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Chloridomethylphenyl(quinoline-2-carboxylato-κ^2N,O)tin(IV)

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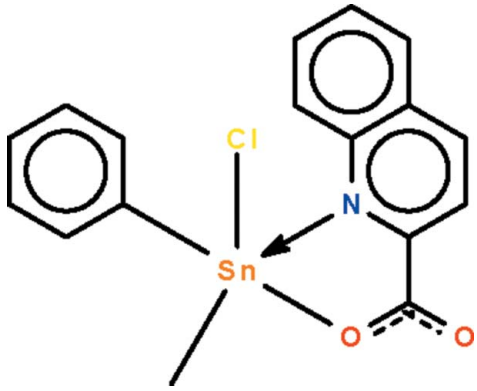
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.035; wR factor = 0.096; data-to-parameter ratio = 18.0.

The Sn atom in the title compound, $[Sn(CH_3)(C_6H_5)(C_{10}H_6NO_2)Cl]$, shows a distorted $C_2SnNOCl$ trigonal-bipyramidal coordination; the apical sites are occupied by the N and Cl atoms.

Related literature

For chloridodimethyl(quinoline-2-carboxylato)tin(IV), see: Wang *et al.* (2007).



Experimental

Crystal data

$[Sn(CH_3)(C_6H_5)(C_{10}H_6NO_2)Cl]$
M_r = 418.43
Monoclinic, $P2_1/n$
a = 10.6942 (5) Å
b = 13.1463 (6) Å
c = 11.2733 (5) Å
β = 93.689 (1)°
V = 1581.6 (1) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.79 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} = 0.616, T_{max} = 0.841
14187 measured reflections
3613 independent reflections
3433 reflections with $I > 2\sigma(I)$
R_{int} = 0.039

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.096
S = 1.40
3613 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.74 e Å^{-3}
$\Delta\rho_{min}$ = −0.94 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.117 (3)	Sn1—O1	2.062 (2)
Sn1—C2	2.122 (2)	Sn1—Cl1	2.4414 (7)
Sn1—N1	2.369 (2)		
C1—Sn1—C2	138.58 (9)		

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: BT5296).

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supporting information

Acta Cryst. (2010). E**66**, m947 [https://doi.org/10.1107/S1600536810027595]

Chloridomethylphenyl(quinoline-2-carboxylato-κ^2N,O)tin(IV)

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S1. Comment

The tin atom in chlorodimethyl(quinoline-2-carboxylate)tin shows *cis*-$C_2SnNOCl$ trigonal bipyramidal coordination, with the C_2Sn skeleton being bent at 131.8 (2) ° (Wang *et al.*, 2007). Replacing one of the methyl groups by a bulkier phenyl group in the title analog (Scheme I, Fig. 1) leads to only a marginal opening of the angle 138.6 (1) °; the *trans* angle is also marginally increased.

S2. Experimental

Sodium quinoline-2-carboxylate was synthesized by reacting sodium hydroxide and quinoline-2-carboxylic acid in toluene in a Dean-Start apparatus. The compound (0.20 g, 1 mmol) was then stirred with methylphenyltin dichloride (0.35 g, 1 mmol) in toluene; no heat was applied. The precipitate that formed was recrystallized from methanol.

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 (1.741eÅ^{-3}) at 0.78 Å from Sn1.

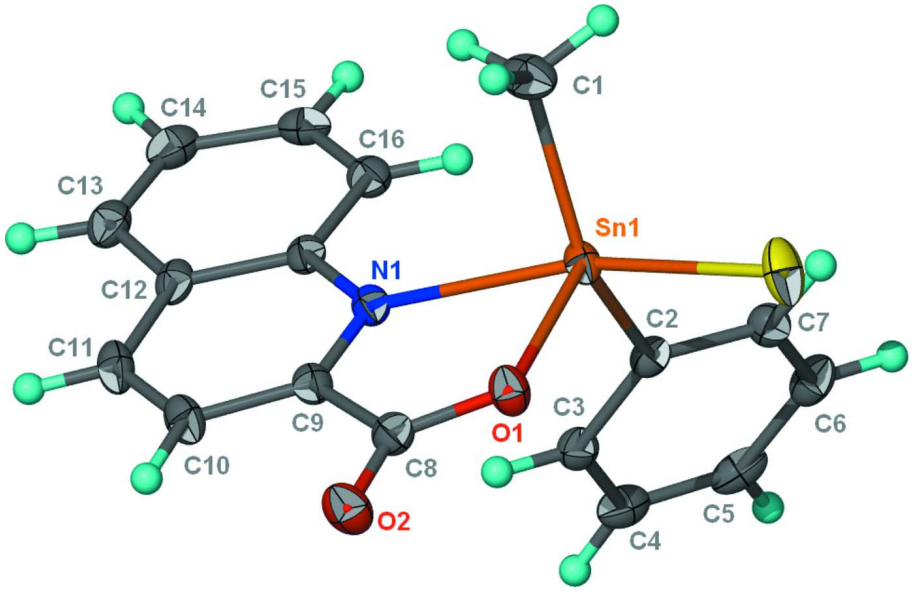

Figure 1

Anisotropic displacement ellipsoid plot (Barbour, 2001) of $SnCl(CH_3)(C_6H_5)(C_{10}H_6NO_2)$ at the 70% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

Chloridomethylphenyl(quinoline-2-carboxylato-κ^2N,O)tin(IV)

Crystal data

$[Sn(CH_3)(C_6H_5)(C_{10}H_6NO_2)Cl]$
$M_r = 418.43$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.6942$ (5) Å
$b = 13.1463$ (6) Å
$c = 11.2733$ (5) Å
$\beta = 93.689$ (1)°
$V = 1581.6$ (1) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.757$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9943 reflections
$\theta = 2.4$–$28.3°$
$\mu = 1.79$ mm^{-1}
$T = 100$ K
Prism, colorless
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)
$T_{min} = 0.616$, $T_{max} = 0.841$
14187 measured reflections
3613 independent reflections
3433 reflections with $I > 2\sigma(I)$
$R_{int} = 0.039$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.4°$
$h = -13 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.035$
$wR(F^2) = 0.096$
$S = 1.40$
3613 reflections
201 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
$w = 1/[\sigma^2(F_o^2) + (0.0523P)^2 + 0.1663P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.74$ e Å^{-3}
$\Delta\rho_{min} = -0.94$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0280 (15)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.813061 (14)	0.776948 (11)	0.733408 (14)	0.01396 (11)
Cl1	1.02998 (6)	0.75394 (6)	0.68330 (7)	0.02452 (16)
O1	0.77940 (15)	0.62981 (12)	0.67664 (15)	0.0176 (3)
O2	0.64876 (17)	0.49885 (13)	0.64587 (16)	0.0217 (4)
C1	0.8465 (3)	0.77556 (17)	0.9205 (3)	0.0226 (6)
H1A	0.7742	0.8046	0.9575	0.034*
H1B	0.9213	0.8160	0.9428	0.034*
H1C	0.8596	0.7054	0.9479	0.034*
C2	0.7644 (2)	0.88296 (16)	0.59620 (19)	0.0139 (4)
C3	0.6502 (2)	0.87698 (17)	0.52921 (19)	0.0161 (4)
H3	0.5931	0.8236	0.5435	0.019*
C4	0.6195 (2)	0.94912 (19)	0.4413 (2)	0.0193 (5)

H4	0.5427	0.9438	0.3945	0.023*
C5	0.7010 (2)	1.02855 (18)	0.4224 (2)	0.0203 (5)
H5	0.6785	1.0791	0.3647	0.024*
C6	0.8157 (2)	1.03451 (17)	0.4877 (2)	0.0197 (5)
H6	0.8719	1.0887	0.4742	0.024*
C7	0.8479 (2)	0.96066 (17)	0.5731 (2)	0.0167 (4)
H7	0.9274	0.9634	0.6158	0.020*
C8	0.6698 (2)	0.58635 (18)	0.6779 (2)	0.0163 (4)
C9	0.5661 (2)	0.65049 (17)	0.72434 (19)	0.0146 (4)
C10	0.4453 (2)	0.61082 (18)	0.7341 (2)	0.0178 (4)
H10	0.4255	0.5435	0.7089	0.021*
C11	0.3567 (2)	0.67171 (19)	0.7810 (2)	0.0187 (5)
H11	0.2747	0.6462	0.7898	0.022*
C12	0.3874 (3)	0.77218 (16)	0.8162 (2)	0.0158 (5)
C13	0.3008 (2)	0.83899 (19)	0.8662 (2)	0.0193 (5)
H13	0.2194	0.8153	0.8813	0.023*
C14	0.3339 (2)	0.9378 (2)	0.8929 (2)	0.0207 (5)
H14	0.2759	0.9819	0.9271	0.025*
C15	0.4546 (2)	0.97368 (18)	0.86940 (19)	0.0186 (5)
H15	0.4754	1.0429	0.8845	0.022*
C16	0.5418 (2)	0.91036 (18)	0.82531 (19)	0.0172 (4)
H16	0.6234	0.9351	0.8126	0.021*
C17	0.5105 (2)	0.80846 (18)	0.79870 (19)	0.0140 (4)
N1	0.5977 (2)	0.74461 (18)	0.75477 (18)	0.0139 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01151 (15)	0.01373 (15)	0.01635 (15)	−0.00098 (4)	−0.00142 (8)	0.00397 (4)
Cl1	0.0122 (3)	0.0219 (3)	0.0395 (4)	0.0004 (3)	0.0017 (2)	0.0078 (3)
O1	0.0146 (8)	0.0141 (8)	0.0244 (9)	−0.0003 (6)	0.0028 (6)	−0.0009 (6)
O2	0.0208 (9)	0.0156 (8)	0.0286 (9)	−0.0014 (7)	0.0008 (7)	−0.0046 (7)
C1	0.0274 (15)	0.0217 (13)	0.0179 (13)	−0.0011 (9)	−0.0052 (11)	0.0035 (8)
C2	0.0152 (10)	0.0134 (10)	0.0133 (9)	0.0019 (8)	0.0027 (8)	0.0011 (8)
C3	0.0148 (11)	0.0176 (11)	0.0162 (10)	0.0009 (8)	0.0020 (8)	−0.0006 (8)
C4	0.0192 (11)	0.0236 (12)	0.0152 (10)	0.0072 (9)	0.0004 (8)	−0.0009 (9)
C5	0.0302 (13)	0.0177 (12)	0.0134 (10)	0.0090 (10)	0.0054 (9)	0.0024 (8)
C6	0.0268 (12)	0.0135 (10)	0.0198 (11)	0.0006 (9)	0.0088 (9)	0.0020 (8)
C7	0.0179 (11)	0.0145 (10)	0.0178 (10)	−0.0005 (8)	0.0021 (8)	−0.0007 (8)
C8	0.0174 (11)	0.0164 (11)	0.0151 (10)	−0.0006 (8)	0.0011 (8)	0.0020 (8)
C9	0.0139 (11)	0.0154 (11)	0.0142 (10)	−0.0005 (8)	−0.0007 (8)	0.0022 (8)
C10	0.0166 (11)	0.0143 (10)	0.0223 (11)	−0.0033 (8)	−0.0002 (9)	0.0030 (8)
C11	0.0142 (11)	0.0196 (12)	0.0223 (11)	−0.0028 (9)	0.0013 (9)	0.0067 (9)
C12	0.0133 (12)	0.0207 (13)	0.0135 (11)	0.0010 (8)	0.0012 (9)	0.0060 (7)
C13	0.0170 (11)	0.0253 (12)	0.0157 (10)	0.0016 (9)	0.0022 (8)	0.0041 (8)
C14	0.0218 (12)	0.0257 (13)	0.0146 (10)	0.0059 (10)	0.0011 (9)	0.0002 (9)
C15	0.0245 (12)	0.0174 (11)	0.0135 (10)	0.0005 (9)	−0.0023 (9)	−0.0012 (8)
C16	0.0193 (11)	0.0176 (11)	0.0147 (10)	−0.0016 (8)	−0.0002 (8)	0.0017 (8)

C17	0.0144 (11)	0.0163 (11)	0.0113 (9)	−0.0004 (9)	0.0001 (8)	0.0029 (8)
N1	0.0136 (10)	0.0142 (9)	0.0139 (9)	−0.0009 (8)	0.0001 (7)	0.0025 (8)

Geometric parameters (Å, º)

Sn1—C1	2.117 (3)	C7—H7	0.9500
Sn1—C2	2.122 (2)	C8—C9	1.513 (3)
Sn1—N1	2.369 (2)	C9—N1	1.322 (3)
Sn1—O1	2.062 (2)	C9—C10	1.404 (3)
Sn1—Cl1	2.4414 (7)	C10—C11	1.373 (3)
O1—C8	1.305 (3)	C10—H10	0.9500
O2—C8	1.222 (3)	C11—C12	1.412 (4)
C1—H1A	0.9800	C11—H11	0.9500
C1—H1B	0.9800	C12—C13	1.420 (3)
C1—H1C	0.9800	C12—C17	1.426 (3)
C2—C7	1.392 (3)	C13—C14	1.375 (4)
C2—C3	1.397 (3)	C13—H13	0.9500
C3—C4	1.395 (3)	C14—C15	1.415 (4)
C3—H3	0.9500	C14—H14	0.9500
C4—C5	1.385 (4)	C15—C16	1.367 (3)
C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.392 (4)	C16—C17	1.408 (3)
C5—H5	0.9500	C16—H16	0.9500
C6—C7	1.394 (3)	C17—N1	1.371 (3)
C6—H6	0.9500		
O1—Sn1—C1	108.43 (8)	C6—C7—H7	119.8
O1—Sn1—C2	111.11 (7)	O2—C8—O1	123.9 (2)
C1—Sn1—C2	138.58 (9)	O2—C8—C9	120.1 (2)
O1—Sn1—N1	73.25 (7)	O1—C8—C9	116.0 (2)
C1—Sn1—N1	90.02 (10)	N1—C9—C10	123.3 (2)
C2—Sn1—N1	89.86 (8)	N1—C9—C8	115.5 (2)
O1—Sn1—Cl1	87.79 (5)	C10—C9—C8	121.2 (2)
C1—Sn1—Cl1	97.31 (9)	C11—C10—C9	118.4 (2)
C2—Sn1—Cl1	96.02 (6)	C11—C10—H10	120.8
N1—Sn1—Cl1	161.00 (7)	C9—C10—H10	120.8
C8—O1—Sn1	123.13 (14)	C10—C11—C12	120.0 (2)
Sn1—C1—H1A	109.5	C10—C11—H11	120.0
Sn1—C1—H1B	109.5	C12—C11—H11	120.0
H1A—C1—H1B	109.5	C11—C12—C13	123.0 (2)
Sn1—C1—H1C	109.5	C11—C12—C17	118.3 (2)
H1A—C1—H1C	109.5	C13—C12—C17	118.7 (2)
H1B—C1—H1C	109.5	C14—C13—C12	120.4 (2)
C7—C2—C3	119.3 (2)	C14—C13—H13	119.8
C7—C2—Sn1	119.21 (16)	C12—C13—H13	119.8
C3—C2—Sn1	121.48 (16)	C13—C14—C15	120.0 (2)
C4—C3—C2	120.2 (2)	C13—C14—H14	120.0
C4—C3—H3	119.9	C15—C14—H14	120.0

C2—C3—H3	119.9	C16—C15—C14	121.1 (2)
C5—C4—C3	120.0 (2)	C16—C15—H15	119.4
C5—C4—H4	120.0	C14—C15—H15	119.4
C3—C4—H4	120.0	C15—C16—C17	119.9 (2)
C4—C5—C6	120.2 (2)	C15—C16—H16	120.1
C4—C5—H5	119.9	C17—C16—H16	120.1
C6—C5—H5	119.9	N1—C17—C16	120.1 (2)
C5—C6—C7	119.7 (2)	N1—C17—C12	120.1 (2)
C5—C6—H6	120.1	C16—C17—C12	119.8 (2)
C7—C6—H6	120.1	C9—N1—C17	119.9 (2)
C2—C7—C6	120.5 (2)	C9—N1—Sn1	112.07 (16)
C2—C7—H7	119.8	C17—N1—Sn1	127.97 (17)

C1—Sn1—O1—C8	83.29 (19)	C10—C11—C12—C13	−179.5 (2)
C2—Sn1—O1—C8	−84.14 (18)	C10—C11—C12—C17	1.6 (4)
N1—Sn1—O1—C8	−0.97 (16)	C11—C12—C13—C14	−176.5 (2)
Cl1—Sn1—O1—C8	−179.74 (16)	C17—C12—C13—C14	2.4 (3)
O1—Sn1—C2—C7	−133.04 (16)	C12—C13—C14—C15	0.7 (3)
C1—Sn1—C2—C7	65.2 (2)	C13—C14—C15—C16	−3.0 (3)
N1—Sn1—C2—C7	155.02 (17)	C14—C15—C16—C17	2.2 (3)
Cl1—Sn1—C2—C7	−43.08 (17)	C15—C16—C17—N1	−179.8 (2)
O1—Sn1—C2—C3	47.46 (19)	C15—C16—C17—C12	1.0 (3)
C1—Sn1—C2—C3	−114.4 (2)	C11—C12—C17—N1	−3.5 (3)
N1—Sn1—C2—C3	−24.49 (18)	C13—C12—C17—N1	177.5 (2)
Cl1—Sn1—C2—C3	137.41 (17)	C11—C12—C17—C16	175.8 (2)
C7—C2—C3—C4	−1.0 (3)	C13—C12—C17—C16	−3.2 (3)
Sn1—C2—C3—C4	178.55 (16)	C10—C9—N1—C17	0.2 (3)
C2—C3—C4—C5	−1.7 (3)	C8—C9—N1—C17	−179.51 (19)
C3—C4—C5—C6	2.5 (3)	C10—C9—N1—Sn1	176.98 (17)
C4—C5—C6—C7	−0.5 (3)	C8—C9—N1—Sn1	−2.7 (2)
C3—C2—C7—C6	2.9 (3)	C16—C17—N1—C9	−176.6 (2)
Sn1—C2—C7—C6	−176.62 (17)	C12—C17—N1—C9	2.6 (3)
C5—C6—C7—C2	−2.2 (3)	C16—C17—N1—Sn1	7.2 (3)
Sn1—O1—C8—O2	−179.09 (17)	C12—C17—N1—Sn1	−173.62 (16)
Sn1—O1—C8—C9	−0.1 (3)	O1—Sn1—N1—C9	2.05 (15)
O2—C8—C9—N1	−178.9 (2)	C1—Sn1—N1—C9	−107.22 (17)
O1—C8—C9—N1	2.1 (3)	C2—Sn1—N1—C9	114.19 (16)
O2—C8—C9—C10	1.4 (3)	Cl1—Sn1—N1—C9	5.8 (3)
O1—C8—C9—C10	−177.6 (2)	O1—Sn1—N1—C17	178.5 (2)
N1—C9—C10—C11	−2.1 (3)	C1—Sn1—N1—C17	69.2 (2)
C8—C9—C10—C11	177.6 (2)	C2—Sn1—N1—C17	−69.4 (2)
C9—C10—C11—C12	1.1 (4)	Cl1—Sn1—N1—C17	−177.71 (13)