)  $x, -y + 2, z + \frac{1}{2}$ ; (iii)  $x, -y + 1, z - \frac{1}{2}$ .

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