metal-organic compounds

catena-Poly[[trimethyltin(IV)]-*μ*-quinaldato]

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The title compound, $[Sn(CH_3)_3(C_{10}H_6NO_2)]_n$, forms an extended one-dimensional chain structure. There are two independent Sn^{IV} ions, both of which are in slightly distorted trigonal-bipyramidal coordination environments with two symmetry-related O atoms in the axial sites. In each case, the Sn^{IV} ion and one of the three equatorial C atoms lie on a crystallographic twofold axis.

Related literature

A series of new triorganotin(IV) pyridinedicarboxylates has been synthesized by the reaction of trimethyltin(IV), triphenyltin(IV) or tribenzyltin(IV) chloride with 2,6(3,5 or 2,5)-H_2pdc (pdc = pyridinedicarboxylate), see: Ma *et al.* (2006)
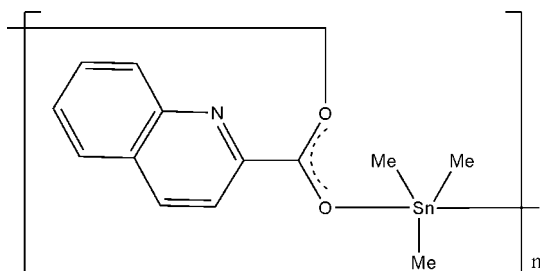
Experimental

Crystal data

$[Sn(CH_3)_3(C_{10}H_6NO_2)]$	a = 7.0487 (14) Å
M_r = 335.95	b = 25.011 (2) Å
Orthorhombic, $C222_1$	c = 15.587 (2) Å

V = 2748.0 (7) Å^3	μ = 1.85 mm^{-1}
Z = 8	T = 298 (2) K
Mo $K\alpha$ radiation	$0.49 \times 0.48 \times 0.37$ mm

Data collection

Bruker SMART CCD diffractometer	7068 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	2439 independent reflections
T_{min} = 0.464, T_{max} = 0.548	2251 reflections with $I > 2\sigma(I)$
(expected range = 0.428–0.504)	R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021	$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$wR(F^2)$ = 0.055	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
S = 1.00	Absolute structure: Flack (1983), 1036 Friedel pairs
2439 reflections	Flack parameter: −0.06 (3)
156 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—C12	2.113 (5)	Sn2—C14	2.100 (5)
Sn1—C11	2.118 (4)	Sn2—C13	2.134 (4)
Sn1—O1	2.267 (2)	Sn2—O2	2.281 (3)
C12—Sn1—C11	121.36 (18)	C14^{ii}—Sn2—C14	131.0 (3)
C11^i—Sn1—C11	117.3 (4)	C14—Sn2—C13	114.51 (14)
O1—Sn1—O1^i	175.41 (15)	O2—Sn2—O2^{ii}	170.34 (14)

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 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*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2573).

References

Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
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supporting information

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### Hongyun Wang, Handong Yin and Daqi Wang

S1. Comment

Organotin esters of carboxylic acids are widely used as biocides, 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 an 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 title compound, (Fig. 1), forms an extended one-dimensional chain structure arising from Sn—O bridges to ligands. The Sn—O distances in (I) (Table 1), are similar to those in related organotin carboxylates (Ma *et al.*, 2006). The two independent Sn^{IV} atoms are in slightly distorted trigonal-bipyramidal coordination geometries, with the O atoms in axial positions and three C atoms of three methyl groups in equatorial positions.

S2. Experimental

The reaction was carried out under N$_2$ 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. Trimethyltin 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).(yield 83%; m.p. 447 K). Analysis calculated (%) for C$_{13}$H$_{15}$NO$_2$Sn (Mr = 335.95): C, 46.47; H, 4.50; N, 4.17. found: C, 46.39; H, 4.62; N, 4.21.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C) where x = 1.5 for methyl H and x = 1.2 for aromatic H atoms.
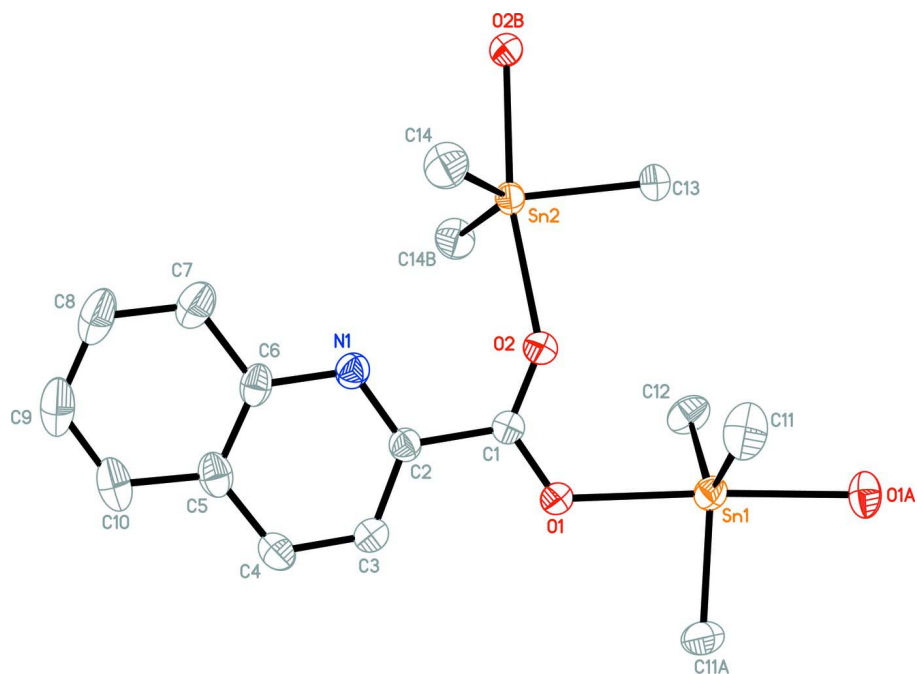
Figure 1

The molecular structure showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity [symmetry code: (A) x, $-y + 1$, $-z + 1$; (B) $-x + 1$, y, $-z + 1/2$].
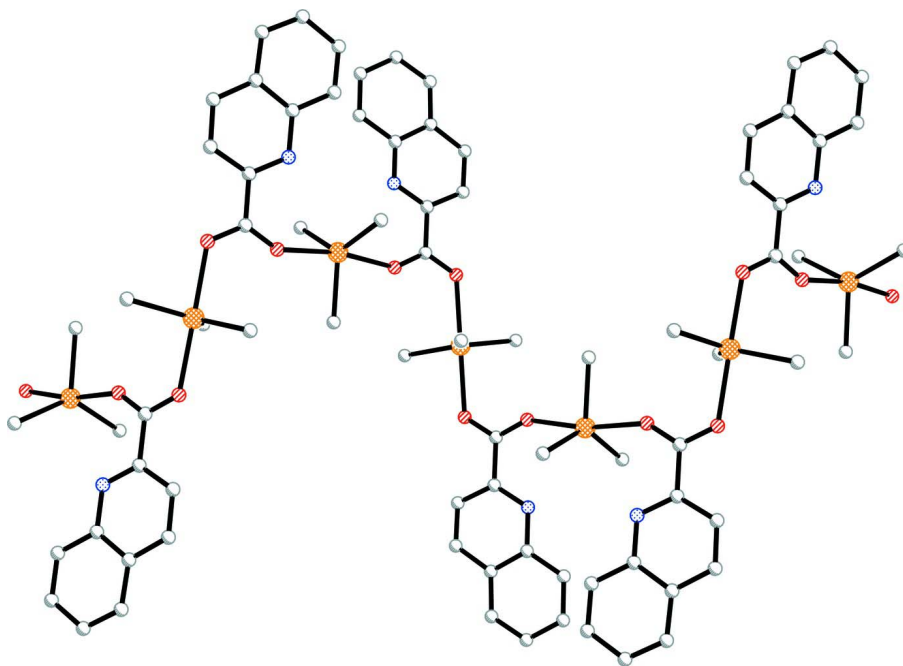
Figure 2

The extended chain structure of with H atoms omitted for clarity.

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Crystal data

$[Sn(CH_3)_3(C_{10}H_6NO_2)]$	$F(000) = 1328$
$M_r = 335.95$	$D_x = 1.624$ Mg m^{-3}
Orthorhombic, $C222_1$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: C 2c 2	Cell parameters from 5374 reflections
$a = 7.0487$ (14) Å	$\theta = 2.6$–28.0°
$b = 25.011$ (2) Å	$\mu = 1.85$ mm^{-1}
$c = 15.587$ (2) Å	$T = 298$ K
$V = 2748.0$ (7) Å^3	Block, colourless
$Z = 8$	$0.49 \times 0.48 \times 0.37$ mm

Data collection

Bruker SMART CCD diffractometer	7068 measured reflections
Radiation source: fine-focus sealed tube	2439 independent reflections
Graphite monochromator	2251 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.035$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$, $\theta_{min} = 1.6°$
$T_{min} = 0.464$, $T_{max} = 0.548$	$h = -8 \rightarrow 8$
	$k = -29 \rightarrow 29$
	$l = -9 \rightarrow 18$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.021$	$w = 1/[\sigma^2(F_o^2) + (0.0295P)^2 + 1.3697P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.055$	
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
2439 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
156 parameters	$\Delta\rho_{min} = -0.24$ e Å^{-3}
0 restraints	Absolute structure: Flack (1983), 1036 Friedel pairs
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: −0.06 (3)
Secondary atom site location: difference Fourier map	

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.85035 (5)	0.5000	0.5000	0.04229 (10)	
Sn2	0.5000	0.597822 (12)	0.2500	0.04016 (10)	
N1	0.7684 (4)	0.69843 (12)	0.3468 (2)	0.0435 (7)	
O1	0.8632 (4)	0.58995 (10)	0.48310 (17)	0.0540 (7)	
O2	0.7139 (4)	0.59014 (11)	0.35911 (18)	0.0558 (7)	
C1	0.7965 (6)	0.61356 (14)	0.4183 (2)	0.0425 (9)	
C2	0.8264 (5)	0.67348 (14)	0.4162 (2)	0.0398 (8)	
C3	0.9083 (5)	0.69858 (14)	0.4871 (3)	0.0480 (9)	
H3	0.9465	0.6786	0.5344	0.058*	
C4	0.9317 (6)	0.75282 (14)	0.4862 (4)	0.0557 (12)	
H4	0.9858	0.7704	0.5327	0.067*	
C5	0.8716 (6)	0.78169 (15)	0.4128 (3)	0.0520 (10)	

C6	0.7940 (6)	0.75296 (15)	0.3438 (3)	0.0455 (9)	
C7	0.7360 (7)	0.78067 (17)	0.2691 (3)	0.0655 (13)	
H7	0.6860	0.7620	0.2227	0.079*	
C8	0.7539 (7)	0.83512 (19)	0.2655 (5)	0.0775 (17)	
H8	0.7158	0.8534	0.2165	0.093*	
C9	0.8285 (9)	0.86342 (19)	0.3346 (4)	0.0766 (16)	
H9	0.8371	0.9005	0.3315	0.092*	
C10	0.8888 (7)	0.83802 (17)	0.4062 (4)	0.0686 (14)	
H10	0.9416	0.8575	0.4510	0.082*	
C11	1.0067 (9)	0.48610 (17)	0.3861 (3)	0.0718 (13)	
H11A	1.1400	0.4876	0.3986	0.108*	
H11B	0.9756	0.5130	0.3445	0.108*	
H11C	0.9755	0.4514	0.3638	0.108*	
C12	0.5506 (8)	0.5000	0.5000	0.0627 (15)	
H12A	0.5052	0.4932	0.4430	0.094*	0.50
H12B	0.5052	0.5342	0.5191	0.094*	0.50
H12C	0.5052	0.4726	0.5380	0.094*	0.50
C13	0.5000	0.51249 (17)	0.2500	0.0531 (13)	
H13A	0.5943	0.4997	0.2106	0.080*	0.50
H13B	0.3774	0.4997	0.2328	0.080*	0.50
H13C	0.5283	0.4997	0.3066	0.080*	0.50
C14	0.6981 (9)	0.63265 (19)	0.1663 (3)	0.0655 (14)	
H14A	0.7675	0.6050	0.1372	0.098*	
H14B	0.7844	0.6545	0.1985	0.098*	
H14C	0.6328	0.6543	0.1249	0.098*	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.04158 (19)	0.04241 (18)	0.04287 (19)	0.000	0.000	0.00532 (19)
Sn2	0.0528 (2)	0.03181 (16)	0.03584 (17)	0.000	0.00173 (17)	0.000
N1	0.0400 (17)	0.0416 (16)	0.0489 (18)	0.0011 (14)	−0.0024 (13)	0.0032 (15)
O1	0.0703 (17)	0.0394 (13)	0.0524 (17)	−0.0040 (12)	−0.0230 (15)	0.0057 (12)
O2	0.0699 (19)	0.0420 (15)	0.0554 (17)	−0.0057 (14)	−0.0224 (15)	0.0013 (13)
C1	0.046 (2)	0.0386 (18)	0.043 (2)	0.0006 (16)	−0.0050 (18)	0.0004 (16)
C2	0.037 (2)	0.0371 (17)	0.045 (2)	0.0010 (16)	−0.0021 (16)	0.0000 (16)
C3	0.052 (2)	0.0444 (19)	0.048 (2)	0.0020 (16)	−0.0093 (19)	0.0040 (19)
C4	0.060 (3)	0.0467 (19)	0.061 (3)	−0.0059 (18)	−0.009 (2)	−0.008 (2)
C5	0.045 (2)	0.041 (2)	0.071 (3)	−0.0004 (18)	0.011 (2)	−0.004 (2)
C6	0.037 (2)	0.0382 (19)	0.061 (3)	0.0052 (16)	0.0081 (19)	0.0097 (18)
C7	0.060 (3)	0.060 (2)	0.076 (4)	0.006 (2)	−0.003 (2)	0.020 (2)
C8	0.063 (3)	0.058 (3)	0.111 (5)	0.009 (2)	0.002 (3)	0.036 (3)
C9	0.064 (4)	0.043 (2)	0.122 (5)	0.001 (2)	0.013 (4)	0.018 (3)
C10	0.068 (3)	0.040 (2)	0.097 (4)	−0.007 (2)	0.015 (3)	−0.008 (2)
C11	0.077 (3)	0.067 (3)	0.072 (3)	0.010 (3)	0.034 (3)	0.012 (2)
C12	0.044 (3)	0.079 (4)	0.065 (3)	0.000	0.000	0.018 (4)
C13	0.070 (4)	0.036 (3)	0.054 (3)	0.000	−0.009 (3)	0.000
C14	0.078 (4)	0.066 (3)	0.052 (3)	−0.008 (3)	0.017 (3)	0.007 (2)

Geometric parameters (Å, º)

Sn1—C12	2.113 (5)	C5—C10	1.418 (6)
Sn1—C11[i]	2.118 (4)	C6—C7	1.415 (6)
Sn1—C11	2.118 (4)	C7—C8	1.369 (6)
Sn1—O1	2.267 (2)	C7—H7	0.9300
Sn1—O1[i]	2.267 (2)	C8—C9	1.392 (9)
Sn2—C14[ii]	2.100 (5)	C8—H8	0.9300
Sn2—C14	2.100 (5)	C9—C10	1.352 (8)
Sn2—C13	2.134 (4)	C9—H9	0.9300
Sn2—O2	2.281 (3)	C10—H10	0.9300
Sn2—O2[ii]	2.281 (3)	C11—H11A	0.9600
N1—C2	1.315 (5)	C11—H11B	0.9600
N1—C6	1.377 (5)	C11—H11C	0.9600
O1—C1	1.261 (4)	C12—H12A	0.9600
O2—C1	1.238 (5)	C12—H12B	0.9600
C1—C2	1.514 (5)	C12—H12C	0.9600
C2—C3	1.395 (5)	C13—H13A	0.9600
C3—C4	1.367 (5)	C13—H13B	0.9600
C3—H3	0.9300	C13—H13C	0.9600
C4—C5	1.418 (7)	C14—H14A	0.9600
C4—H4	0.9300	C14—H14B	0.9600
C5—C6	1.404 (6)	C14—H14C	0.9600
C12—Sn1—C11[i]	121.36 (18)	N1—C6—C7	118.4 (4)
C12—Sn1—C11	121.36 (18)	C5—C6—C7	119.5 (4)
C11[i]—Sn1—C11	117.3 (4)	C8—C7—C6	119.6 (5)
C12—Sn1—O1	92.29 (7)	C8—C7—H7	120.2
C11[i]—Sn1—O1	85.04 (13)	C6—C7—H7	120.2
C11—Sn1—O1	92.56 (14)	C7—C8—C9	120.6 (5)
C12—Sn1—O1[i]	92.29 (7)	C7—C8—H8	119.7
C11[i]—Sn1—O1[i]	92.56 (14)	C9—C8—H8	119.7
C11—Sn1—O1[i]	85.04 (13)	C10—C9—C8	121.2 (4)
O1—Sn1—O1[i]	175.41 (15)	C10—C9—H9	119.4
C14[ii]—Sn2—C14	131.0 (3)	C8—C9—H9	119.4
C14[ii]—Sn2—C13	114.51 (14)	C9—C10—C5	120.0 (5)
C14—Sn2—C13	114.51 (14)	C9—C10—H10	120.0
C14[ii]—Sn2—O2	90.63 (17)	C5—C10—H10	120.0
C14—Sn2—O2	93.37 (18)	Sn1—C11—H11A	109.5
C13—Sn2—O2	85.17 (7)	Sn1—C11—H11B	109.5
C14[ii]—Sn2—O2[ii]	93.37 (18)	H11A—C11—H11B	109.5
C14—Sn2—O2[ii]	90.63 (17)	Sn1—C11—H11C	109.5
C13—Sn2—O2[ii]	85.17 (7)	H11A—C11—H11C	109.5
O2—Sn2—O2[ii]	170.34 (14)	H11B—C11—H11C	109.5
C2—N1—C6	117.2 (3)	Sn1—C12—H12A	109.5
C1—O1—Sn1	122.9 (2)	Sn1—C12—H12B	109.5
C1—O2—Sn2	145.8 (3)	H12A—C12—H12B	109.5
O2—C1—O1	123.4 (3)	Sn1—C12—H12C	109.5

O2—C1—C2	121.2 (3)	H12A—C12—H12C	109.5
O1—C1—C2	115.4 (3)	H12B—C12—H12C	109.5
N1—C2—C3	124.5 (3)	Sn2—C13—H13A	109.5
N1—C2—C1	116.4 (3)	Sn2—C13—H13B	109.5
C3—C2—C1	119.1 (3)	H13A—C13—H13B	109.5
C4—C3—C2	119.2 (4)	Sn2—C13—H13C	109.5
C4—C3—H3	120.4	H13A—C13—H13C	109.5
C2—C3—H3	120.4	H13B—C13—H13C	109.5
C3—C4—C5	118.5 (4)	Sn2—C14—H14A	109.5
C3—C4—H4	120.7	Sn2—C14—H14B	109.5
C5—C4—H4	120.7	H14A—C14—H14B	109.5
C6—C5—C4	118.3 (3)	Sn2—C14—H14C	109.5
C6—C5—C10	119.1 (4)	H14A—C14—H14C	109.5
C4—C5—C10	122.6 (4)	H14B—C14—H14C	109.5
N1—C6—C5	122.1 (4)		

Symmetry codes: (i) x, $-y+1$, $-z+1$; (ii) $-x+1$, y, $-z+1/2$.