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Bis[μ-1-pyruvic acid (4-chlorobenzoyl)-hydrazonato(2−)]bis[ethanoldimethyltin(IV)]

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In the title centrosymmetric dimeric complex of Sn^{IV}, $[Sn_2(CH_3)_4(C_{10}H_7ClN_2O_3)_2(C_2H_6O)_2]$, each Sn atom has a distorted pentagonal–bipyramidal configuration, being coordinated by three O atoms and one N atom from the pyruvic acid 4-chlorobenzoylhydrazone ligands, one O atom from an ethanol molecule and two axial C atoms from *trans* methyl groups.

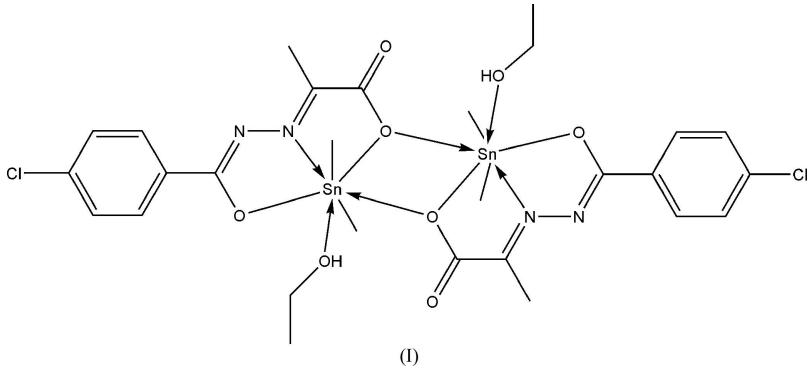
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.009 Å
R factor = 0.045
wR factor = 0.093
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

As part of our ongoing investigation of Sn chemistry, we present here the crystal structure of the title compound, (I).



(I)

The molecular structure of (I) is shown in Fig. 1. In the centrosymmetric molecule, each Sn atom displays a distorted pentagonal–bipyramidal coordination environment, formed by an ethanol molecule, a tridentate pyruvic acid 4-chlorobenzoylhydrazone ligand and two methyl groups. The bond distances involving the C—N—N—C part show electron delocalization (Table 1). The bridging Sn1—O1^{i} bond is much longer than the Sn1—O1 bond [symmetry code: (i) $-x, -y+1, -z+1$], comparable to analogous bond distances found in related seven-coordinate diorganotin systems (Gielen *et al.*, 1998; Yin *et al.*, 2003).

The Sn1—O4(ethanol) bond distance is longer than those found in analogous compounds (Yin *et al.*, 2003; Gielen *et al.*,1998), perhaps due to the formation of O4–H4$\cdots$O2^{i} hydrogen bonds within the dimeric molecule (Table 2).

Experimental

The reaction was carried out under a nitrogen atmosphere. Pyruvic acid 4-chlorobenzoylhydrazone (1 mmol) and sodium ethoxide (1 mmol) were dissolved in benzene (30 ml) in a Schlenk flask and the solution was stirred for 0.5 h. Dimethyltin(IV) chloride (1 mmol) was then added and the mixture was stirred for 8 h at 313 K. The resulting clear solution was evaporated under vacuum. The product was

recrystallized from a solution in a mixture of dichloromethane and methanol (1:1 *v*/*v*). Elemental analysis, calculated for $C_{14}H_{19}ClN_2O_4Sn$: C 38.79, H 4.42, N 6.46%; found: C 38.61, H 4.35, N 6.57%.

Crystal data

$[Sn_2(CH_3)_4(C_{10}H_7ClN_2O_3)_2\cdot(C_2H_6O)_2]$	β = 105.757 (3)°
M_r = 866.94	γ = 99.499 (2)°
Triclinic, $P\overline{1}$	V = 856.1 (3) Å^3
a = 7.8870 (17) Å	Z = 1
b = 10.4730 (19) Å	Mo $K\alpha$ radiation
c = 11.753 (2) Å	μ = 1.67 mm^{-1}
α = 107.846 (3)°	T = 298 (2) K
	0.31 × 0.17 × 0.07 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4353 measured reflections
	2921 independent reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2154 reflections with $I > 2\sigma(I)$
T_{min} = 0.626, T_{max} = 0.892	R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045	199 parameters
$wR(F^2)$ = 0.093	H-atom parameters constrained
S = 1.01	$\Delta\rho_{max}$ = 0.78 e Å^{-3}
2921 reflections	$\Delta\rho_{min}$ = −0.81 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—N1	2.246 (5)	Sn1—C14	2.097 (6)
Sn1—O1	2.333 (4)	N1—C2	1.294 (7)
Sn1—O1^{i}	2.688 (4)	N1—N2	1.377 (6)
Sn1—O3	2.175 (4)	N2—C4	1.338 (7)
Sn1—O4	2.458 (4)	O1—C1	1.280 (6)
Sn1—C13	2.109 (6)		
C14—Sn1—C13	161.7 (2)	O3—Sn1—O4	75.31 (14)
C14—Sn1—O3	94.1 (2)	N1—Sn1—O4	145.49 (16)
C14—Sn1—N1	100.4 (2)	O1—Sn1—O4	145.02 (14)
O3—Sn1—N1	70.19 (16)	C14—Sn1—O1^{i}	81.6 (2)
C14—Sn1—O1	92.0 (2)	O3—Sn1—O1^{i}	153.94 (14)
O3—Sn1—O1	139.67 (14)	N1—Sn1—O1^{i}	135.87 (14)
N1—Sn1—O1	69.50 (15)	O1—Sn1—O1^{i}	66.37 (14)
C14—Sn1—O4	82.6 (2)	O4—Sn1—O1^{i}	78.64 (12)

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O2^{i}	0.82	1.89	2.685 (6)	164

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

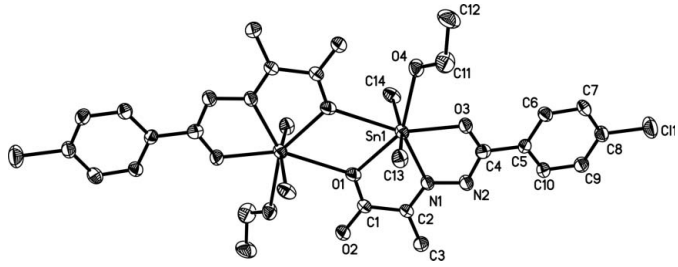


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids. H atoms have been omitted. Unlabelled atoms are related to labelled atoms by the symmetry operator $(-x, -y+1, -z+1)$.

All H atoms were positioned geometrically and treated as riding on their parent atoms, with aromatic C—H distances of 0.93 Å, methylene C—H distances of 0.97 Å and methyl C—H distances of 0.96 Å, and with an O—H distance of 0.82 Å. The U_{iso}(H) values were set at $1.5U_{eq}$(C) for the methyl H atoms $1.2U_{eq}$(C) for the other C-bound H atoms, and $1.5U_{eq}$(O).

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

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