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Bis(μ-quinolin-8-olato)-$\kappa^3N,O:O$;-$\kappa^3O:N,O$-bis[chloridomethylphenyltin(IV)]

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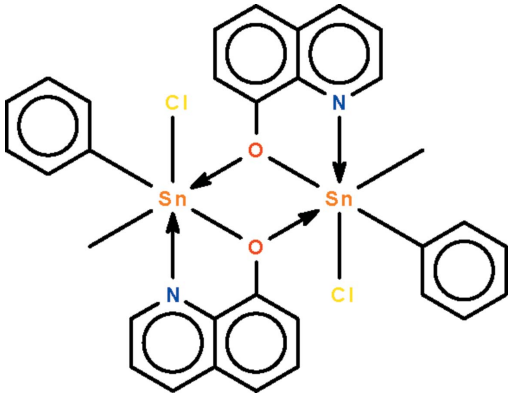
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.018; wR factor = 0.047; data-to-parameter ratio = 17.8.

The Sn^{IV} atom in the centrosymmetric dinuclear title compound, $[Sn_2(CH_3)_2(C_6H_5)_2(C_9H_6NO)_2Cl_2]$, shows a *trans*-$C_2SnNO_2Cl$ distorted octahedral coordination [C–Sn–C = 157.83 (8)°]. The quinolin-8-olate anion chelates to the Sn atom; its O atom also binds to the inversion-related Sn atom, forming the dinuclear compound. In the crystal structure, weak intermolecular C—H···Cl hydrogen bonding links the molecules, forming supramolecular chains running along [100].

Related literature

For related structures, see: Ng *et al.* (1989); Shi & Hu (1987).



Experimental

Crystal data

$[Sn_2(CH_3)_2(C_6H_5)_2(C_9H_6NO)_2Cl_2]$
M_r = 780.84
Monoclinic, $P2_1/c$
a = 7.9967 (5) Å
b = 17.8081 (10) Å
c = 10.1623 (6) Å
β = 95.232 (1)°
V = 1441.14 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.95 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.592, T_{max} = 0.829
9127 measured reflections
3245 independent reflections
3088 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.047
S = 1.09
3245 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.52 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···Cl1^{i}	0.95	2.76	3.710 (2)	174

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU2799).

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supporting information

Acta Cryst. (2010). E**66**, m964 [https://doi.org/10.1107/S1600536810027765]

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S1. Comment

The anion of 8-hydroxyquinoline is known to chelate to tin in organotin(IV) quinolinolates; however, for the chloro-organotin quinolinates, the chlorine atom sometimes participates in weak intermolecular bridging. In chloridoodiethyl-(quinolin-8-olato)tin, the carbon–tin–carbon angle is opened to 140.9 (3) ° owing to a tin···chlorine contact of 3.690 (2) Å (Shi & Hu, 1987). With the bis(2-carbomethoxyethyl) analog, the tin atom is six-coordinate owing to an intramolecular bond with the oxygen atom of the organo radical (Ng *et al.*, 1989). The chloridomethylphenyltin analog exists as a centrosymmetric dimer in which the quinolin-8-olate anion *N*,*O*-chelates to the tin atom (Fig. 1). However, its oxygen atom also binds to the inversion-related tin atom so that bridging by the chlorine atom is precluded for the *trans*-C_2SnNO_2Cl octahedral dinuclear molecule. Intermolecular weak C—H···Cl hydrogen bonding links the molecules to form the one dimensional supra-molecular chain in the crystal structure (Table 1).

S2. Experimental

Methylphenyltin dichloride (0.35 g, 1 mmol) and 8-hydroxyquinoline (0.15 g, 1 mmol) were dissolved in methanol (10 ml) to give a faint yellow solution. The solution was set aside for the growth of crystals over a few days. Slow evaporation of methanol furnished crystals.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.95–0.98 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U_{eq}(C).

The final difference Fourier map had a peak in the vicinity of Sn1.

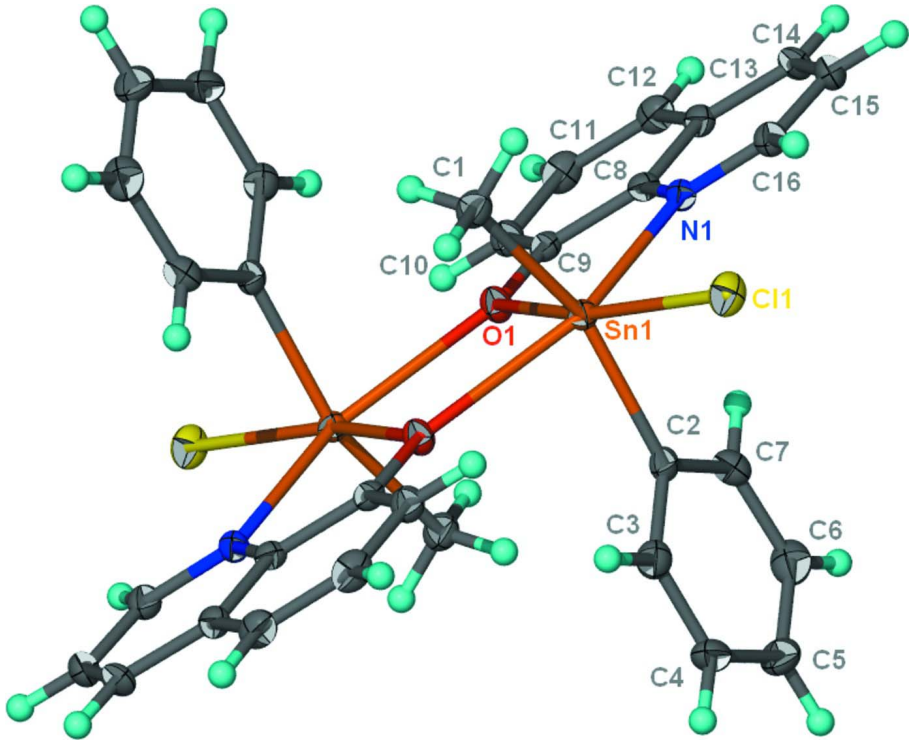

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $[SnCl(CH_3)(C_6H_5)(C_9H_6NO)]_2$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

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Crystal data

$[Sn_2(CH_3)_2(C_6H_5)_2(C_9H_6NO)_2Cl_2]$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.9967\ (5)$ Å
$b = 17.8081\ (10)$ Å
$c = 10.1623\ (6)$ Å
$\beta = 95.232\ (1)°$
$V = 1441.14\ (15)$ Å^3
$Z = 2$
$F(000) = 768$
$D_x = 1.799$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 6739 reflections
$\theta = 2.3–28.3°$
$\mu = 1.95$ mm^{-1}
$T = 100$ K
Block, yellow
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.592$, $T_{max} = 0.829$
9127 measured reflections
3245 independent reflections
3088 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -10\rightarrow6$
$k = -23\rightarrow23$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.018$
$wR(F^2) = 0.047$
$S = 1.09$
3245 reflections
182 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
$w = 1/[\sigma^2(F_o^2) + (0.021P)^2 + 1.1915P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.43$ e Å^{-3}
$\Delta\rho_{min} = -0.52$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.569331 (15)	0.585876 (6)	0.601796 (12)	0.01090 (5)
Cl1	0.70000 (6)	0.71504 (2)	0.65698 (5)	0.01757 (10)
O1	0.42527 (16)	0.48265 (7)	0.60854 (13)	0.0135 (3)
N1	0.4714 (2)	0.58459 (8)	0.80183 (16)	0.0121 (3)
C1	0.8095 (2)	0.53633 (10)	0.6389 (2)	0.0167 (4)
H1A	0.7981	0.4816	0.6403	0.025*
H1B	0.8618	0.5536	0.7245	0.025*
H1C	0.8800	0.5508	0.5691	0.025*
C2	0.3678 (2)	0.64342 (9)	0.49452 (19)	0.0130 (4)
C3	0.3885 (3)	0.67691 (11)	0.3733 (2)	0.0169 (4)
H3	0.4928	0.6723	0.3361	0.020*
C4	0.2584 (3)	0.71696 (11)	0.3060 (2)	0.0195 (4)
H4	0.2734	0.7388	0.2226	0.023*
C5	0.1060 (3)	0.72510 (11)	0.3607 (2)	0.0207 (4)
H5	0.0176	0.7533	0.3156	0.025*
C6	0.0837 (3)	0.69195 (11)	0.4814 (2)	0.0206 (4)
H6	−0.0198	0.6975	0.5194	0.025*
C7	0.2136 (2)	0.65061 (10)	0.5464 (2)	0.0164 (4)
H7	0.1967	0.6268	0.6279	0.020*
C8	0.3633 (2)	0.52614 (10)	0.81865 (18)	0.0119 (3)
C9	0.3396 (2)	0.47262 (10)	0.71380 (18)	0.0124 (3)
C10	0.2317 (2)	0.41329 (10)	0.7296 (2)	0.0147 (4)
H10	0.2124	0.3772	0.6611	0.018*
C11	0.1502 (2)	0.40557 (10)	0.8459 (2)	0.0173 (4)
H11	0.0772	0.3641	0.8544	0.021*
C12	0.1735 (2)	0.45627 (10)	0.9470 (2)	0.0162 (4)
H12	0.1177	0.4497	1.0248	0.019*
C13	0.2812 (2)	0.51873 (10)	0.93531 (19)	0.0133 (4)
C14	0.3148 (3)	0.57403 (11)	1.0345 (2)	0.0160 (4)
H14	0.2616	0.5713	1.1142	0.019*
C15	0.4242 (2)	0.63159 (10)	1.0154 (2)	0.0165 (4)
H15	0.4471	0.6688	1.0816	0.020*
C16	0.5016 (2)	0.63503 (10)	0.89730 (19)	0.0146 (4)
H16	0.5781	0.6747	0.8851	0.018*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01182 (7)	0.01028 (7)	0.01071 (8)	0.00014 (4)	0.00166 (5)	0.00028 (4)
Cl1	0.0161 (2)	0.01251 (19)	0.0241 (3)	−0.00307 (15)	0.00144 (18)	−0.00177 (16)
O1	0.0167 (6)	0.0120 (6)	0.0123 (7)	−0.0016 (5)	0.0041 (5)	−0.0008 (5)
N1	0.0147 (8)	0.0107 (7)	0.0110 (8)	0.0009 (5)	0.0018 (6)	0.0001 (5)
C1	0.0155 (9)	0.0161 (8)	0.0185 (10)	0.0022 (7)	0.0006 (7)	−0.0006 (7)
C2	0.0149 (9)	0.0093 (7)	0.0144 (9)	−0.0004 (6)	−0.0006 (7)	−0.0027 (6)
C3	0.0181 (9)	0.0157 (8)	0.0170 (10)	0.0016 (7)	0.0027 (8)	−0.0005 (7)
C4	0.0269 (11)	0.0179 (9)	0.0133 (10)	0.0027 (8)	−0.0012 (8)	0.0020 (7)
C5	0.0206 (10)	0.0178 (9)	0.0221 (11)	0.0035 (7)	−0.0064 (8)	−0.0015 (8)
C6	0.0146 (9)	0.0228 (10)	0.0242 (11)	0.0002 (7)	0.0009 (8)	−0.0043 (8)
C7	0.0179 (9)	0.0182 (9)	0.0131 (10)	−0.0013 (7)	0.0014 (7)	−0.0010 (7)
C8	0.0128 (8)	0.0120 (8)	0.0107 (9)	0.0014 (6)	0.0005 (7)	0.0015 (6)
C9	0.0125 (8)	0.0125 (8)	0.0121 (9)	0.0027 (6)	0.0007 (7)	0.0012 (7)
C10	0.0154 (9)	0.0127 (8)	0.0159 (10)	−0.0003 (6)	0.0006 (7)	−0.0013 (7)
C11	0.0147 (9)	0.0143 (8)	0.0232 (11)	−0.0018 (7)	0.0030 (8)	0.0026 (7)
C12	0.0149 (9)	0.0178 (9)	0.0169 (10)	0.0018 (7)	0.0057 (7)	0.0032 (7)
C13	0.0135 (9)	0.0145 (8)	0.0122 (9)	0.0030 (6)	0.0019 (7)	0.0002 (7)
C14	0.0207 (10)	0.0196 (9)	0.0084 (9)	0.0042 (7)	0.0045 (7)	−0.0001 (7)
C15	0.0208 (10)	0.0157 (8)	0.0128 (10)	0.0035 (7)	−0.0001 (8)	−0.0033 (7)
C16	0.0155 (9)	0.0132 (8)	0.0148 (10)	0.0007 (7)	−0.0003 (7)	−0.0010 (7)

Geometric parameters (Å, º)

Sn1—C1	2.1162 (19)	C5—H5	0.9500
Sn1—C2	2.1248 (18)	C6—C7	1.390 (3)
Sn1—O1	2.1739 (13)	C6—H6	0.9500
Sn1—O1^{i}	2.4651 (13)	C7—H7	0.9500
Sn1—N1	2.2442 (16)	C8—C13	1.413 (3)
Sn1—Cl1	2.5672 (5)	C8—C9	1.429 (2)
O1—C9	1.334 (2)	C9—C10	1.383 (3)
O1—Sn1^{i}	2.4651 (13)	C10—C11	1.408 (3)
N1—C16	1.328 (2)	C10—H10	0.9500
N1—C8	1.373 (2)	C11—C12	1.367 (3)
C1—H1A	0.9800	C11—H11	0.9500
C1—H1B	0.9800	C12—C13	1.419 (3)
C1—H1C	0.9800	C12—H12	0.9500
C2—C3	1.392 (3)	C13—C14	1.417 (3)
C2—C7	1.391 (3)	C14—C15	1.373 (3)
C3—C4	1.388 (3)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.401 (3)
C4—C5	1.393 (3)	C15—H15	0.9500
C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.387 (3)		
C1—Sn1—C2	157.83 (8)	C6—C5—C4	119.75 (19)

C1—Sn1—O1	96.71 (6)	C6—C5—H5	120.1
C2—Sn1—O1	92.56 (6)	C4—C5—H5	120.1
C1—Sn1—N1	102.73 (7)	C5—C6—C7	119.69 (19)
C2—Sn1—N1	99.13 (7)	C5—C6—H6	120.2
O1—Sn1—N1	74.52 (5)	C7—C6—H6	120.2
C1—Sn1—O1^{i}	81.99 (6)	C2—C7—C6	121.21 (19)
C2—Sn1—O1^{i}	82.31 (6)	C2—C7—H7	119.4
O1—Sn1—O1^{i}	70.12 (5)	C6—C7—H7	119.4
N1—Sn1—O1^{i}	144.64 (5)	N1—C8—C13	121.40 (16)
C1—Sn1—Cl1	89.42 (5)	N1—C8—C9	117.06 (16)
C2—Sn1—Cl1	87.39 (5)	C13—C8—C9	121.54 (16)
O1—Sn1—Cl1	163.16 (4)	O1—C9—C10	124.56 (17)
N1—Sn1—Cl1	88.85 (4)	O1—C9—C8	117.74 (16)
O1^{i}—Sn1—Cl1	126.44 (3)	C10—C9—C8	117.69 (17)
C9—O1—Sn1	116.80 (11)	C9—C10—C11	120.93 (18)
C9—O1—Sn1^{i}	132.84 (11)	C9—C10—H10	119.5
Sn1—O1—Sn1^{i}	109.88 (5)	C11—C10—H10	119.5
C16—N1—C8	119.75 (17)	C12—C11—C10	121.63 (18)
C16—N1—Sn1	126.85 (13)	C12—C11—H11	119.2
C8—N1—Sn1	113.33 (12)	C10—C11—H11	119.2
Sn1—C1—H1A	109.5	C11—C12—C13	119.79 (18)
Sn1—C1—H1B	109.5	C11—C12—H12	120.1
H1A—C1—H1B	109.5	C13—C12—H12	120.1
Sn1—C1—H1C	109.5	C14—C13—C8	117.37 (17)
H1A—C1—H1C	109.5	C14—C13—C12	124.21 (18)
H1B—C1—H1C	109.5	C8—C13—C12	118.41 (17)
C3—C2—C7	118.50 (18)	C15—C14—C13	119.99 (18)
C3—C2—Sn1	121.01 (14)	C15—C14—H14	120.0
C7—C2—Sn1	120.46 (14)	C13—C14—H14	120.0
C2—C3—C4	120.78 (19)	C14—C15—C16	119.41 (18)
C2—C3—H3	119.6	C14—C15—H15	120.3
C4—C3—H3	119.6	C16—C15—H15	120.3
C5—C4—C3	120.03 (19)	N1—C16—C15	122.08 (17)
C5—C4—H4	120.0	N1—C16—H16	119.0
C3—C4—H4	120.0	C15—C16—H16	119.0

C1—Sn1—O1—C9	107.94 (13)	C3—C4—C5—C6	−1.1 (3)
C2—Sn1—O1—C9	−92.24 (13)	C4—C5—C6—C7	−0.2 (3)
N1—Sn1—O1—C9	6.53 (12)	C3—C2—C7—C6	−1.8 (3)
O1^{i}—Sn1—O1—C9	−173.12 (15)	Sn1—C2—C7—C6	176.04 (14)
Cl1—Sn1—O1—C9	−2.8 (2)	C5—C6—C7—C2	1.7 (3)
C1—Sn1—O1—Sn1^{i}	−78.95 (7)	C16—N1—C8—C13	0.7 (3)
C2—Sn1—O1—Sn1^{i}	80.88 (7)	Sn1—N1—C8—C13	−176.16 (13)
N1—Sn1—O1—Sn1^{i}	179.65 (7)	C16—N1—C8—C9	−178.36 (16)
O1^{i}—Sn1—O1—Sn1^{i}	0.0	Sn1—N1—C8—C9	4.7 (2)
Cl1—Sn1—O1—Sn1^{i}	170.35 (8)	Sn1—O1—C9—C10	174.90 (14)
C1—Sn1—N1—C16	83.99 (16)	Sn1^{i}—O1—C9—C10	3.7 (3)
C2—Sn1—N1—C16	−92.33 (16)	Sn1—O1—C9—C8	−6.4 (2)

O1—Sn1—N1—C16	177.53 (16)	Sn1^{i}—O1—C9—C8	−177.52 (11)
O1^{i}—Sn1—N1—C16	178.10 (13)	N1—C8—C9—O1	0.9 (2)
Cl1—Sn1—N1—C16	−5.16 (15)	C13—C8—C9—O1	−178.23 (16)
C1—Sn1—N1—C8	−99.37 (13)	N1—C8—C9—C10	179.70 (16)
C2—Sn1—N1—C8	84.31 (13)	C13—C8—C9—C10	0.6 (3)
O1—Sn1—N1—C8	−5.84 (12)	O1—C9—C10—C11	177.91 (17)
O1^{i}—Sn1—N1—C8	−5.27 (17)	C8—C9—C10—C11	−0.8 (3)
Cl1—Sn1—N1—C8	171.48 (12)	C9—C10—C11—C12	0.3 (3)
C1—Sn1—C2—C3	−8.7 (3)	C10—C11—C12—C13	0.4 (3)
O1—Sn1—C2—C3	−123.54 (15)	N1—C8—C13—C14	0.0 (3)
N1—Sn1—C2—C3	161.73 (14)	C9—C8—C13—C14	179.06 (17)
O1^{i}—Sn1—C2—C3	−53.99 (15)	N1—C8—C13—C12	−178.93 (16)
Cl1—Sn1—C2—C3	73.32 (14)	C9—C8—C13—C12	0.1 (3)
C1—Sn1—C2—C7	173.51 (16)	C11—C12—C13—C14	−179.50 (19)
O1—Sn1—C2—C7	58.69 (15)	C11—C12—C13—C8	−0.6 (3)
N1—Sn1—C2—C7	−16.04 (15)	C8—C13—C14—C15	−0.4 (3)
O1^{i}—Sn1—C2—C7	128.23 (15)	C12—C13—C14—C15	178.46 (18)
Cl1—Sn1—C2—C7	−104.46 (14)	C13—C14—C15—C16	0.1 (3)
C7—C2—C3—C4	0.4 (3)	C8—N1—C16—C15	−1.1 (3)
Sn1—C2—C3—C4	−177.45 (14)	Sn1—N1—C16—C15	175.35 (13)
C2—C3—C4—C5	1.1 (3)	C14—C15—C16—N1	0.7 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C6—H6···Cl1^{ii}	0.95	2.76	3.710 (2)	174

Symmetry code: (ii) *x*−1, *y*, *z*.