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## Key indicators

Single-crystal X-ray study  
 $T = 297\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.005\text{ \AA}$   
 $R$  factor = 0.025  
 $wR$  factor = 0.060  
Data-to-parameter ratio = 20.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>. $\mu$ -Hydroxo-bis[[2-(dimethylaminomethyl)phenyl]-  
dimethyltin(IV)] iodide

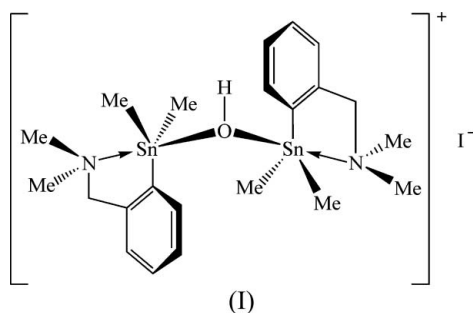
The cation of the title compound,  $[\text{Sn}_2(\text{CH}_3)_4(\text{OH})-(\text{C}_9\text{H}_{12}\text{N})_2]\text{I}$ , consists of two  $[2-(\text{Me}_2\text{NCH}_2)\text{C}_6\text{H}_4]\text{SnMe}_2$  units bridged by a hydroxy group, located on a twofold rotation axis. Both Sn atoms are pentacoordinated in a distorted trigonal-bipyramidal coordination geometry as the result of a strong intramolecular  $\text{N}\rightarrow\text{Sn}$  interaction *trans* to the  $\text{Sn}-\text{O}$  bond  $[\text{N}-\text{Sn}-\text{O} = 168.70(7)^\circ]$ . The iodide ion also lies on a twofold rotation axis.

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## Comment

During our work on organotin(IV) halides containing the  $[2-(\text{Me}_2\text{NCH}_2)\text{C}_6\text{H}_4]$  group (Varga *et al.*, 2001, 2005, 2006) we isolated the title compound, (I), with two organotin(IV) fragments bridged by a hydroxy group, forming the cation of the ionic compound, and with  $\text{I}^-$  as a counter-anion. The bridging hydroxy group and iodide ion are located on the special position 4(*e*), a twofold axis of the space group  $C2/c$ .



The Sn atoms have a trigonal-bipyramidal coordination owing to the strong intramolecular  $\text{N}\rightarrow\text{Sn}$  interaction *trans* to the  $\text{Sn}-\text{O}$  bond, with the C atoms from the organic ligands in equatorial positions (Fig. 1). The  $(\text{C},\text{N})\text{C}_2\text{SnO}$  cores are distorted from the ideal geometry as a consequence of the small 'bite' of the pendant arm ligand. The deviation of the metal atom from the equatorial plane (C1/C10/C11) is  $0.13\text{ \AA}$  towards the O atom.

The intramolecular  $\text{N}\rightarrow\text{Sn}$  interaction induces planar chirality at the metal centre (Varga *et al.*, 2005, 2006) and the compound crystallizes as a racemate, a mixture of *RR* and *SS* isomers (1:1).

In the crystal packing there is a hydrogen bond between the hydroxy group and the iodide ion [ $\text{H1}\cdots\text{I1} = 2.77\text{ \AA}$ ,  $\text{O1}\cdots\text{I1} = 3.579(3)\text{ \AA}$  and  $\text{O1}-\text{H1}\cdots\text{I1} = 179.98(3)^\circ$ ].

## Experimental

Compound (I) was obtained after recrystallization of *C,N*-[2-(dimethylaminomethyl)phenyl]dimethyltin(IV) iodide from hot DMSO (Varga, 2003).

## Crystal data

[Sn<sub>2</sub>(CH<sub>3</sub>)<sub>4</sub>(OH)(C<sub>9</sub>H<sub>12</sub>N)<sub>2</sub>] $M_r = 709.86$ Monoclinic,  $C2/c$  $a = 9.4994$  (14) Å $b = 18.762$  (3) Å $c = 14.778$  (2) Å $\beta = 92.240$  (2)° $V = 2631.8$  (7) Å<sup>3</sup> $Z = 4$  $D_x = 1.791$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation $\mu = 3.09$  mm<sup>-1</sup> $T = 297$  (2) K

Block, colourless

 $0.42 \times 0.35 \times 0.20$  mm

## Data collection

Bruker SMART CCD area-detector diffractometer

 $\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Bruker, 2000)

 $T_{\min} = 0.293$ ,  $T_{\max} = 0.537$ 

10450 measured reflections

2697 independent reflections

2509 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.026$  $\theta_{\text{max}} = 26.4^\circ$ 

## Refinement

Refinement on  $F^2$  $R[F^2 > 2\sigma(F^2)] = 0.025$  $wR(F^2) = 0.061$  $S = 1.11$ 

2697 reflections

134 parameters

H atoms treated by a mixture of independent and constrained refinement

 $w = 1/[\sigma^2(F_o^2) + (0.0274P)^2 + 2.4944P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\text{max}} = 0.002$  $\Delta\rho_{\text{max}} = 0.51$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -0.61$  e Å<sup>-3</sup>

Table 1

Selected geometric parameters (Å, °).

Sn1—C1	2.126 (3)	Sn1—O1	2.1459 (11)
Sn1—C10	2.130 (3)	Sn1—N1	2.470 (3)
Sn1—C11	2.118 (3)		
C11—Sn1—C1	126.43 (14)	C11—Sn1—N1	91.56 (12)
C11—Sn1—C10	116.19 (15)	C1—Sn1—N1	75.46 (11)
C1—Sn1—C10	116.29 (13)	C10—Sn1—N1	93.36 (12)
C11—Sn1—O1	92.22 (12)	O1—Sn1—N1	168.70 (7)
C1—Sn1—O1	93.76 (8)	Sn1—O1—Sn1 <sup>i</sup>	136.92 (15)
C10—Sn1—O1	94.52 (11)		

Symmetry code: (i)  $-x, y, -z + \frac{1}{2}$ .

All C-bound H atoms were placed in calculated positions ( $C-H = 0.93-0.97$  Å) and treated using a riding model with  $U_{\text{iso}} = 1.5U_{\text{eq}}(C)$  for methyl and  $U_{\text{iso}} = 1.2U_{\text{eq}}(C)$  for aryl H atoms; the methyl groups were allowed to rotate but not to tip. Atom H1 bonded to the O atom was calculated and fixed at the standard O—H distance of  $0.81$  (2) Å.

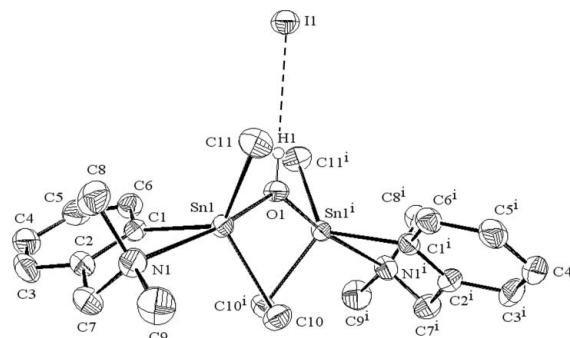


Figure 1

View of compound (I), with the labelling of all non-H atoms. Displacement ellipsoids are shown at the 30% probability levels. C-bound H atoms have been omitted. Symmetry code (i) as in Table 1. The dashed line indicates the  $H1 \cdots O1$  hydrogen bond.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2000); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXTL (Bruker, 2001); program(s) used to refine structure: SHELXTL; molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg & Putz, 2001); software used to prepare material for publication: publCIF (Westrip, 2006).

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## References

- Brandenburg, K. & Putz, H. (2001). DIAMOND. Crystal Impact GbR, Bonn, Germany.
- Bruker (2000). SADABS (Version 2.03), SMART (Version 5.625) and SAINT-Plus (Version 6.29). Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (2001). SHELXTL. Version 6.10.12. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Varga, R. A. (2003). PhD thesis, 'Babes-Bolyai' University, Cluj-Napoca, Romania.
- Varga, R. A., Rotar, A., Schuermann, M., Jurkschat, K. & Silvestru, C. (2006). *Eur. J. Inorg. Chem.* **7**, 1475–1486.
- Varga, R. A., Schuermann, M. & Silvestru, C. (2001). *J. Organomet. Chem.* **623**, 161–167.
- Varga, R. A., Silvestru, C. & Deleanu, C. (2005). *Appl. Organomet. Chem.* **19**, 153–160.
- Westrip, S. P. (2006). publCIF. In preparation.