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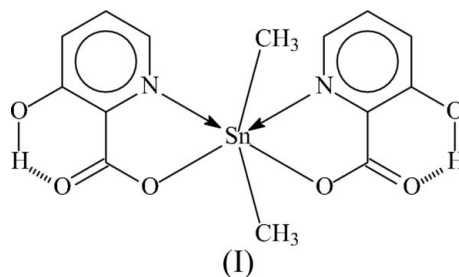
Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å
 R factor = 0.034
 wR factor = 0.090
Data-to-parameter ratio = 13.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Bis(3-hydroxypyridine-2-carboxylato)dimethyltin(IV)

The six-coordinate Sn atom (site symmetry 2) in the monomeric title complex, $[\text{Sn}(\text{CH}_3)_2(\text{C}_6\text{H}_4\text{NO}_3)_2]$, exists in a skew-trapezoidal geometry [$\text{C}-\text{Sn}-\text{C} = 149.4(3)^\circ$].Received 6 October 2005
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Comment

Dialkyltin(IV) dicarboxylates generally exist as monomeric six-coordinate compounds that display *O,O*-chelation to tin from the carboxylate groups (Tiekink, 1991, 1994). However, if there is a suitable Lewis basic site in the ligand, this site can compete for coordination. Thus, the 2-pyridylcarboxylate anion should be able to bind in the *O,N* mode, and this feature has been observed in the di-*n*-butyltin (Dakternieks *et al.*, 2003; Szorcsik *et al.*, 2004) and di-*t*-butyltin (Jurkschat & Tiekink, 1994) derivatives. Small chelate bite angles lead to the manifestation of a skew-trapezoidal geometry (Ng *et al.*, 1987), a geometry for which the diorganotin skeleton shows a $\text{C}-\text{Sn}-\text{C}$ angle of about 135° , this value being midway between a *cis* angle and a *trans* angle in an idealized octahedral system. The dimethyltin dipicolinate homolog is seven-coordinate arising from carboxylate bridging (Lockhart & Davidson, 1987), and is an exception owing to the small size of the methyl groups.

On the other hand, in some diorganotin dipicolinates, the diorganotin skeleton can open wide enough to admit another atom into the tin coordination sphere. For example, the dicyclohexyltin derivative is an aqua adduct (Dakternieks *et al.*, 2003, 2004), and an aqua adduct of dibutyltin dipicolinate has been reported (Yin *et al.*, 2002). The title dimethyltin bis-3-picolinate, (I), has a potentially basic hydroxy site, but the tin, with site symmetry 2, is only six-coordinate in a skew-trapezoidal bipyramidal geometry (Fig. 1 and Table 1). The reason that a higher coordination number or a polymeric structure is not attained is probably that the hydroxy groups are involved in intramolecular hydrogen bonding (Table 2) to the non-coordinated carboxyl O atoms. This strong hydrogen bond reduces the Lewis basicity of the donor O atom so that it is unable to bind to an adjacent Sn atom.

Experimental

The reaction was carried out under a nitrogen atmosphere. 3-Hydroxy-2-pyridylcarboxylic acid (0.28 g, 2 mmol) was reacted with triethylamine (0.20 g, 2 mmol) in benzene (20 ml), then dimethyltin dichloride (0.22 g, 1 mmol) was added to the mixture. The mixture was heated at 313 K for 12 h. The solvent was removed and the product purified by recrystallization from a dichloromethane–hexane (1:1) mixture to afford colorless crystals of (I), which melt at 433 K, in about 85% yield. Analysis calculated for $C_{14}H_{14}N_2O_6Sn$: C 39.50, H 3.32%; found: C 39.27, H 3.45%.

Crystal data

$[Sn(CH_3)_2(C_6H_4NO_3)_2]$	$D_x = 1.818 \text{ Mg m}^{-3}$
$M_r = 424.96$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 3129 reflections
$a = 9.228 (1) \text{ \AA}$	$\theta = 2.7\text{--}28.3^\circ$
$b = 13.363 (2) \text{ \AA}$	$\mu = 1.68 \text{ mm}^{-1}$
$c = 13.222 (2) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\beta = 107.783 (1)^\circ$	Block, colorless
$V = 1552.5 (3) \text{ \AA}^3$	$0.45 \times 0.27 \times 0.23 \text{ mm}$
$Z = 4$	

Data collection

Bruker SMART area-detector diffractometer	1783 independent reflections
φ and ω scans	1605 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.039$
$T_{min} = 0.416$, $T_{max} = 0.699$	$\theta_{max} = 27.5^\circ$
4512 measured reflections	$h = -11 \rightarrow 11$
	$k = -11 \rightarrow 17$
	$l = -14 \rightarrow 17$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0461P)^2 + 2.0757P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.090$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.06$	$\Delta\rho_{max} = 1.25 \text{ e \AA}^{-3}$
1783 reflections	$\Delta\rho_{min} = -0.82 \text{ e \AA}^{-3}$
133 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Sn1—C1	2.102 (4)	Sn1—O1	2.120 (3)
Sn1—N1	2.485 (3)		
C1—Sn1—C1 ⁱ	149.4 (3)	N1—Sn1—N1 ⁱ	139.9 (1)
C1—Sn1—O1	101.4 (2)	N1—Sn1—O1	70.9 (1)
C1—Sn1—O1 ⁱ	102.2 (2)	N1—Sn1—O1 ⁱ	149.2 (1)
C1—Sn1—N1	84.7 (1)	O1—Sn1—O1 ⁱ	78.3 (1)
C1—Sn1—N1 ⁱ	84.9 (1)		

Symmetry code: (i) $-x + 1, y, -z + \frac{3}{2}$.

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O3—H3O \cdots O2	0.85 (1)	1.82 (3)	2.578 (5)	149 (6)

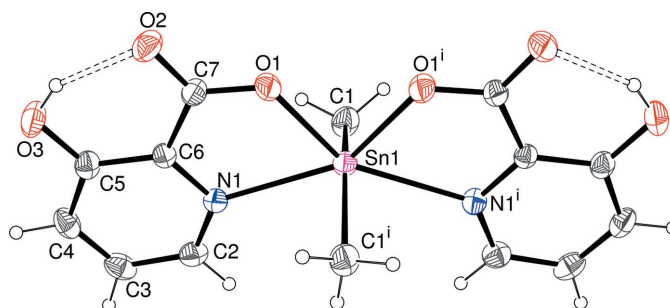


Figure 1

View of (I), showing 30% probability displacement ellipsoids (arbitrary spheres for the H atoms). The hydrogen bonds are indicated by dashed lines. (Symmetry code as in Table 1.)

All H atoms were located in difference maps and refined with distance restraints of O—H = 0.85 (1) \AA , C—H = 0.95 (1) \AA and H \cdots H = 1.55 (1) \AA . Their U_{iso} values were freely refined. The highest difference peak is 1 \AA from atom Sn1.

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINTE* (Bruker, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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