Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[trimethyltin(IV)]-μ-2,4,6-trichlorobenzoato]

Liyuan Wen, Handong Yin,* Wenkuan Li and Daqi Wang

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

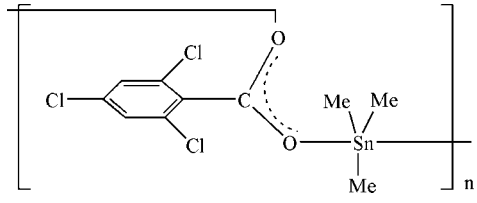
Received 15 November 2008; accepted 3 December 2008

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.028; wR factor = 0.085; data-to-parameter ratio = 17.0.

In the title compound, $[Sn(CH_3)_3(C_7H_2Cl_3O_2)]_n$, the tin(IV) atom exhibits a slightly distorted trigonal-bipyramidal geometry with two O atoms of symmetry-related carboxylate groups in the axial positions and three methyl groups in the equatorial positions. In the crystal structure, the metal atoms are linked by carboxylate bridges into polymeric chains extending along the b axis.

Related literature

For related structures, see: Wang *et al.* (2007); Ma *et al.* (2006).



Experimental

Crystal data

$[Sn(CH_3)_3(C_7H_2Cl_3O_2)]$
M_r = 388.25
Monoclinic, $P2_1/c$
a = 9.8457 (10) Å
b = 9.6891 (9) Å
c = 15.3028 (19) Å
β = 106.761 (1)°
V = 1397.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.38 mm^{-1}
T = 298 (2) K
0.42 × 0.18 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.434, T_{max} = 0.832
6983 measured reflections
2469 independent reflections
1996 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.085
S = 1.01
2469 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.68 e Å^{-3}
$\Delta\rho_{min}$ = −0.37 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C9	2.107 (5)	Sn1—O1	2.212 (3)
Sn1—C10	2.116 (5)	Sn1—O2^{i}	2.467 (3)
Sn1—C8	2.123 (4)		

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*

We acknowledge the National Natural Foundation of China (grant No. 20771053), and the Natural Science Foundation of Shandong Province (2005ZX09) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2273).

References

Ma, C., Li, J., Zhang, R. & Wang, D. (2006). *J. Organomet. Chem.*, **691**, 1713-1721.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, H., Yin, H. & Wang, D. (2007). *Acta Cryst.* E**63**, m2955.

supplementary materials

Acta Cryst. (2009). E**65**, m30 [**doi:10.1107/S1600536808040798**]

catena-Poly[[trimethyltin(IV)]-μ-2,4,6-trichlorobenzoato]

L. Wen, H. Yin, W. Li and D. Wang

Comment

Organoantin(IV) derivatives have recently attracted considerable attention due to the significant antimicrobial properties (Wang *et al.*, 2007). As a part of our ongoing investigations in this field, we have synthesized the title compound and present its crystal structure here.

In the title compound (Fig. 1), the Sn—O bond distances (Table 1) are comparable to those found in related organotin carboxylates (Ma *et al.*, 2006). The Sn atom assumes a slightly distorted trigonal-bipyramidal coordination geometry, provided by two O atoms of symmetry related carboxylate groups at the axial positions and three methyl groups at the equatorial positions. In the crystal structure, the metal atoms are linked by carboxylate bridges into polymeric chains extending along the *b* axis (Fig. 2).

Experimental

The reaction was carried out under nitrogen atmosphere. 2,4,6-Trichlorobenzoic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to a stirred solution of benzene (30 ml) in a Schlenk flask and stirred for 0.5 h. Trimethyltin chloride (1 mmol) was then added and the reaction mixture was stirred for 12 h at room temperature. The resulting clear solution was evaporated under vacuum. Colourless crystals suitable for X-ray analysis were obtained by slow evaporation of a dichloromethane/methanol (1:1 v/v) solution (yield 83%. m. p. 403K). Anal. Calcd (%) for $C_{10}H_{11}Cl_3O_2Sn$: C, 30.94; H, 2.86; O, 8.24; Sn, 30.58; Found (%): C, 30.89; H, 2.90; O, 8.31; Sn, 30.62.

Refinement

H atoms were positioned geometrically, with methyl C—H distances of 0.96 Å and aromatic C—H distances of 0.93 Å, and refined as riding on their parent atoms, with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 U_{eq}(C) for the methyl groups.

Figures

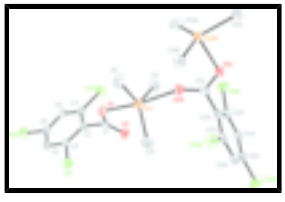


Fig. 1. The molecular structure of the compound, showing 50% probability displacement ellipsoids. H atoms are omitted for clarity. Symmetry code: (A) = -*x* + 1,*y* + 1/2,-*z* + 1/2.

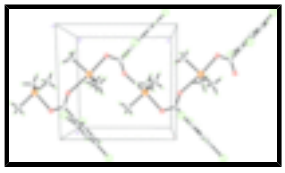


Fig. 2. View of the one-dimensional chain structure extending along the *b* axis.

catena-Poly[[trimethyltin(IV)]-μ-2,4,6-trichlorobenzoato]

Crystal data

$[Sn(CH_3)_3(C_7H_2Cl_3O_2)]$	F_{000} = 752
M_r = 388.25	D_x = 1.845 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 3337 reflections
a = 9.8457 (10) Å	θ = 2.5–27.6º
b = 9.6891 (9) Å	μ = 2.38 mm^{-1}
c = 15.3028 (19) Å	T = 298 (2) K
β = 106.7610 (10)º	Block, colourless
V = 1397.8 (3) Å^3	0.42 × 0.18 × 0.08 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	2469 independent reflections
Radiation source: fine-focus sealed tube	1996 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.025
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→11
T_{min} = 0.434, T_{max} = 0.832	k = −10→11
6983 measured reflections	l = −18→15

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.028	H-atom parameters constrained
$wR(F^2)$ = 0.085	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 1.1107P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.01	$(\Delta/\sigma)_{max} < 0.001$
2469 reflections	$\Delta\rho_{max}$ = 0.68 e Å^{-3}
145 parameters	$\Delta\rho_{min}$ = −0.37 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	0.41662 (3)	0.26723 (3)	0.24850 (2)	0.03954 (13)
Cl1	0.13395 (13)	−0.14643 (14)	0.30795 (8)	0.0553 (3)
Cl2	−0.17245 (14)	−0.41671 (14)	0.00986 (9)	0.0685 (4)
Cl3	0.21742 (14)	−0.04603 (14)	−0.01909 (8)	0.0589 (3)
O1	0.2441 (3)	0.1152 (3)	0.1981 (2)	0.0436 (7)
O2	0.4091 (3)	−0.0438 (3)	0.2076 (2)	0.0483 (8)
C1	0.2834 (4)	−0.0058 (4)	0.1860 (3)	0.0368 (9)
C2	0.1682 (4)	−0.1073 (4)	0.1414 (3)	0.0357 (9)
C3	0.0947 (4)	−0.1793 (4)	0.1922 (3)	0.0379 (9)
C4	−0.0092 (5)	−0.2761 (4)	0.1529 (3)	0.0416 (10)
H4	−0.0557	−0.3248	0.1881	0.050*
C5	−0.0410 (5)	−0.2974 (4)	0.0609 (3)	0.0429 (11)
C6	0.0256 (5)	−0.2269 (4)	0.0067 (3)	0.0449 (11)
H6	0.0004	−0.2414	−0.0560	0.054*
C7	0.1307 (4)	−0.1341 (4)	0.0483 (3)	0.0396 (10)
C8	0.2673 (5)	0.4245 (5)	0.2502 (4)	0.0582 (13)
H8A	0.3162	0.5044	0.2809	0.087*
H8B	0.2023	0.3917	0.2818	0.087*
H8C	0.2158	0.4484	0.1887	0.087*
C9	0.4924 (6)	0.2466 (5)	0.1337 (3)	0.0510 (12)
H9A	0.5867	0.2092	0.1523	0.077*
H9B	0.4938	0.3355	0.1062	0.077*
H9C	0.4312	0.1857	0.0902	0.077*
C10	0.5129 (6)	0.1758 (6)	0.3770 (3)	0.0617 (14)
H10A	0.6022	0.1359	0.3770	0.093*
H10B	0.4520	0.1051	0.3886	0.093*
H10C	0.5283	0.2449	0.4238	0.093*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03773 (19)	0.0345 (2)	0.0475 (2)	−0.00090 (12)	0.01410 (14)	−0.00256 (13)
Cl1	0.0537 (7)	0.0745 (9)	0.0398 (7)	−0.0114 (6)	0.0167 (5)	−0.0052 (6)
Cl2	0.0641 (8)	0.0599 (8)	0.0692 (9)	−0.0214 (7)	−0.0003 (6)	−0.0076 (7)
Cl3	0.0717 (8)	0.0616 (8)	0.0511 (7)	−0.0064 (6)	0.0300 (6)	0.0062 (6)
O1	0.0357 (15)	0.0308 (16)	0.066 (2)	−0.0010 (12)	0.0176 (14)	−0.0100 (14)
O2	0.0367 (17)	0.0375 (17)	0.068 (2)	0.0041 (13)	0.0106 (14)	0.0015 (15)
C1	0.038 (2)	0.034 (2)	0.040 (2)	−0.0021 (18)	0.0155 (19)	0.0017 (18)
C2	0.035 (2)	0.028 (2)	0.042 (2)	0.0022 (17)	0.0089 (18)	−0.0017 (18)
C3	0.040 (2)	0.037 (2)	0.038 (2)	−0.0023 (19)	0.0133 (19)	−0.0009 (19)
C4	0.038 (2)	0.036 (2)	0.051 (3)	−0.0047 (18)	0.012 (2)	0.003 (2)
C5	0.039 (2)	0.033 (2)	0.051 (3)	−0.0032 (19)	0.005 (2)	−0.007 (2)
C6	0.049 (3)	0.045 (3)	0.038 (3)	0.004 (2)	0.009 (2)	−0.005 (2)
C7	0.041 (2)	0.035 (2)	0.045 (3)	0.0037 (18)	0.0144 (19)	0.0031 (19)
C8	0.045 (3)	0.045 (3)	0.086 (4)	−0.004 (2)	0.022 (3)	−0.019 (3)
C9	0.055 (3)	0.052 (3)	0.051 (3)	−0.002 (2)	0.023 (2)	0.001 (2)
C10	0.078 (4)	0.056 (3)	0.047 (3)	−0.014 (3)	0.011 (3)	0.004 (2)

Geometric parameters (Å, °)

Sn1—C9	2.107 (5)	C4—C5	1.366 (6)
Sn1—C10	2.116 (5)	C4—H4	0.9300
Sn1—C8	2.123 (4)	C5—C6	1.377 (7)
Sn1—O1	2.212 (3)	C6—C7	1.380 (6)
Sn1—O2^{i}	2.467 (3)	C6—H6	0.9300
Cl1—C3	1.730 (4)	C8—H8A	0.9600
Cl2—C5	1.744 (4)	C8—H8B	0.9600
Cl3—C7	1.740 (4)	C8—H8C	0.9600
O1—C1	1.265 (5)	C9—H9A	0.9600
O2—C1	1.241 (5)	C9—H9B	0.9600
O2—Sn1^{ii}	2.467 (3)	C9—H9C	0.9600
C1—C2	1.508 (5)	C10—H10A	0.9600
C2—C7	1.390 (6)	C10—H10B	0.9600
C2—C3	1.392 (6)	C10—H10C	0.9600
C3—C4	1.390 (6)		
C9—Sn1—C10	124.3 (2)	C6—C5—Cl2	118.7 (4)
C9—Sn1—C8	119.4 (2)	C5—C6—C7	118.0 (4)
C10—Sn1—C8	114.6 (2)	C5—C6—H6	121.0
C9—Sn1—O1	93.83 (16)	C7—C6—H6	121.0
C10—Sn1—O1	97.96 (16)	C6—C7—C2	122.4 (4)
C8—Sn1—O1	91.00 (15)	C6—C7—Cl3	118.5 (4)
C9—Sn1—O2^{i}	84.92 (15)	C2—C7—Cl3	119.1 (3)
C10—Sn1—O2^{i}	88.16 (16)	Sn1—C8—H8A	109.5
C8—Sn1—O2^{i}	83.90 (15)	Sn1—C8—H8B	109.5
O1—Sn1—O2^{i}	173.28 (10)	H8A—C8—H8B	109.5
C1—O1—Sn1	115.6 (2)	Sn1—C8—H8C	109.5
C1—O2—Sn1^{ii}	148.7 (3)	H8A—C8—H8C	109.5
O2—C1—O1	124.0 (4)	H8B—C8—H8C	109.5
O2—C1—C2	119.3 (4)	Sn1—C9—H9A	109.5
O1—C1—C2	116.6 (3)	Sn1—C9—H9B	109.5
C7—C2—C3	116.9 (4)	H9A—C9—H9B	109.5
C7—C2—C1	121.9 (4)	Sn1—C9—H9C	109.5
C3—C2—C1	121.2 (4)	H9A—C9—H9C	109.5
C4—C3—C2	122.1 (4)	H9B—C9—H9C	109.5
C4—C3—Cl1	119.1 (3)	Sn1—C10—H10A	109.5
C2—C3—Cl1	118.7 (3)	Sn1—C10—H10B	109.5
C5—C4—C3	118.0 (4)	H10A—C10—H10B	109.5
C5—C4—H4	121.0	Sn1—C10—H10C	109.5
C3—C4—H4	121.0	H10A—C10—H10C	109.5
C4—C5—C6	122.6 (4)	H10B—C10—H10C	109.5
C4—C5—Cl2	118.8 (4)		
C9—Sn1—O1—C1	61.1 (3)	C1—C2—C3—Cl1	2.0 (5)
C10—Sn1—O1—C1	−64.4 (3)	C2—C3—C4—C5	−1.5 (7)
C8—Sn1—O1—C1	−179.3 (3)	Cl1—C3—C4—C5	178.2 (3)

Sn1^{ii}—O2—C1—O1	154.5 (4)	C3—C4—C5—C6	−0.1 (7)
Sn1^{ii}—O2—C1—C2	−26.3 (8)	C3—C4—C5—Cl2	−179.2 (3)
Sn1—O1—C1—O2	6.1 (5)	C4—C5—C6—C7	1.7 (7)
Sn1—O1—C1—C2	−173.0 (3)	Cl2—C5—C6—C7	−179.2 (3)
O2—C1—C2—C7	−82.9 (5)	C5—C6—C7—C2	−1.8 (7)
O1—C1—C2—C7	96.3 (5)	C5—C6—C7—Cl3	179.1 (3)
O2—C1—C2—C3	96.8 (5)	C3—C2—C7—C6	0.2 (6)
O1—C1—C2—C3	−84.0 (5)	C1—C2—C7—C6	179.9 (4)
C7—C2—C3—C4	1.5 (6)	C3—C2—C7—Cl3	179.3 (3)
C1—C2—C3—C4	−178.2 (4)	C1—C2—C7—Cl3	−1.0 (5)
C7—C2—C3—Cl1	−178.3 (3)		

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

Fig. 1

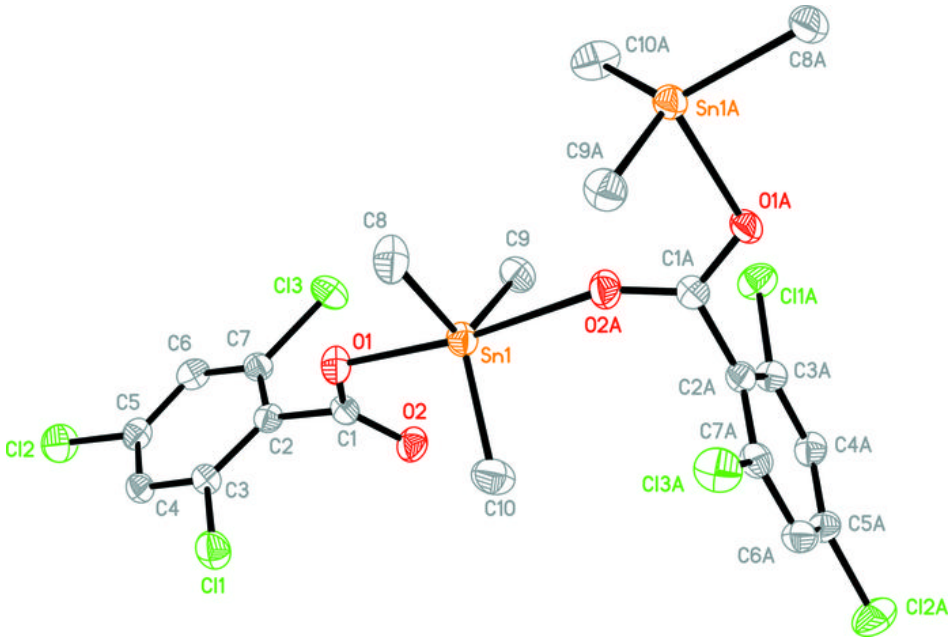

C10A
C8A
Sn1A
C9A
O1A
C8
C9
C1A
Cl3
Cl1A
O2A
O1
Sn1
C6
C7
C2A
C3A
C5
O2
C7A
C4A
Cl2
C2
C1
Cl3A
C3
C4
C10
C5A
C6A
Cl1
Cl2A

Fig. 2