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Bis(acetohydroxamato-κ^2O,O')diphenyltin(IV)

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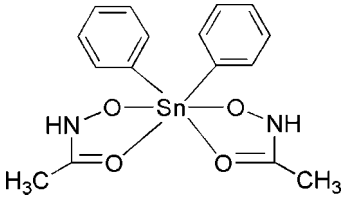
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.030; wR factor = 0.077; data-to-parameter ratio = 14.5.

The complex molecule of the title compound, $[Sn(C_6H_5)_2(C_2H_4NO_2)_2]$, has crystallographically imposed twofold symmetry. The Sn atom is coordinated by four O atoms from two acetohydroxamate ligands and by two C atoms from phenyl groups in a distorted octahedral geometry. In the crystal, molecules are connected by N—H···O hydrogen-bonding interactions, forming a chain structure along the c axis

Related literature

For the biological activity of diorganotin(IV) complexes with hydroxamates, see: Shang *et al.* (2007). For a related structure, see: Harrison *et al.* (1976). For van der Waals radii, see: Bondi (1964).



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_2H_4NO_2)_2]$ M_r = 421.01
Monoclinic, $C2/c$
a = 18.7713 (17) Å
b = 10.2683 (8) Å
c = 9.8326 (6) Å
β = 112.842 (1)°
V = 1746.6 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.48 mm^{-1}
T = 298 K
0.38 × 0.33 × 0.19 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.603, T_{max} = 0.766
4295 measured reflections
1542 independent reflections
1367 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.077
S = 1.00
1542 reflections
106 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.86	2.03	2.847 (4)	159

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2612).

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supplementary materials

Acta Cryst. (2011). E**67**, m1034 [**doi:10.1107/S160053681102558X**]

Bis(acetohydroxamato-κ^2O,O')diphenyltin(IV)

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Comment

Among many multidentate organic ligands, hydroxamic acids are of particular importance, because of their remarkable structural diversity and biological applications (Shang *et al.* , 2007). As a continuation of our interest in this area, we have synthesized the title compound and report its crystal structure herein.

The molecular structure of the compound is depicted in Fig. 1. The complex molecule has crystallographically imposed two-fold symmetry. The tin atom is six-coordinated in a distorted octahedral geometry. The Sn–O bond distances (Sn1–O2 = 2.103 (2) Å; Sn1–O = 2.275 (3) Å) are close to the sum of the covalent radii (2.13 Å; Bondi, 1964), and the Sn–C distance (Sn1–C3 = 2.147 (4) Å) are in the range observed in a related compound (2.14–2.18 Å; Harrison *et al.*, 1976). In the crystal packing, the molecules are linked by N—H···O hydrogen bonds (Table 1) into a one-dimensional chains parallel to the *c* axis (Fig. 2).

Experimental

The reaction was carried out under nitrogen atmosphere. Acetohydroxamic acid (0.4 mmol) and KOH (0.4 mmol) in methanol (30 ml) were added to a Schlenk flask and stirred for 30 min. Diphenyltin dichloride (0.2 mmol) was then added to the reactor. The reaction mixture was stirred for 8 h at room temperature and then filtrated. The filtrate was evaporated *in vacuo* to dryness. The obtained solid was recrystallized from a dichloromethane-petroleum ether (3:1 *v*/*v*) solution (yield 86%; m. p. 431 K). Anal. Calcd (%) for $C_{16}H_{18}N_2O_4Sn$ (Mr = 421.01): C, 45.64; H, 4.31; N, 6.65; O, 15.20. Found (%): C, 45.60; H, 4.25; N, 6.62; O,15.16.

Refinement

All H atoms were positioned with idealized geometry (C—H = 0.83-0.96 Å; N—H = 0.86 Å) and were refined isotropically with U_{iso}(H) = 1.2 U_{eq}(C, N) or 1.5 U_{eq}(C) for methyl H atoms.

Figures

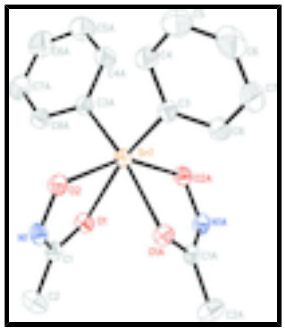


Fig. 1. The molecular structure of the compound, showing 50% probability displacement ellipsoids. H atoms are omitted for clarity. Symmetry code: (A) = -x, y, -z + 1/2.

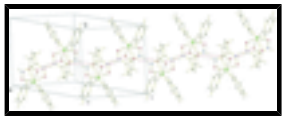


Fig. 2. View of the one-dimensional linear chain structure in the title compound.

Bis(acetohydroxamato-κ^2*O*,*O*')diphenyltin(IV)

Crystal data

$[Sn(C_6H_5)_2(C_2H_4NO_2)_2]$	$F(000) = 840$
$M_r = 421.01$	$D_x = 1.601$ Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation, λ = 0.71073 Å
Hall symbol: -C 2yc	Cell parameters from 2602 reflections
a = 18.7713 (17) Å	θ = 2.3–26.2°
b = 10.2683 (8) Å	μ = 1.48 mm^{-1}
c = 9.8326 (6) Å	*T* = 298 K
β = 112.842 (1)°	Block, colourless
V = 1746.6 (2) Å^3	0.38 × 0.33 × 0.19 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	1542 independent reflections
Radiation source: fine-focus sealed tube	1367 reflections with $I > 2\sigma(I)$
graphite	$R_{int} = 0.048$
phi and ω scans	$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$h = -22 \rightarrow 14$
$T_{min} = 0.603$, $T_{max} = 0.766$	$k = -12 \rightarrow 11$
4295 measured reflections	$l = -11 \rightarrow 11$

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.030$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.077$	H-atom parameters constrained
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 6.1631P]$ where $P = (F_o^2 + 2F_c^2)/3$
1542 reflections	$(\Delta/\sigma)_{max} < 0.001$
106 parameters	$\Delta\rho_{max} = 0.72$ e Å^{-3}
0 restraints	$\Delta\rho_{min} = -0.94$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.0000	0.27983 (4)	0.2500	0.03426 (15)
O1	−0.07784 (14)	0.4550 (3)	0.2287 (3)	0.0377 (6)
O2	−0.04374 (15)	0.3345 (3)	0.0264 (3)	0.0399 (6)
N1	−0.07653 (16)	0.4552 (3)	0.0036 (3)	0.0371 (7)
H1	−0.0874	0.4929	−0.0802	0.045*
C1	−0.0919 (2)	0.5148 (4)	0.1067 (4)	0.0356 (8)
C2	−0.1242 (3)	0.6484 (5)	0.0813 (5)	0.0599 (12)
H2A	−0.1762	0.6467	0.0766	0.090*
H2B	−0.1241	0.6812	−0.0101	0.090*
H2C	−0.0932	0.7039	0.1608	0.090*
C3	0.0918 (2)	0.1575 (4)	0.2454 (4)	0.0393 (9)
C4	0.0752 (3)	0.0355 (5)	0.1751 (5)	0.0591 (12)
H4	0.0244	0.0061	0.1339	0.071*
C5	0.1343 (4)	−0.0411 (6)	0.1669 (7)	0.0833 (19)
H5	0.1228	−0.1216	0.1200	0.100*
C6	0.2094 (3)	0.0010 (7)	0.2273 (7)	0.0827 (18)
H6	0.2485	−0.0494	0.2182	0.099*
C7	0.2269 (3)	0.1177 (6)	0.3013 (6)	0.0710 (15)
H7	0.2781	0.1450	0.3452	0.085*
C8	0.1685 (2)	0.1946 (5)	0.3103 (5)	0.0506 (11)
H8	0.1811	0.2731	0.3612	0.061*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0343 (2)	0.0369 (2)	0.0340 (2)	0.000	0.01590 (15)	0.000
O1	0.0429 (14)	0.0422 (16)	0.0321 (13)	0.0038 (12)	0.0190 (11)	0.0018 (11)
O2	0.0462 (15)	0.0414 (16)	0.0324 (13)	−0.0006 (13)	0.0158 (11)	−0.0028 (12)
N1	0.0322 (16)	0.049 (2)	0.0299 (16)	−0.0002 (14)	0.0117 (13)	0.0062 (14)
C1	0.0300 (18)	0.043 (2)	0.0332 (19)	−0.0028 (16)	0.0122 (15)	0.0030 (16)
C2	0.073 (3)	0.055 (3)	0.061 (3)	0.019 (3)	0.036 (2)	0.015 (2)
C3	0.040 (2)	0.043 (2)	0.0341 (19)	0.0034 (18)	0.0137 (16)	−0.0027 (17)
C4	0.057 (3)	0.051 (3)	0.061 (3)	0.003 (2)	0.014 (2)	−0.017 (2)
C5	0.089 (4)	0.069 (4)	0.087 (4)	0.020 (3)	0.029 (3)	−0.031 (3)
C6	0.068 (4)	0.091 (5)	0.091 (4)	0.033 (3)	0.034 (3)	−0.012 (4)
C7	0.043 (3)	0.080 (4)	0.087 (4)	0.014 (3)	0.022 (2)	0.002 (3)
C8	0.042 (2)	0.046 (3)	0.063 (3)	0.0045 (19)	0.019 (2)	−0.003 (2)

Geometric parameters (Å, °)

Sn1—O2^{i}	2.103 (2)	C2—H2C	0.9600
Sn1—O2	2.103 (2)	C3—C8	1.383 (6)
Sn1—C3^{i}	2.147 (4)	C3—C4	1.406 (6)
Sn1—C3	2.147 (4)	C4—C5	1.388 (7)

Sn1—O1^{i}	2.275 (3)	C4—H4	0.9300
Sn1—O1	2.275 (3)	C5—C6	1.371 (9)
O1—C1	1.281 (4)	C5—H5	0.9300
O2—N1	1.363 (4)	C6—C7	1.374 (8)
N1—C1	1.308 (5)	C6—H6	0.9300
N1—H1	0.8600	C7—C8	1.381 (7)
C1—C2	1.482 (6)	C7—H7	0.9300
C2—H2A	0.9600	C8—H8	0.9300
C2—H2B	0.9600		
O2^{i}—Sn1—O2	149.02 (16)	C1—C2—H2B	109.5
O2^{i}—Sn1—C3^{i}	97.18 (12)	H2A—C2—H2B	109.5
O2—Sn1—C3^{i}	100.81 (12)	C1—C2—H2C	109.5
O2^{i}—Sn1—C3	100.81 (12)	H2A—C2—H2C	109.5
O2—Sn1—C3	97.18 (12)	H2B—C2—H2C	109.5
C3^{i}—Sn1—C3	108.4 (2)	C8—C3—C4	117.7 (4)
O2^{i}—Sn1—O1^{i}	73.53 (10)	C8—C3—Sn1	122.0 (3)
O2—Sn1—O1^{i}	82.02 (10)	C4—C3—Sn1	120.3 (3)
C3^{i}—Sn1—O1^{i}	162.29 (13)	C5—C4—C3	120.2 (5)
C3—Sn1—O1^{i}	88.41 (13)	C5—C4—H4	119.9
O2^{i}—Sn1—O1	82.02 (10)	C3—C4—H4	119.9
O2—Sn1—O1	73.53 (10)	C6—C5—C4	120.5 (5)
C3^{i}—Sn1—O1	88.41 (13)	C6—C5—H5	119.7
C3—Sn1—O1	162.29 (13)	C4—C5—H5	119.7
O1^{i}—Sn1—O1	75.54 (13)	C5—C6—C7	119.9 (5)
C1—O1—Sn1	110.9 (2)	C5—C6—H6	120.1
N1—O2—Sn1	112.5 (2)	C7—C6—H6	120.1
C1—N1—O2	121.3 (3)	C6—C7—C8	120.0 (5)
C1—N1—H1	119.4	C6—C7—H7	120.0
O2—N1—H1	119.4	C8—C7—H7	120.0
O1—C1—N1	118.3 (4)	C7—C8—C3	121.5 (5)
O1—C1—C2	121.6 (4)	C7—C8—H8	119.2
N1—C1—C2	120.1 (3)	C3—C8—H8	119.2
C1—C2—H2A	109.5		
O2^{i}—Sn1—O1—C1	144.7 (2)	C3^{i}—Sn1—C3—C8	−148.3 (4)
O2—Sn1—O1—C1	−16.0 (2)	O1^{i}—Sn1—C3—C8	26.0 (4)
C3^{i}—Sn1—O1—C1	−117.8 (3)	O1—Sn1—C3—C8	50.8 (6)
C3—Sn1—O1—C1	44.1 (5)	O2^{i}—Sn1—C3—C4	133.1 (4)
O1^{i}—Sn1—O1—C1	69.8 (2)	O2—Sn1—C3—C4	−72.2 (4)
O2^{i}—Sn1—O2—N1	−24.99 (19)	C3^{i}—Sn1—C3—C4	31.7 (3)
C3^{i}—Sn1—O2—N1	99.4 (2)	O1^{i}—Sn1—C3—C4	−154.0 (4)
C3—Sn1—O2—N1	−150.2 (2)	O1—Sn1—C3—C4	−129.2 (4)
O1^{i}—Sn1—O2—N1	−62.9 (2)	C8—C3—C4—C5	−2.7 (7)
O1—Sn1—O2—N1	14.3 (2)	Sn1—C3—C4—C5	177.3 (4)
Sn1—O2—N1—C1	−12.8 (4)	C3—C4—C5—C6	0.1 (9)

Sn1—O1—C1—N1	15.1 (4)	C4—C5—C6—C7	2.3 (10)
Sn1—O1—C1—C2	−164.6 (3)	C5—C6—C7—C8	−2.2 (10)
O2—N1—C1—O1	−2.5 (5)	C6—C7—C8—C3	−0.4 (9)
O2—N1—C1—C2	177.2 (3)	C4—C3—C8—C7	2.8 (7)
O2^{i}—Sn1—C3—C8	−46.9 (4)	Sn1—C3—C8—C7	−177.2 (4)
O2—Sn1—C3—C8	107.8 (4)		

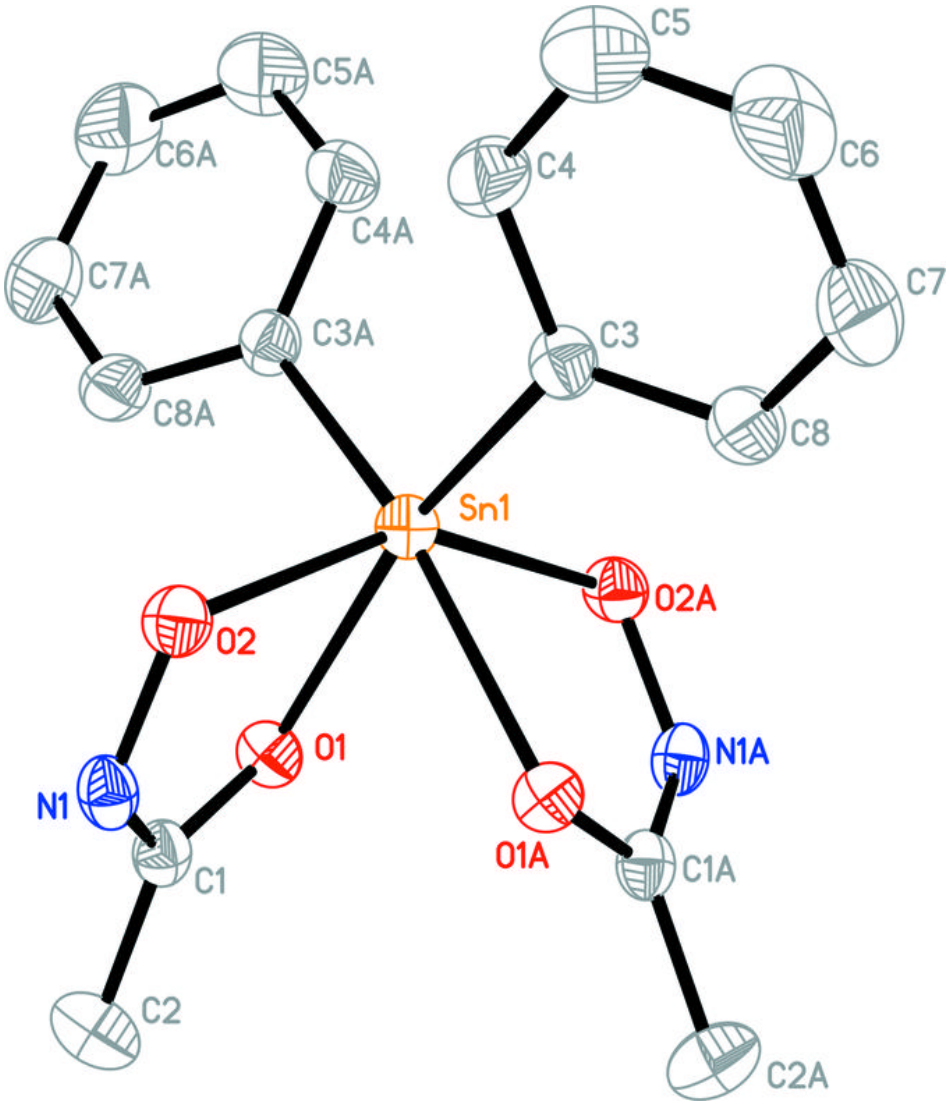
Symmetry codes: (i) −*x*, *y*, −*z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{ii}	0.86	2.03	2.847 (4)	159

Symmetry codes: (ii) *x*, −*y*+1, *z*−1/2.

Fig. 1


C5
C5A
C6A
C6
C4
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C7A
C7
C3A
C3
C8A
C8
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O2
O1
N1A
N1
O1A
C1A
C1
C2
C2A

Fig. 2