Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

{4-Amino-*N*′-[(2-oxidonaphthalen-1-yl)-methylidene]benzohydrazidato}dimethyltin(IV)

Miao Cheng, Yuhong Zhao, Tiantian Dong and Jichun Cui*

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: jchcui@163.com

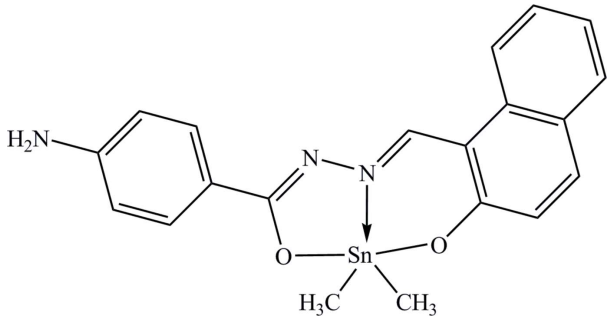
Received 10 June 2014; accepted 21 June 2014

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.009 Å; R factor = 0.052; wR factor = 0.121; data-to-parameter ratio = 13.8.

In the title compound, $[Sn(CH_3)_2(C_{18}H_{13}N_3O_2)]$, the Sn^{IV} ion is coordinated by one N and two O atoms from the tridentate 4-amino-*N*′-[(2-oxidonaphthalen-1-yl)methylidene]benzohydrazidate(2−) ligand and two C atoms from methyl ligands in a distorted trigonal–bipyramidal geometry. The dihedral angle between the naphthalene ring system and the benzene ring is 19.2 (2)°. In the crystal, weak N—H···O hydrogen bonds link the molecules into zigzag chains along [010].

Related literature

For the biological activity of organotin compounds, see: Hong *et al.* (2013). For a related crystal structure, see: Cui *et al.* (2013).



Experimental

Crystal data

$[Sn(CH_3)_2(C_{18}H_{13}N_3O_2)]$
M_r = 452.07
Orthorhombic, *Pbca*
a = 8.3545 (7) Å
b = 12.9503 (11) Å
c = 34.291 (2) Å
V = 3710.1 (5) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.40 mm^{-1}
T = 293 K
0.35 × 0.20 × 0.15 mm

Data collection

Bruker SMART 1000 diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.641, T_{max} = 0.818
8234 measured reflections
3265 independent reflections
2382 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.121
S = 1.14
3265 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −1.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{i}	0.86	2.46	3.245 (7)	152

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

We acknowledge the Students Science and Technology Innovation Fund of Liaocheng University (SF2012053).

Supporting information for this paper is available from the IUCr electronic archives (Reference: CV5466).

References

Bruker (2007). *SMART*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Cui, J., Qiao, Y. & Wang, F. (2013). *Acta Cryst.* E**69**, m688.
Hong, M., Yin, H., Zhang, X., Li, C., Yue, C. & Cheng, S. (2013). *J. Organomet. Chem.* **724**, 23–31.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2014). E**70**, m283 [https://doi.org/10.1107/S1600536814014652]

{4-Amino-*N*′-[(2-oxidonaphthalen-1-yl)methylidene]benzohydrazidato}dimethyltin(IV)

Miao Cheng, Yuhong Zhao, Tiantian Dong and Jichun Cui

S1. Comment

The chemistry of organotin(IV) derivatives is a subject of study with growing interest due to their significant antimicrobial properties as well as antitumor activities (Hong *et al.*, 2013). As a part of our ongoing investigations in this field (Cui *et al.*, 2013) we have synthesized the title compound, (I), and present its crystal structure here.

In (I) (Fig. 1), the Sn^{IV} ion has distorted trigonal-bipyramidal coordination geometry, with atoms O1 and O2 in axial positions [O1—Sn1—O3 = 154.81 (18) °] and the atoms C19, C20 and N2 in equatorial positions. This coordination geometry is similar to that observed in the related compound {4-chloro-N′-[(2-oxidonaphthalen-1-yl*κ*O) methylidene]benzohydrazidato-κ^2N′,O}dimethyltin(IV) (Cui *et al.*, 2013).

In the crystal, weak intermolecular N—H···O hydrogen bonds (Table 1) link molecules into zigzag chains in [010].

S2. Experimental

[4-Azyl-N′-(2-hydroxy-1-naphthaldehyde)benzohydrazide (1 mmol) and sodium ethoxide (2 mmol) were added to the solution of dry methanol(30 ml) and stirred for 10 min. Dimethyltin(IV) dichloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 4 h. The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/ethanol(1:1) to yield orange blocks of the title compound (yield 86%).

S3. Refinement

The H atoms were fixed geometrically and treated as riding atoms: N—H = 0.86 Å, with U_{iso}(H) = 1.2 U_{eq}(N), and C—H = 0.93 - 0.97 Å, with U_{iso}(H) = 1.2 or 1.5 U_{eq}(C)

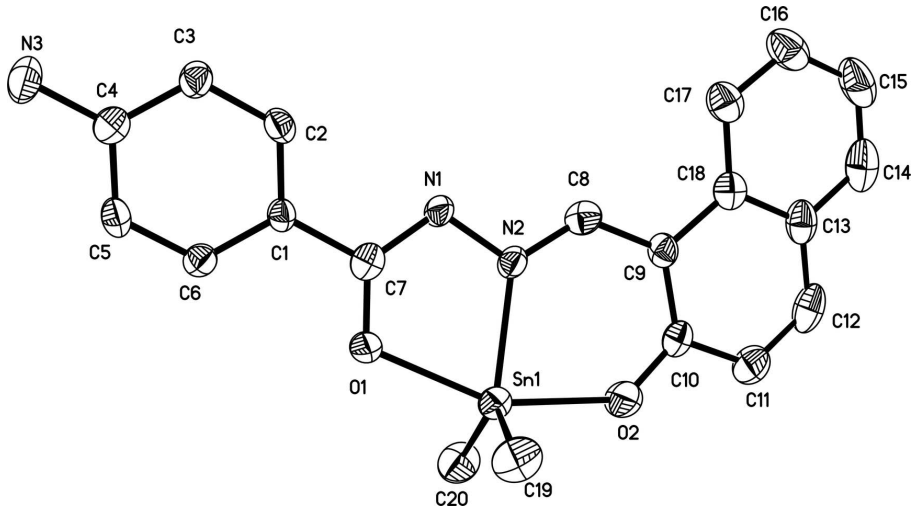


Figure 1

The molecular strucure of (I) showing showing the atomic numbering and 40% probability displacement ellipsoids. H atoms omitted for clarity.

{4-Amino-*N*′-[(2-oxidonaphthalen-1-yl)methylidene]benzohydrazidato}dimethyltin(IV)

Crystal data

$[Sn(CH_3)_2(C_{18}H_{13}N_3O_2)]$
$M_r = 452.07$
Orthorhombic, *Pbca*
$a = 8.3545$ (7) Å
$b = 12.9503$ (11) Å
$c = 34.291$ (2) Å
$V = 3710.1$ (5) Å^3
$Z = 8$
$F(000) = 1808$
$D_x = 1.619$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1667 reflections
$\theta = 2.7$–$28.4°$
$\mu = 1.40$ mm^{-1}
$T = 293$ K
Block, orange
0.35 × 0.20 × 0.15 mm

Data collection

Bruker SMART 1000 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
$T_{min} = 0.641$, $T_{max} = 0.818$
8234 measured reflections
3265 independent reflections
2382 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -9\rightarrow4$
$k = -8\rightarrow15$
$l = -33\rightarrow40$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.121$
$S = 1.14$
3265 reflections
237 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 1.7722P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -1.27$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.22653 (5)	0.82846 (3)	0.350360 (13)	0.03635 (18)
C1	0.6096 (7)	1.0398 (4)	0.31885 (17)	0.0282 (13)
C2	0.6565 (7)	1.1338 (4)	0.33421 (18)	0.0333 (14)
H2	0.6144	1.1553	0.3580	0.040*
C3	0.7651 (7)	1.1966 (5)	0.3149 (2)	0.0357 (16)
H3	0.7940	1.2599	0.3256	0.043*
C4	0.8311 (7)	1.1654 (5)	0.27934 (19)	0.0346 (14)
C5	0.7822 (7)	1.0706 (5)	0.26347 (19)	0.0361 (15)
H5	0.8241	1.0488	0.2397	0.043*
C6	0.6718 (7)	1.0092 (4)	0.28297 (18)	0.0326 (14)
H6	0.6391	0.9471	0.2720	0.039*
C7	0.4895 (7)	0.9742 (5)	0.33911 (19)	0.0337 (15)
C8	0.3081 (8)	0.9472 (4)	0.4283 (2)	0.0358 (15)
H8	0.3624	1.0011	0.4404	0.043*
C9	0.1988 (7)	0.8916 (5)	0.45182 (18)	0.0331 (15)
C10	0.1039 (7)	0.8101 (4)	0.43669 (19)	0.0365 (15)
C18	0.1849 (7)	0.9175 (5)	0.4931 (2)	0.0366 (15)
C11	0.0086 (9)	0.7509 (5)	0.4619 (2)	0.052 (2)
H11	−0.0513	0.6962	0.4521	0.062*
C12	0.0036 (9)	0.7732 (6)	0.5005 (2)	0.057 (2)
H12	−0.0591	0.7321	0.5167	0.069*
C13	0.0892 (8)	0.8557 (5)	0.5173 (2)	0.0456 (18)
C14	0.0800 (10)	0.8798 (7)	0.5574 (2)	0.065 (2)
H14	0.0174	0.8382	0.5734	0.078*
C15	0.1576 (10)	0.9600 (7)	0.5734 (2)	0.067 (2)
H15	0.1495	0.9737	0.5999	0.081*
C16	0.2504 (9)	1.0222 (7)	0.5491 (2)	0.058 (2)
H16	0.3037	1.0788	0.5596	0.070*
C17	0.2644 (8)	1.0012 (6)	0.5102 (2)	0.0485 (19)
H17	0.3282	1.0435	0.4948	0.058*
C19	0.0383 (9)	0.9080 (5)	0.3224 (2)	0.057 (2)
H19A	−0.0545	0.9080	0.3389	0.085*
H19B	0.0132	0.8742	0.2982	0.085*
H19C	0.0705	0.9778	0.3173	0.085*
C20	0.3138 (9)	0.6763 (5)	0.3414 (2)	0.056 (2)
H20A	0.2512	0.6286	0.3564	0.084*
H20B	0.4237	0.6726	0.3495	0.084*
H20C	0.3059	0.6590	0.3142	0.084*
N1	0.4605 (6)	0.9964 (3)	0.37632 (14)	0.0331 (12)
N2	0.3417 (6)	0.9318 (3)	0.39137 (15)	0.0323 (12)
N3	0.9344 (7)	1.2295 (4)	0.25953 (17)	0.0493 (15)
H3A	0.9585	1.2890	0.2690	0.059*
H3B	0.9749	1.2101	0.2377	0.059*
O1	0.4219 (5)	0.9000 (3)	0.31939 (12)	0.0393 (11)
O2	0.0996 (6)	0.7846 (4)	0.39985 (14)	0.0609 (15)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0369 (3)	0.0357 (3)	0.0364 (3)	−0.00536 (19)	0.0007 (2)	−0.0002 (2)
C1	0.029 (3)	0.032 (3)	0.023 (3)	0.000 (3)	0.002 (3)	0.004 (3)
C2	0.032 (3)	0.040 (3)	0.027 (3)	0.003 (3)	0.004 (3)	−0.005 (3)
C3	0.041 (3)	0.030 (3)	0.036 (4)	−0.002 (3)	0.007 (3)	0.003 (3)
C4	0.024 (3)	0.039 (3)	0.041 (4)	0.004 (3)	−0.002 (3)	0.002 (3)
C5	0.034 (3)	0.048 (4)	0.026 (3)	0.003 (3)	0.004 (3)	0.004 (3)
C6	0.032 (3)	0.033 (3)	0.033 (4)	−0.002 (3)	−0.003 (3)	0.003 (3)
C7	0.026 (3)	0.035 (3)	0.040 (4)	0.007 (3)	−0.002 (3)	0.006 (3)
C8	0.043 (3)	0.027 (3)	0.037 (4)	−0.004 (3)	−0.003 (3)	0.009 (3)
C9	0.036 (3)	0.039 (3)	0.024 (3)	−0.001 (3)	0.001 (3)	0.007 (3)
C10	0.032 (3)	0.039 (3)	0.039 (4)	−0.003 (3)	0.005 (3)	0.007 (3)
C18	0.033 (3)	0.038 (4)	0.038 (4)	0.009 (3)	−0.001 (3)	0.006 (3)
C11	0.054 (4)	0.043 (4)	0.057 (6)	−0.014 (4)	0.008 (4)	0.005 (4)
C12	0.048 (4)	0.064 (5)	0.060 (6)	−0.006 (4)	0.018 (4)	0.026 (4)
C13	0.039 (4)	0.062 (5)	0.036 (4)	0.009 (3)	0.005 (4)	0.013 (4)
C14	0.053 (5)	0.086 (6)	0.055 (6)	0.010 (5)	0.017 (5)	0.018 (5)
C15	0.073 (6)	0.097 (7)	0.032 (4)	0.015 (5)	0.006 (5)	−0.005 (5)
C16	0.059 (5)	0.071 (5)	0.044 (5)	0.014 (4)	−0.010 (4)	−0.013 (4)
C17	0.052 (4)	0.054 (4)	0.039 (4)	0.005 (3)	0.001 (4)	0.000 (4)
C19	0.053 (4)	0.052 (4)	0.066 (5)	0.001 (4)	−0.010 (4)	0.007 (4)
C20	0.055 (4)	0.038 (4)	0.075 (6)	0.002 (4)	0.005 (4)	−0.004 (4)
N1	0.035 (3)	0.041 (3)	0.023 (3)	−0.013 (2)	0.000 (3)	0.005 (2)
N2	0.030 (3)	0.037 (3)	0.030 (3)	−0.007 (2)	0.002 (3)	0.004 (2)
N3	0.050 (3)	0.043 (3)	0.054 (4)	−0.004 (3)	0.020 (3)	0.006 (3)
O1	0.048 (2)	0.037 (2)	0.033 (3)	−0.014 (2)	0.006 (2)	−0.005 (2)
O2	0.075 (4)	0.065 (3)	0.043 (3)	−0.039 (3)	0.012 (3)	−0.001 (3)

Geometric parameters (Å, º)

Sn1—O2	2.080 (5)	C10—C11	1.403 (9)
Sn1—C19	2.110 (7)	C18—C17	1.401 (9)
Sn1—C20	2.123 (6)	C18—C13	1.402 (9)
Sn1—O1	2.157 (4)	C11—C12	1.356 (10)
Sn1—N2	2.167 (5)	C11—H11	0.9300
C1—C2	1.383 (8)	C12—C13	1.409 (10)
C1—C6	1.393 (8)	C12—H12	0.9300
C1—C7	1.487 (8)	C13—C14	1.412 (10)
C2—C3	1.388 (8)	C14—C15	1.342 (11)
C2—H2	0.9300	C14—H14	0.9300
C3—C4	1.397 (9)	C15—C16	1.394 (11)
C3—H3	0.9300	C15—H15	0.9300
C4—N3	1.377 (8)	C16—C17	1.366 (10)
C4—C5	1.403 (8)	C16—H16	0.9300
C5—C6	1.389 (8)	C17—H17	0.9300
C5—H5	0.9300	C19—H19A	0.9600

C6—H6	0.9300	C19—H19B	0.9600
C7—O1	1.304 (7)	C19—H19C	0.9600
C7—N1	1.330 (8)	C20—H20A	0.9600
C8—N2	1.311 (8)	C20—H20B	0.9600
C8—C9	1.416 (8)	C20—H20C	0.9600
C8—H8	0.9300	N1—N2	1.397 (6)
C9—C10	1.418 (8)	N3—H3A	0.8600
C9—C18	1.458 (9)	N3—H3B	0.8600
C10—O2	1.306 (7)		

O2—Sn1—C19	97.1 (3)	C12—C11—C10	120.2 (7)
O2—Sn1—C20	92.3 (3)	C12—C11—H11	119.9
C19—Sn1—C20	130.0 (3)	C10—C11—H11	119.9
O2—Sn1—O1	154.81 (18)	C11—C12—C13	122.9 (7)
C19—Sn1—O1	97.5 (2)	C11—C12—H12	118.5
C20—Sn1—O1	93.9 (2)	C13—C12—H12	118.5
O2—Sn1—N2	82.28 (18)	C18—C13—C12	118.8 (7)
C19—Sn1—N2	108.9 (2)	C18—C13—C14	118.8 (7)
C20—Sn1—N2	121.0 (2)	C12—C13—C14	122.5 (7)
O1—Sn1—N2	73.63 (17)	C15—C14—C13	122.9 (8)
C2—C1—C6	118.8 (5)	C15—C14—H14	118.5
C2—C1—C7	121.0 (5)	C13—C14—H14	118.5
C6—C1—C7	120.1 (5)	C14—C15—C16	118.1 (7)
C1—C2—C3	121.3 (6)	C14—C15—H15	120.9
C1—C2—H2	119.4	C16—C15—H15	120.9
C3—C2—H2	119.4	C17—C16—C15	121.0 (8)
C2—C3—C4	120.3 (6)	C17—C16—H16	119.5
C2—C3—H3	119.8	C15—C16—H16	119.5
C4—C3—H3	119.8	C16—C17—C18	121.6 (8)
N3—C4—C3	120.2 (6)	C16—C17—H17	119.2
N3—C4—C5	121.2 (6)	C18—C17—H17	119.2
C3—C4—C5	118.5 (6)	Sn1—C19—H19A	109.5
C6—C5—C4	120.4 (6)	Sn1—C19—H19B	109.5
C6—C5—H5	119.8	H19A—C19—H19B	109.5
C4—C5—H5	119.8	Sn1—C19—H19C	109.5
C5—C6—C1	120.7 (6)	H19A—C19—H19C	109.5
C5—C6—H6	119.7	H19B—C19—H19C	109.5
C1—C6—H6	119.7	Sn1—C20—H20A	109.5
O1—C7—N1	125.3 (5)	Sn1—C20—H20B	109.5
O1—C7—C1	118.1 (5)	H20A—C20—H20B	109.5
N1—C7—C1	116.6 (5)	Sn1—C20—H20C	109.5
N2—C8—C9	127.7 (6)	H20A—C20—H20C	109.5
N2—C8—H8	116.2	H20B—C20—H20C	109.5
C9—C8—H8	116.2	C7—N1—N2	110.8 (5)
C8—C9—C10	122.0 (6)	C8—N2—N1	114.7 (5)
C8—C9—C18	119.2 (6)	C8—N2—Sn1	128.7 (4)
C10—C9—C18	118.8 (6)	N1—N2—Sn1	116.5 (4)
O2—C10—C11	116.2 (6)	C4—N3—H3A	120.0

O2—C10—C9	123.9 (6)	C4—N3—H3B	120.0
C11—C10—C9	119.9 (6)	H3A—N3—H3B	120.0
C17—C18—C13	117.6 (7)	C7—O1—Sn1	112.9 (4)
C17—C18—C9	123.2 (6)	C10—O2—Sn1	134.9 (4)
C13—C18—C9	119.2 (6)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1^{i}	0.86	2.46	3.245 (7)	152

Symmetry code: (i) −*x*+3/2, *y*+1/2, *z*.