Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

Tetrachlorobis(dimethylamine)tin(IV)

Yong Zhang, Hong-Bo Tong, Dian-Sheng Liu,* Su-Ping Huang and Mei-Su Zhou

Institute of Modern Chemistry, Shanxi University, Shanxi, People's Republic of China

Correspondence e-mail: dsliu@sxu.edu.cn

Received 11 July 2005
Accepted 28 July 2005
Online 6 August 2005

Key indicators

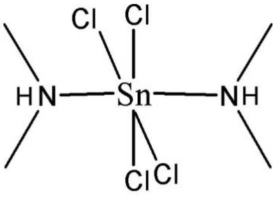
Single-crystal X-ray study
T = 202 K
Mean σ(N–C) = 0.009 Å
R factor = 0.050
wR factor = 0.108
Data-to-parameter ratio = 18.1

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

In the title compound, $[SnCl_4(C_3H_7N)_2]$, the coordination geometry around the Sn atom is octahedral, with the two N atoms of dimethylamine in the axial sites. The Sn atom is at the center of the square formed by four Cl atoms. The title molecule lies on a crystallographic center of symmetry. The crystal structure has a moderate N—H···Cl hydrogen bond.

Comment

Tin compounds are classified into two main groups, *viz*. inorganic tin and organotin compounds. The organotin compounds are defined as compounds in which at least one Sn—C bond exists, but the inorganic tin compounds do not contain carbon as the principal element. Inorganic tin compounds are relatively simple in their molecular structure and, like tin itself, are not considered to be toxic. Sn atoms can replace C atoms in chemical compounds and a great variety of organotin compounds is known.



(I)

Recently, we synthesized the title compound, (I). It contains two dimethylamine ligands coordinated to tin tetrachloride, and its crystal structure is presented here. The coordination geometry around the Sn atom is octahedral, with the two

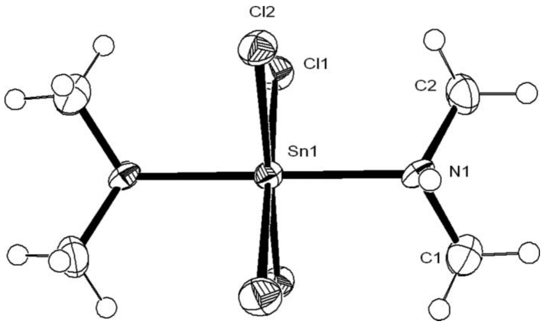


Figure 1
View of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by small spheres of arbitrary radii. (Symmetry code for unlabeled atoms: $-x$, $1 - y$, $-z$.)

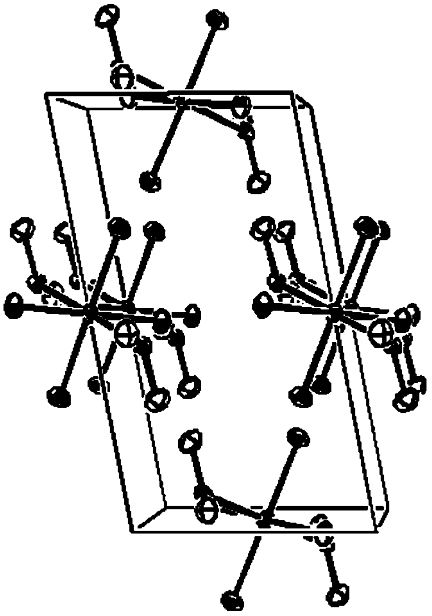


Figure 2
The packing of the title complex. H atoms have been omitted.

dimethylamine N atoms in axial positions. The Sn atom lies on a center of symmetry. Although the H-atom positions are of low precision, the geometry around the amine N atom is essentially tetrahedral. It can be noted from Table 1 that the bond Sn1—N1 of (I) is slightly longer than the Sn—N bonds [2.177 (5) and 2.204 (4) Å] in {tris[*N*-(salicylidene)-2-aminoethyl]amine}tin(IV) iodide acetonitrile solvate (Watson *et al.*, 1997). One possible reason is that the previous structure has an N—H···Cl intermolecular hydrogen-bond interaction. As the packing plot shows, a chain is formed by intermolecular hydrogen-bond interactions (Fig. 2).

Experimental

Dimethylamine (10 ml) in diethyl ether (0.1 mol l^{-1}) was added dropwise to a solution of tin tetrachloride (0.5 mmol) in dichloromethane at 273 K, and then the temperature was allowed to rise to room temperature. The mixture was stirred for more than 5 h and then carefully concentrated in a vacuum until colorless crystals of (I) appeared. All reactions were performed under argon using standard Schlenk techniques. The CH_2Cl_2 was distilled from CaH_2, and diethyl ether was distilled from sodium.

Crystal data

$[SnCl_4(C_2H_7N)_2]$
M_r = 350.66
Monoclinic, $P2_1/n$
a = 6.319 (2) Å
b = 8.153 (3) Å
c = 11.529 (4) Å
β = 100.786 (4)°
V = 583.5 (3) Å^3
Z = 2
D_x = 1.996 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1059 reflections
θ = 3.1–26.5°
μ = 3.06 mm^{-1}
T = 202 (2) K
Block, colorless
0.10 × 0.10 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.750, $T_{\max}$ = 0.862
2328 measured reflections
1034 independent reflections
942 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.031
$\theta_{\max}$ = 25.0°
$h = -6 \rightarrow 7$
$k = -9 \rightarrow 9$
$l = -13 \rightarrow 12$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.108
S = 1.17
1034 reflections
57 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2 + 0.6995P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 1.35 e Å^{-3}
$\Delta\rho_{\min}$ = −0.79 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—N1	2.224 (6)		
C1—N1—Sn1	115.8 (5)	C1—N1—H1	99 (6)
C2—N1—H1	111 (6)	Sn1—N1—H1	104 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···Cl2^{i}	0.89 (8)	2.49 (9)	3.276 (6)	148 (7)

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

The methyl H atoms were constrained to an ideal geometry, with C—H = 0.98 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C), but each group was allowed to rotate freely about its C—C bond. The position of the amine H atom was refined freely along with an isotropic displacement parameter.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the Natural Science Foundation of China (Nos. 20171030 and 29872024, to DSL), the Natural Science Foundation of ShanXi province (No. 20011008, to DSL) and the Youth Foundation of Shanxi Province (No. 20031015).

References

Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Watson, S., Errington, W., Fenn, D., Moore, P. & Wallbridge, M. G. H. (1997). *Acta Cryst.* C**53**, 1031–1034.

m1698 Zhang *et al.* • $[SnCl_4(C_2H_7N)_2]$ *Acta Cryst.* (2005). E**61**, m1697–m1698