

Min Hong, Han-Dong Yin* and
Da-Qi WangCollege of Chemistry and Chemical Engineering,
Liaocheng University, Shandong 252059,
People's Republic of ChinaCorrespondence e-mail:
handongyin@lctu.edu.cn

Key indicators

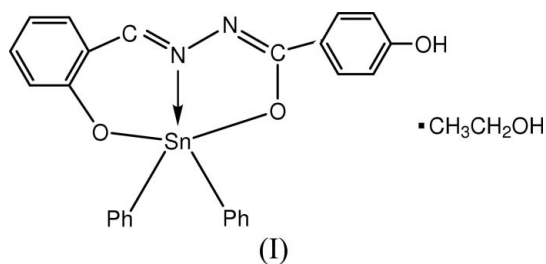
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.011\text{ \AA}$
 R factor = 0.053
 wR factor = 0.129
Data-to-parameter ratio = 14.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.[2-Oxidobenzaldehyde (4-hydroxybenzoyl)-
hydrazonato]diphenyltin(IV) ethanol solvate

In the title complex, $[\text{Sn}(\text{C}_6\text{H}_5)_2(\text{C}_{14}\text{H}_{10}\text{N}_2\text{O}_3)] \cdot \text{C}_2\text{H}_6\text{O}$, the Sn atom is in a distorted trigonal-bipyramidal geometry, with Sn—O distances of 2.077 (4) and 2.130 (4) Å. The crystal packing shows a hydrogen-bonded dimeric arrangement of two Sn complexes and two ethanol solvent molecules located about a crystallographic inversion centre.

Received 15 May 2006
Accepted 31 May 2006

Comment

Diorganotin(IV) compounds are of current interest owing to their wide range of applications as biocides and homogeneous catalysts in industry (Yamamoto, 1997). In line with these developments, we have recently reported some diorganotin compounds of salicylaldehyde isonicotinylhydrazone (Yin *et al.*, 2005). As a continuation of this line of investigation, we have now synthesized the title diorganotin compound, (I), with salicylaldehyde 4-hydroxybenzhydrazone and present its structure here.



The structure of (I) shows that the complex is a monomer in which the Sn atom adopts a five-coordinate geometry, coordinated by two O atoms, two C atoms and one N atom (Fig. 1). The coordination environment is a distorted trigonal bipyramid. The Schiff base coordinates to the Sn atom as a tridentate ligand *via* the azomethine N atom, the hydroxyl O atom and the carbonyl O atom. The C—N—N—C chain shows conjugation, as evidenced by the intermediate values for the bond lengths (Table 1). The Sn1···N1 distance is 2.153 (5) Å, close to the sum of the non-polar covalent radii (2.15 Å; Sanderson, 1967), indicating an Sn···N interaction. The O atoms are coordinated to the Sn atom with one short and one long Sn—O bond.

The crystal packing of (I) shows an ethanol solvent molecule which links two adjacent molecules through O—H···N and O—H···O hydrogen bonds, contributing to the crystal stability and compactness and resulting in a hydrogen-bonded dimeric arrangement, located about a crystallographic inversion centre (Fig. 2).

Experimental

Salicylaldehyde 4-hydroxybenzhydrazone (1.0 mmol) and triethylamine (3.0 mmol) were added to dry benzene (20 ml) in a Schlenk flask and stirred for 0.5 h. Diphenyltin dichloride (1.0 mmol) was then added to the reactor dropwise and the reaction mixture was stirred for 4 h at room temperature and then filtered. The solvent was gradually removed by evaporation under vacuum until a sticky product was obtained. The product was then recrystallized from ethanol and yellow crystals of (I) suitable for X-ray diffraction were obtained (m.p. 462 K). Elemental analysis, calculated for $C_{28}H_{26}N_2O_4Sn$: C 58.67, H 4.57, N 4.89%; found: C 58.59, H 4.63, N 4.80%.

Crystal data

$[Sn(C_6H_5)_2(C_{14}H_{10}N_2O_3)] \cdot C_2H_6O$	$V = 1282 (2) \text{ \AA}^3$
$M_r = 573.20$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.485 \text{ Mg m}^{-3}$
$a = 9.565 (10) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 10.230 (11) \text{ \AA}$	$\mu = 1.03 \text{ mm}^{-1}$
$c = 14.110 (15) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\alpha = 78.031 (17)^\circ$	Block, yellow
$\beta = 71.855 (15)^\circ$	$0.31 \times 0.25 \times 0.21 \text{ mm}$
$\gamma = 88.474 (18)^\circ$	

Data collection

Bruker SMART CCD area-detector diffractometer	6799 measured reflections
φ and ω scans	4501 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3093 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.740$, $T_{\max} = 0.812$	$R_{\text{int}} = 0.032$
	$\theta_{\max} = 25.1^\circ$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2]$
$wR(F^2) = 0.129$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} < 0.001$
4501 reflections	$\Delta\rho_{\max} = 1.89 \text{ e \AA}^{-3}$
319 parameters	$\Delta\rho_{\min} = -0.45 \text{ e \AA}^{-3}$

Table 1

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

Sn1—O1	2.077 (4)	N1—C8	1.310 (7)
Sn1—O2	2.130 (4)	N1—N2	1.398 (6)
Sn1—N2	2.153 (5)	N2—C7	1.282 (7)
O1—Sn1—C15	97.1 (2)	O1—Sn1—N2	83.37 (18)
C15—Sn1—C21	125.7 (2)	C21—Sn1—N2	114.5 (2)
O1—Sn1—O2	156.22 (16)	O2—Sn1—N2	72.87 (17)
C21—Sn1—O2	92.9 (2)		

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O4—H4A \cdots N1 ⁱ	0.82	2.07	2.860 (7)	163
O3—H3 \cdots O4 ⁱⁱ	0.82	1.88	2.691 (7)	171

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

H atoms attached to C atoms were positioned geometrically and treated as riding on their parent atoms, with aromatic C—H distances of 0.93 \AA , methyl C—H distances of 0.96 \AA and methylene C—H

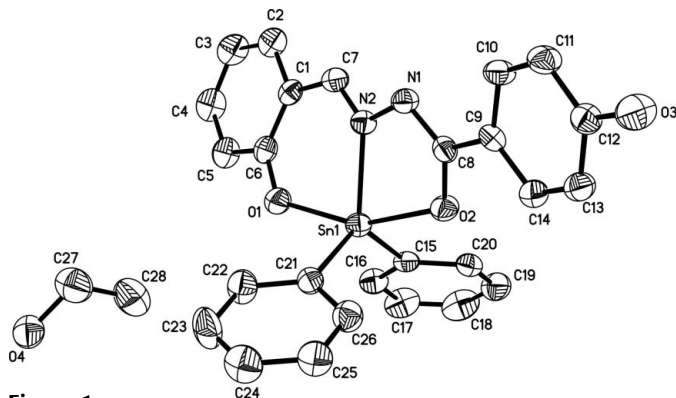


Figure 1

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

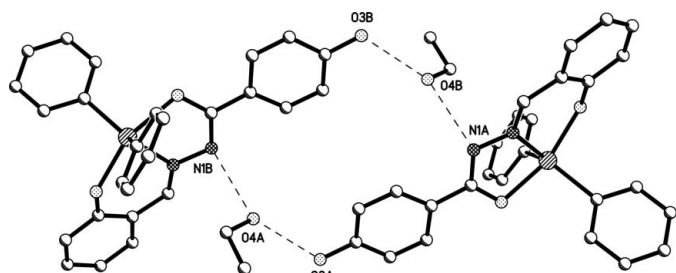


Figure 2

The dimeric arrangement of the title complex formed via intermolecular hydrogen bonding. H atoms have been omitted. Symmetry codes: (A) $x, y + 1, z - 1$; (B) $-x, -y + 2, -z + 1$.

distances of 0.97 \AA , and a fixed O—H distance of 0.82 \AA for O3—H3 and O4—H4A. The $U_{\text{iso}}(\text{H})$ values were set at $1.5U_{\text{eq}}(\text{C})$ for the methyl and hydroxyl H atoms, and at $1.2U_{\text{eq}}(\text{C})$ for the other C-bound H atoms. The highest residual electron-density peak was located 1.05 \AA from Sn1.

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.

The authors acknowledge the financial support of the Shandong Province Science Foundation and the State Key Laboratory of Crystalline Materials, Shandong University, China.

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