Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Chloridodimethyl(quinaldato)tin(IV)

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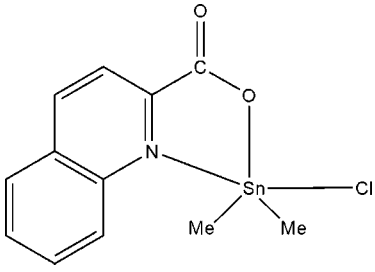
Received 9 November 2007; accepted 12 November 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.031; wR factor = 0.091; data-to-parameter ratio = 15.4.

The Sn atom in the title compound, $[Sn(CH_3)_2(C_{10}H_6NO_2)Cl]$, has a distorted SnC_2NOCl trigonal–bipyramidal geometry with the quinoline N atom and Cl atom occupying the axial sites.

Related literature

For related materials, see: Ma *et al.* (2004).



Experimental

Crystal data

$[Sn(CH_3)_2(C_{10}H_6NO_2)Cl]$
M_r = 356.37
Monoclinic, $P2_1/c$
a = 10.093 (10) Å
b = 10.245 (10) Å
c = 13.763 (7) Å
β = 107.811 (10)°
V = 1355 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.07 mm^{-1}
T = 298 (2) K
0.43 × 0.22 × 0.10 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.470, T_{max} = 0.820
6777 measured reflections
2370 independent reflections
1864 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.092
S = 1.00
2370 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—O1	2.040 (3)	Sn1—N1	2.390 (4)
Sn1—C11	2.098 (5)	Sn1—Cl1	2.448 (2)
Sn1—C12	2.109 (5)		

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*.

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

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2653).

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 doi:10.1107/S1600536807058229

supplementary materials

Acta Cryst. (2007). E**63**, m3059 [**doi:10.1107/S1600536807058229**]

Chloridodimethyl(quinaldato)tin(IV)

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Comment

Organotin esters of carboxylic acids are widely used as biocides, as fungicides and, in industry, as homogeneous catalysts. Studies on organotin complexes containing carboxylate ligands with an additional donor atom (*e.g.* N, O or S) that is available for coordinating to the Sn atom have revealed that new structural types may lead to different activities. We have therefore synthesized the title compound, (I), and present its crystal structure here.

The molecular structure of (I) is shown in Fig. 1. The Sn1 assumes a trigonal-bipyramidal coordination geometry (Table 1) with atoms N1 and Cl1 in axial positions [N1—Sn1—Cl1 = 156.47 (10) °] and the C atoms of the two methyl groups and the ligand Cl atom in equatorial positions. Associated with the sum of the angles subtended at the Sn1 in the equatorial plane is 358.7°, indicating approximate coplanarity for these atoms;. The Sn—O and Sn—N distnaces in (I) are close to those in related compounds (Ma *et al.*, 2004).

Experimental

The reaction was carried out under nitrogen atmosphere. Quinaldic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to benzene (30 ml) in a Schlenk flask and stirred for 0.5 h. Dimethyltin chloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 12 h at 313 K. The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/methanol (1:1 *v*/*v*) to yield colourless blocks of (I) (yield 85%; m.p. 422 K). Analysis calculated (%) for $C_{12}H_{12}ClNO_2Sn$ (Mr = 356.37): C, 40.44; H, 3.39; N, 3.93. found: C, 40.37; H, 3.42; N, 4.06.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

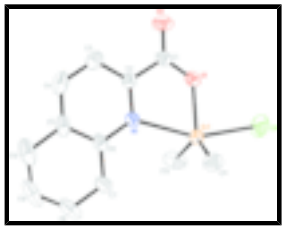

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

Chloridodimethyl(quinaldato)tin(IV)

Crystal data

$[Sn(CH_3)_2(C_{10}H_6NO_2)Cl]$	$F_{000} = 696$
$M_r = 356.37$	$D_x = 1.747$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 3020 reflections
$a = 10.093$ (10) Å	$\theta = 2.2$–26.9^o
$b = 10.245$ (10) Å	$\mu = 2.07$ mm^{-1}
$c = 13.763$ (7) Å	$T = 298$ (2) K
$\beta = 107.811$ (10)^o	Block, colourless
$V = 1355$ (2) Å^3	0.43 × 0.22 × 0.10 mm
$Z = 4$	

Data collection

Siemens SMART CCD diffractometer	2370 independent reflections
Radiation source: fine-focus sealed tube	1864 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.035$
$T = 298$(2) K	$\theta_{max} = 25.0^o$
ω scans	$\theta_{min} = 2.1^o$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.470$, $T_{max} = 0.820$	$k = -11 \rightarrow 12$
6777 measured reflections	$l = -16 \rightarrow 12$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H-atom parameters constrained
$wR(F^2) = 0.092$	$w = 1/[\sigma^2(F_o^2) + (0.050P)^2 + 1.111P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2370 reflections	$\Delta\rho_{max} = 0.52$ e Å^{-3}
154 parameters	$\Delta\rho_{min} = -0.64$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}

Sn1	0.84595 (3)	0.38500 (3)	0.11961 (2)	0.04570 (15)
Cl1	0.9399 (2)	0.58899 (17)	0.20610 (15)	0.1085 (7)
N1	0.6902 (3)	0.2501 (3)	−0.0062 (2)	0.0404 (8)
O1	0.7184 (3)	0.5072 (3)	0.0152 (2)	0.0527 (8)
O2	0.5316 (4)	0.5410 (4)	−0.1171 (3)	0.0745 (11)
C1	0.6110 (5)	0.4669 (5)	−0.0584 (4)	0.0491 (11)
C2	0.5919 (4)	0.3224 (4)	−0.0701 (3)	0.0432 (10)
C3	0.4796 (5)	0.2692 (5)	−0.1459 (3)	0.0559 (12)
H3	0.4110	0.3226	−0.1876	0.067*
C4	0.4729 (6)	0.1371 (6)	−0.1573 (4)	0.0630 (15)
H4	0.3993	0.0996	−0.2077	0.076*
C5	0.5757 (5)	0.0577 (5)	−0.0939 (4)	0.0557 (12)
C6	0.6834 (5)	0.1170 (4)	−0.0167 (4)	0.0472 (11)
C7	0.7870 (5)	0.0395 (5)	0.0500 (4)	0.0608 (13)
H7	0.8583	0.0780	0.1016	0.073*
C8	0.7814 (7)	−0.0936 (5)	0.0380 (6)	0.0799 (19)
H8	0.8493	−0.1453	0.0822	0.096*
C9	0.6768 (8)	−0.1520 (6)	−0.0385 (6)	0.085 (2)
H9	0.6765	−0.2423	−0.0453	0.102*
C10	0.5746 (8)	−0.0815 (6)	−0.1038 (5)	0.0765 (19)
H10	0.5045	−0.1229	−0.1545	0.092*
C11	0.7655 (5)	0.3133 (5)	0.2328 (4)	0.0623 (13)
H11A	0.6855	0.3638	0.2332	0.093*
H11B	0.8351	0.3197	0.2982	0.093*
H11C	0.7389	0.2237	0.2188	0.093*
C12	1.0181 (5)	0.3270 (6)	0.0735 (5)	0.0815 (18)
H12A	1.0249	0.3822	0.0188	0.122*
H12B	1.0060	0.2381	0.0505	0.122*
H12C	1.1016	0.3344	0.1301	0.122*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0431 (2)	0.0443 (2)	0.0489 (2)	−0.00363 (13)	0.01283 (14)	0.00114 (14)
Cl1	0.1292 (16)	0.0709 (11)	0.0931 (13)	−0.0353 (10)	−0.0139 (11)	−0.0156 (9)
N1	0.051 (2)	0.035 (2)	0.0390 (19)	0.0010 (16)	0.0183 (16)	−0.0001 (15)
O1	0.0593 (19)	0.0362 (18)	0.060 (2)	0.0000 (14)	0.0143 (16)	0.0035 (15)
O2	0.079 (2)	0.062 (2)	0.072 (2)	0.016 (2)	0.007 (2)	0.024 (2)
C1	0.056 (3)	0.045 (3)	0.050 (3)	0.005 (2)	0.021 (2)	0.007 (2)
C2	0.048 (2)	0.044 (3)	0.040 (2)	−0.003 (2)	0.0166 (19)	−0.001 (2)
C3	0.056 (3)	0.071 (4)	0.041 (3)	−0.007 (2)	0.015 (2)	0.001 (2)
C4	0.062 (3)	0.084 (4)	0.048 (3)	−0.028 (3)	0.024 (2)	−0.023 (3)
C5	0.071 (3)	0.053 (3)	0.055 (3)	−0.018 (3)	0.037 (3)	−0.018 (3)
C6	0.062 (3)	0.035 (2)	0.056 (3)	−0.004 (2)	0.035 (2)	−0.005 (2)
C7	0.073 (3)	0.041 (3)	0.070 (3)	0.008 (2)	0.024 (3)	0.002 (2)
C8	0.109 (5)	0.038 (3)	0.111 (5)	0.017 (3)	0.060 (4)	0.011 (3)
C9	0.124 (6)	0.036 (3)	0.128 (6)	−0.017 (4)	0.089 (5)	−0.022 (4)
C10	0.108 (5)	0.055 (4)	0.095 (5)	−0.027 (3)	0.074 (4)	−0.028 (3)

C11	0.065 (3)	0.072 (4)	0.052 (3)	0.012 (3)	0.021 (2)	0.007 (3)
C12	0.057 (3)	0.082 (4)	0.120 (5)	0.012 (3)	0.049 (3)	0.029 (4)

Geometric parameters (Å, °)

Sn1—O1	2.040 (3)	C5—C10	1.433 (8)
Sn1—C11	2.098 (5)	C6—C7	1.407 (7)
Sn1—C12	2.109 (5)	C7—C8	1.373 (7)
Sn1—N1	2.390 (4)	C7—H7	0.9300
Sn1—Cl1	2.448 (2)	C8—C9	1.379 (9)
N1—C2	1.333 (5)	C8—H8	0.9300
N1—C6	1.371 (5)	C9—C10	1.351 (10)
O1—C1	1.304 (5)	C9—H9	0.9300
O2—C1	1.215 (5)	C10—H10	0.9300
C1—C2	1.495 (7)	C11—H11A	0.9600
C2—C3	1.395 (6)	C11—H11B	0.9600
C3—C4	1.362 (7)	C11—H11C	0.9600
C3—H3	0.9300	C12—H12A	0.9600
C4—C5	1.396 (8)	C12—H12B	0.9600
C4—H4	0.9300	C12—H12C	0.9600
C5—C6	1.404 (7)		
O1—Sn1—C11	115.73 (17)	C6—C5—C10	119.0 (6)
O1—Sn1—C12	111.2 (2)	N1—C6—C5	120.8 (5)
C11—Sn1—C12	131.8 (2)	N1—C6—C7	119.3 (4)
O1—Sn1—N1	73.22 (14)	C5—C6—C7	119.9 (4)
C11—Sn1—N1	90.98 (18)	C8—C7—C6	119.1 (6)
C12—Sn1—N1	92.2 (2)	C8—C7—H7	120.4
O1—Sn1—Cl1	83.42 (11)	C6—C7—H7	120.4
C11—Sn1—Cl1	96.77 (17)	C7—C8—C9	121.1 (6)
C12—Sn1—Cl1	98.9 (2)	C7—C8—H8	119.4
N1—Sn1—Cl1	156.47 (10)	C9—C8—H8	119.4
C2—N1—C6	118.7 (4)	C10—C9—C8	121.8 (6)
C2—N1—Sn1	110.4 (3)	C10—C9—H9	119.1
C6—N1—Sn1	130.7 (3)	C8—C9—H9	119.1
C1—O1—Sn1	123.3 (3)	C9—C10—C5	119.1 (6)
O2—C1—O1	122.8 (4)	C9—C10—H10	120.5
O2—C1—C2	120.6 (4)	C5—C10—H10	120.5
O1—C1—C2	116.5 (4)	Sn1—C11—H11A	109.5
N1—C2—C3	123.2 (4)	Sn1—C11—H11B	109.5
N1—C2—C1	115.7 (4)	H11A—C11—H11B	109.5
C3—C2—C1	121.1 (4)	Sn1—C11—H11C	109.5
C4—C3—C2	118.4 (5)	H11A—C11—H11C	109.5
C4—C3—H3	120.8	H11B—C11—H11C	109.5
C2—C3—H3	120.8	Sn1—C12—H12A	109.5
C3—C4—C5	120.4 (5)	Sn1—C12—H12B	109.5
C3—C4—H4	119.8	H12A—C12—H12B	109.5
C5—C4—H4	119.8	Sn1—C12—H12C	109.5
C4—C5—C6	118.5 (5)	H12A—C12—H12C	109.5
C4—C5—C10	122.6 (6)	H12B—C12—H12C	109.5

Fig. 1