Intramolecular interactions in μ-oxido-bis{bis[2-(dimethylamino-methyl)phenyl]stannol}

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The title compound, $[Sn_2(C_9H_{12}N)_4O(OH)_2]$, consists of two $[2-(Me_2NCH_2)C_6H_4]_2SnOH$ units bridged by an O atom located on a twofold rotation axis. The unique Sn atom is six-coordinated with a $(C,N)_2SnO_2$ octahedral core, as a result of the strong intramolecular N→Sn dative coordination *trans* to the Sn—O bonds [N—Sn—O = 170.24 (12) and 167.83 (10)°]. Owing to the presence of intermolecular H···phenyl contacts, the molecules are arranged in a ladder-like structure.

Comment

During our work on hypercoordinated organotin(IV) compounds with the $[2-(Me_2NCH_2)C_6H_4]Sn$ fragment (Varga *et al.*, 2001, 2005, 2006), the title compound, (I), was isolated. It contains two $[2-(Me_2NCH_2)C_6H_4]_2SnOH$ units bridged by an O atom (Fig. 1), which lies on a twofold axis of the space group $C2/c$. The angle around the bridging O2 atom [Sn1—O2—Sn1^i = 137.1 (2)°; symmetry code: (i) $-x, y, -z + \frac{1}{2}$] is larger than a typical bonding angle for oxygen owing to the steric constraints imposed by the organic groups bonded to the Sn atoms.

(I)
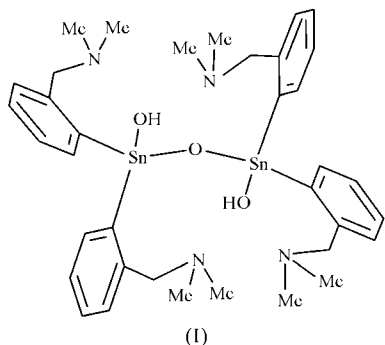
The Sn atoms are six-coordinated as a result of strong intramolecular N→Sn dative coordination. The two N→Sn distances are almost of the same magnitude (Table 1), the bond *trans* to the Sn1—O2 bond being slightly stronger.

Both $(C,N)_2SnO_2$ cores are distorted from an ideal geometry as a consequence of the small 'bite' of the pendant arm ligand [C1—Sn1—N1 = 70.94 (13)° and C10—Sn1—N2 = 71.41 (14)°] and the steric repulsion between the organic groups bonded to the Sn atoms.

The intramolecular N→Sn interaction induces planar chirality at the metal centre (Varga *et al.*, 2005, 2006) and the compound crystallizes as a racemate, *i.e.* a mixture of $S_{N1}R_{N2}S_{N1}{}^iR_{N2}{}^i$ and $R_{N1}S_{N2}R_{N1}{}^iS_{N2}{}^i$ isomers.

Atom H1 of the hydroxy group is involved in an intramolecular H···π interaction (H···centroid = 3.11 Å; Table 2), thus explaining the orientation of the O1—H1 bond and the absence of an acceptor for an eventual hydrogen bond involving H1. Aromatic atom H3 also participates in an intermolecular H···π interaction (H···centroid = 2.88 Å; Table 2), with a phenyl ring from a neighbouring molecule. These interactions lead to the formation of a one-dimensional polymer (Fig. 2), with alternating $S_{N1}R_{N2}S_{N1}{}^iR_{N2}{}^i$ and $R_{N1}S_{N2}R_{N1}{}^iS_{N2}{}^i$ isomers. In the crystal structure, the polymers run parallel to the c axis with no further inter-chain interactions (Fig. 3).
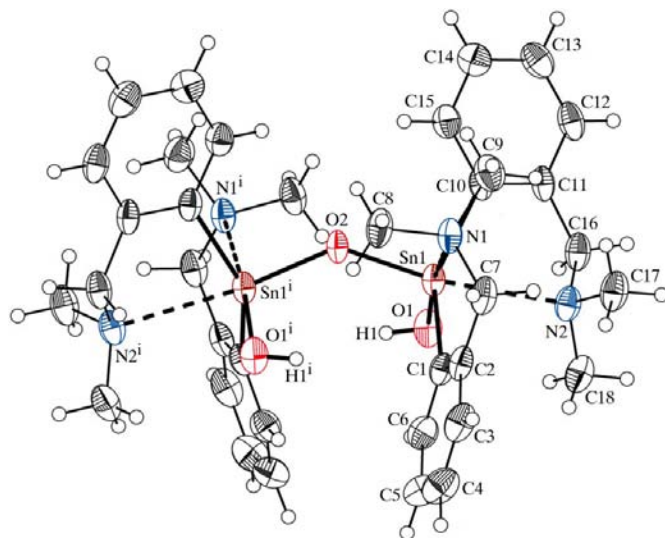

Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms as spheres of arbitrary radii. [Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.]
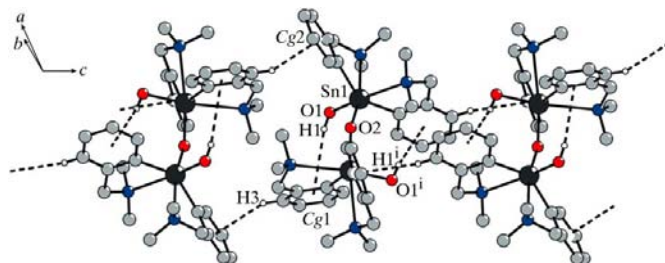

Figure 2
Intra- and intermolecular interactions (represented with dashed lines) in the crystal structure of (I). The symmetry code is as given in Table 2.
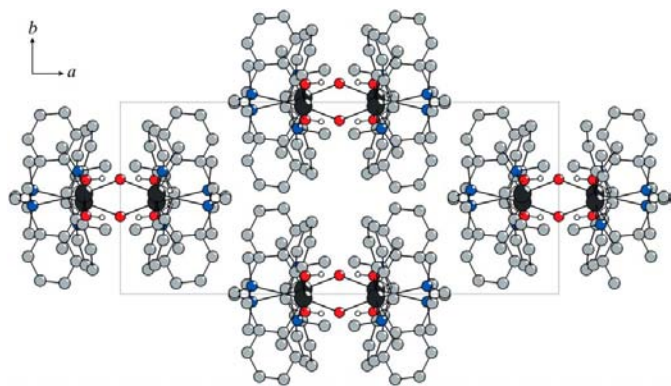
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metal-organic compounds

Figure 3
The crystal packing of (I), viewed along the c axis.

Experimental

The title compound was obtained by reacting [2-(Me$_2$NCH$_2$)C$_6$H$_4$]$_2$-SnCl$_2$ with an excess of KOH in a dichloromethane/water (1:1) mixture. Crystals suitable for X-ray diffraction analysis were obtained from CDCl$_3$.

Crystal data

[Sn$_2$(C$_9$H$_{12}$N)$_4$O(OH)$_2$]	$V = 3592.9\ (8)$ Å^3
$M_r = 824.18$	$Z = 4$
Monoclinic, $C2/c$	Mo $K\alpha$ radiation
$a = 25.518\ (3)$ Å	$\mu = 1.43$ mm^{-1}
$b = 9.7060\ (12)$ Å	$T = 297\ (2)$ K
$c = 16.758\ (2)$ Å	$0.25 \times 0.17 \times 0.12$ mm
$\beta = 120.045\ (2)°$	

Data collection

Bruker SMART CCD area-detector diffractometer	14057 measured reflections
Absorption correction: multi-scan (*SHELXTL*; Bruker, 2001)	3662 independent reflections
$T_{min} = 0.716$, $T_{max} = 0.847$	2986 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.046$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.090$	
$S = 1.13$	$\Delta\rho_{max} = 0.73$ e Å^{-3}
3662 reflections	$\Delta\rho_{min} = -0.48$ e Å^{-3}
212 parameters	
2 restraints	

Table 1
Selected bond lengths (Å).

Sn1—O1	2.036 (3)	Sn1—N1	2.751 (3)
Sn1—O2	1.9705 (15)	Sn1—C10	2.141 (4)
Sn1—N2	2.697 (3)	Sn1—C1	2.155 (4)

Table 2
X—H$\cdots\pi$-ring interactions (Å, °).

$Cg1$ is the centroid of the C1–C6 benzene ring and $Cg2$ is the centroid of the C10–C15 benzene ring.

Y—$X\cdots Cg$	X—H	H$\cdots Cg$	$X\cdots Cg$	X—H$\cdots Cg$
O1—H1$\cdots Cg1^{ii}$	0.83	3.11	3.89 (1)	159
C3—H3$\cdots Cg2^{i}$	0.93	2.88	3.69 (2)	147

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

All H atoms were placed at calculated positions using a riding model, with C—H distances of 0.93–0.97 Å and with U_{iso}(H) values of $1.5U_{eq}$(C) for methyl and $1.2U_{eq}$(C) for aryl H atoms. The methyl groups were allowed to rotate but not to tip. The H atom bonded to O1 was found in a difference map and refined with a restrained O—H distance of 0.83 (3) Å.

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: *DIAMOND* (Brandenburg & Putz, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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