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Dichlorodiphenylbis(pyridine-κN)tin(IV)

Handong Yin,* Shaowen Chen and Daqi Wang

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China

Correspondence e-mail: handongyin@lctu.edu.cn

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Key indicators

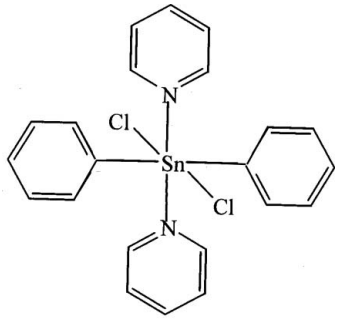
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.008 Å
R factor = 0.038
wR factor = 0.101
Data-to-parameter ratio = 21.1

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

In the mononuclear title complex, $[Sn(C_6H_5)_2Cl_2(C_5H_5N)_2]$, the central Sn^{IV} atom is octahedrally coordinated by two Cl atoms, two pyridine N atoms, and two benzene C atoms. The dihedral angle between the pyridine ring and the SnN_2Cl_2 plane is 19.2 (9)°.

Comment

The molecular structure of the title compound, (I), is shown in Fig. 1. The Sn atom is octahedrally coordinated (Table 1) by two pyridine (py) N atoms, two benzene C atoms and two chloride ions in an all-*trans* configuration.



(I)

The $SnC_2N_2Cl_2$ octahedron is relatively undistorted. The Sn—C, Sn—Cl and Sn—N bond lengths in (I) are in good agreement with those in $py_2Et_2SnCl_2$ (Casas *et al.*, 2000) and $py_2Me_2SnCl_2$ (Aslanov *et al.*, 1978). The bond angles around Sn in (I) are all very close to 90° [range = 88.37 (14)–91.84 (14)°].

Experimental

To a benzene suspension of $(C_6H_5)_2SnCl_2$ (5 mmol) was added a benzene (30 ml) solution of pyridine (10 mmol). The mixture was heated under reflux with stirring for 7 h, and the resulting clear solution was evaporated under vacuum to leave a colourless solid. This was recrystallized from dichloromethane–hexane (3:1 *v*/*v*, resulting in crystals of (I) suitable for X-ray analysis (m.p. 439 K) after 7 d. Analysis for $C_{22}H_{20}Cl_2N_2Sn$, calculated: C 52.63, H 4.02%; found: C 52.45, H 4.13%.

Crystal data

$[Sn(C_6H_5)_2Cl_2(C_5H_5N)_2]$
M_r = 501.99
Monoclinic, $P2_1/n$
a = 9.445 (3) Å
b = 16.720 (5) Å
c = 13.474 (4) Å
β = 91.584 (4)°
V = 2127.0 (10) Å^3
Z = 4
D_x = 1.568 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3361 reflections
θ = 2.4–25.7°
μ = 1.46 mm^{-1}
T = 298 (2) K
Block, colourless
0.48 × 0.39 × 0.36 mm

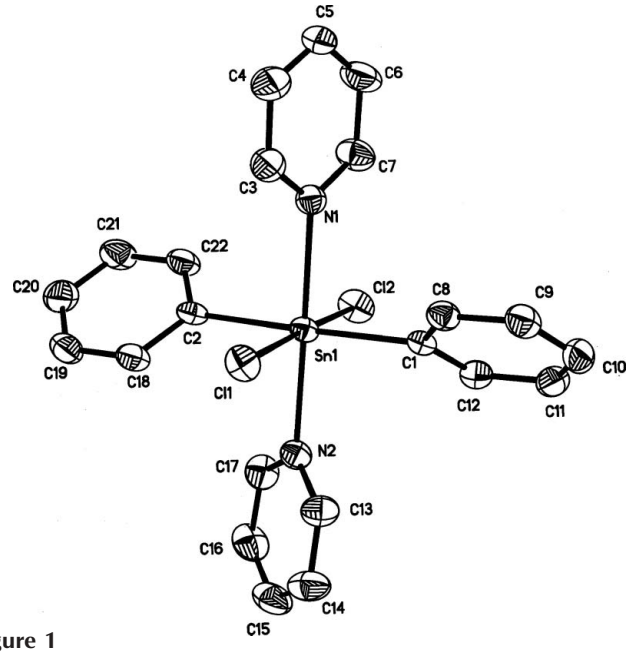


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids. H atoms have been omitted for clarity.

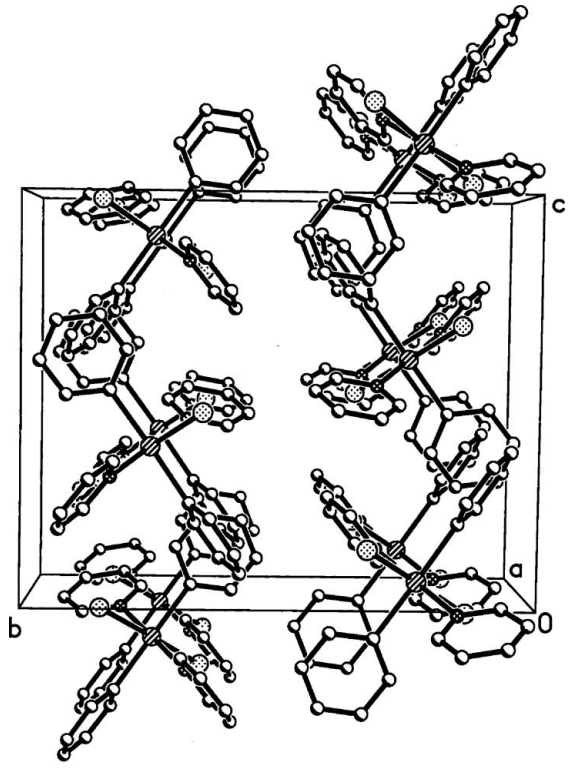


Figure 2
The packing of (I). H atoms have been omitted.

Data collection

Siemens SMART CCD diffractometer	5142 independent reflections
φ and ω scans	2752 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.042$
$T_{min} = 0.541$, $T_{max} = 0.621$	$\theta_{max} = 28.4^\circ$
13388 measured reflections	$h = -11 \rightarrow 12$
	$k = -16 \rightarrow 22$
	$l = -14 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0399P)^2 + 0.5683P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.038$	
$wR(F^2) = 0.101$	
$S = 1.00$	$(\Delta/\sigma)_{max} = 0.001$
5142 reflections	$\Delta\rho_{max} = 1.12$ e Å^{-3}
244 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected bond lengths (Å).

Sn1—C2	2.192 (4)	Sn1—N1	2.331 (4)
Sn1—C1	2.194 (4)	Sn1—Cl2	2.5310 (12)
Sn1—N2	2.314 (4)	Sn1—Cl1	2.5331 (12)

All H atoms were positioned geometrically and refined as riding, with C—H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum and minimum electron-density peaks are located 1.38 Å from atom H18 and 1.40 Å from atom Cl2, respectively.

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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