Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

n-Butyldichlorido{4-cyclohexyl-1-[1-(pyridin-2-yl-κN)ethylidene]thiosemicarbazidato-$\kappa^2 N^1,S$}tin(IV)

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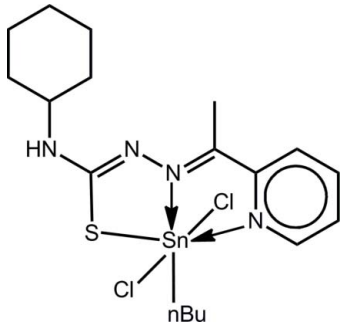
Received 5 June 2012; accepted 7 June 2012

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.035; wR factor = 0.085; data-to-parameter ratio = 20.9.

Two independent molecules comprise the asymmetric unit in the title compound, $[Sn(C_4H_9)(C_{14}H_{19}N_4S)Cl_2]$. In each molecule, the Sn^{IV} atom exists within a distorted octahedral geometry defined by the *N*,*N*′,*S*-tridentate mono-deprotonated Schiff base ligand, two mutually *trans* Cl atoms, and the α-C atom of the *n*-butyl group; the latter is *trans* to the azo-N atom. The greatest distortion from the ideal geometry is found in the nominally *trans* angle formed by the S and pyridyl-N atoms at Sn [151.72 (7) and 152.04 (7)°, respectively]. In the crystal, molecules are consolidated into a three-dimensional architecture by a combination of N—H···Cl, C—H···π and π–π interactions [inter-centroid distances = 3.6718 (19) and 3.675 (2) Å].

Related literature

For the structures of the methyltin and phenyltin derivatives, see: Salam *et al.* (2010*a*,*b*).



Experimental

Crystal data

$[Sn(C_4H_9)(C_{14}H_{19}N_4S)Cl_2]$
M_r = 522.09
Monoclinic, $P2_1/n$
a = 12.1229 (3) Å
b = 15.4518 (4) Å
c = 23.6868 (6) Å
β = 103.894 (3)°
V = 4307.21 (19) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.54 mm^{-1}
T = 100 K
0.25 × 0.25 × 0.25 mm

Data collection

Agilent SuperNova Dual diffractometer with Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
T_{min} = 0.794, T_{max} = 1.000
18205 measured reflections
9861 independent reflections
8503 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.085
S = 1.04
9860 reflections
471 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.64 e Å^{-3}
$\Delta\rho_{min}$ = −1.11 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C1	2.187 (3)	Sn2—C19	2.182 (3)
Sn1—N1	2.269 (2)	Sn2—N5	2.255 (3)
Sn1—N2	2.209 (2)	Sn2—N6	2.215 (3)
Sn1—S1	2.4785 (8)	Sn2—S2	2.4806 (8)
Sn1—Cl1	2.5123 (8)	Sn2—Cl3	2.4959 (8)
Sn1—Cl2	2.4959 (8)	Sn2—Cl4	2.5124 (8)

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

*Cg*1 is the centroid of the N1,C5–C9 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···Cl3	0.88	2.65	3.516 (3)	167
C15—H15A···$Cg1^{i}$	0.99	2.85	3.692 (4)	143

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997), *QMol* (Gans & Shalloway, 2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

This work was supported financially by the Ministry of Science Technology and Innovation (MOSTI) under research grant No. 06–01-09-SF0046. The authors would like to thank Universiti Malaysia Sarawak (UNIMAS) for the facilities to carry out the research work. They also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12).