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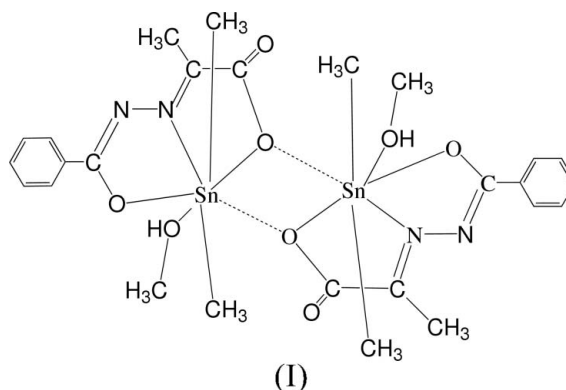
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Key indicators

Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.009\text{ \AA}$
 R factor = 0.034
 wR factor = 0.084
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.[μ -Pyruvic acid benzoylhydrazonato(2-)]-
bis[methanoldimethyltin(IV)]In the title complex, $[\text{Sn}_2(\text{CH}_3)_4(\text{C}_{10}\text{H}_8\text{N}_2\text{O}_3)_2(\text{CH}_4\text{O})_2]$, the Sn^{IV} ion has a distorted pentagonal-bipyramidal coordination geometry. The carboxylate O atom bridges two Sn^{IV} ions to form the dimeric complex, which is located on an inversion center. Hydrogen bonding between the methanol and carboxylate groups helps to stabilize the crystal structure.Received 12 December 2006
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Comment

As a part of an investigation on organotin(IV) complexes we recently synthesized the title complex, (I), and present here its structure.



The Sn^{IV} ion has a distorted pentagonal-bipyramidal coordination geometry, formed by one methanol molecule, two tridentate Schiff base ligands of pyruvic acid benzoylhydrazone and two methyl groups (Fig. 1). Atoms O1, O4, O1ⁱ, O3 and N1 are coplanar within 0.0220 Å [symmetry code (i): $-x, -y + 1, -z + 2$], forming the equatorial plane. The carboxylate atom O1 bridges two Sn^{IV} ions to form the dimeric complex, which is located on an inversion center. The $\text{Sn}-\text{O1}^i$ bond distance (Table 1) is significantly longer than the typical $\text{Sn}-\text{O}$ bond, but shorter than the sum of the van der Waals radii for Sn and O (3.68 Å; Bondi, 1964). Thus, the structure of this complex can be described as a weakly bridged dimer. The formation of the dimer leads to a short $\text{O} \cdots \text{O}^i$ separation of 2.827 (2) Å. The $\text{Sn}-\text{O}(\text{methanol})$ bond distance is longer than those found in analogous complexes (Yin *et al.*, 2003; Parulekar *et al.*, 1989).

Hydrogen bonding between the methanol and carboxylate groups helps to stabilize the crystal structure (Table 2).

Experimental

Pyruvic acid benzoylhydrazone (1 mmol) and sodium ethoxide (1 mmol) were added to dry benzene (20 ml) in a Schlenk flask and

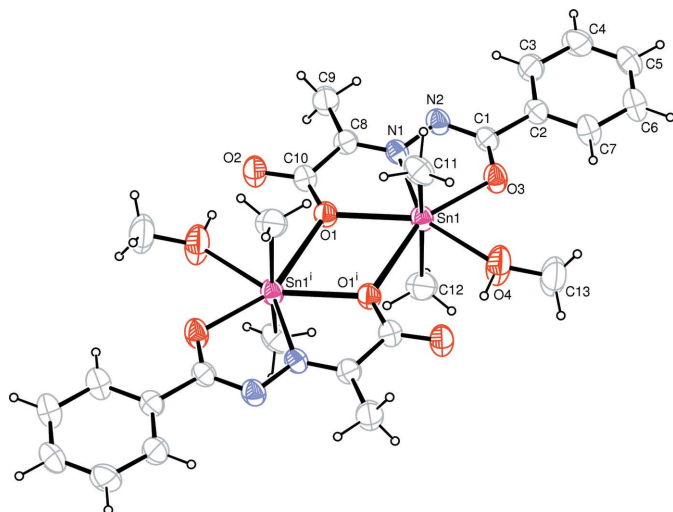


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids [symmetry code (i): $-x, -y + 1, -z + 2$].

stirred for 0.5 h. Dimethyltin dichloride (1 mmol) was added, and the reaction mixture was stirred for 12 h at 313 K and then filtered. The solvent was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from methanol and colorless single crystals were obtained. Elemental analysis, calculated for $C_{13}H_{18}N_2O_4Sn$: C 40.52, H 4.68, N 7.27%; found: C 40.31, H 4.73, N 7.40%.

Crystal data

$[Sn_2(CH_3)_4(C_{10}H_8N_2O_3)_2(CH_4O)_2]$	$Z = 2$
$M_r = 769.96$	$D_x = 1.613 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 10.408 (10) \text{ \AA}$	$\mu = 1.63 \text{ mm}^{-1}$
$b = 18.910 (17) \text{ \AA}$	$T = 298 (2) \text{ K}$
$c = 8.911 (8) \text{ \AA}$	Block, colorless
$\beta = 115.346 (15)^\circ$	$0.47 \times 0.42 \times 0.18 \text{ mm}$
$V = 1585 (3) \text{ \AA}^3$	

Data collection

Bruker SMART CCD area-detector diffractometer	8215 measured reflections
φ and ω scans	2809 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	2060 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.470, T_{\max} = 0.750$	$R_{\text{int}} = 0.036$
	$\theta_{\max} = 25.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0338P)^2 + 2.1392P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.084$	$(\Delta\sigma)_{\max} = 0.004$
$S = 1.00$	$\Delta\rho_{\max} = 0.57 \text{ e \AA}^{-3}$
2809 reflections	$\Delta\rho_{\min} = -0.55 \text{ e \AA}^{-3}$
187 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters ($\text{\AA}, ^\circ$).

Sn1—O1	2.312 (3)	Sn1—N1	2.263 (4)
Sn1—O1 ⁱ	2.751 (4)	Sn1—C11	2.094 (5)
Sn1—O3	2.184 (3)	Sn1—C12	2.094 (5)
Sn1—O4	2.427 (4)		
C11—Sn1—C12	161.5 (2)	C11—Sn1—O4	82.5 (2)
C11—Sn1—O3	96.22 (19)	O3—Sn1—O4	77.39 (14)
C12—Sn1—O3	96.15 (19)	N1—Sn1—O4	146.79 (14)
C11—Sn1—N1	99.24 (19)	O1—Sn1—O4	142.83 (13)
C12—Sn1—N1	98.0 (2)	C11—Sn1—O1 ⁱ	81.59 (17)
O3—Sn1—N1	69.44 (14)	O3—Sn1—O1 ⁱ	153.03 (11)
C11—Sn1—O1	90.07 (18)	O1—Sn1—O1 ⁱ	67.21 (12)
O3—Sn1—O1	139.76 (12)	O4—Sn1—O1 ⁱ	75.68 (13)
N1—Sn1—O1	70.31 (13)		

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

Table 2
Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O4—H14 \cdots O2 ⁱ	0.93 (7)	1.74 (7)	2.648 (6)	165 (6)

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

H atoms attached to C atoms were all positioned geometrically and treated as riding on their parent atoms, with aromatic C—H distances of 0.93 \AA and methyl C—H distances of 0.96 \AA . The $U_{\text{iso}}(\text{H})$ values were set at $1.5U_{\text{eq}}(\text{C})$ for the methyl H atoms and at $1.2U_{\text{eq}}(\text{C})$ for the other C-bound H atoms. The H atom bonded to the O atom was refined isotropically, giving an O—H distance of 0.93 (7) \AA .

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

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