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catena-Poly[[dimethyltin(IV)]-μ-*cis*-cyclohexane-1,2-dicarboxylato]

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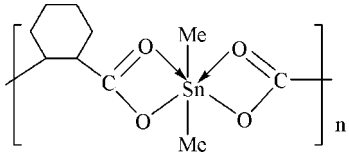
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.031; wR factor = 0.062; data-to-parameter ratio = 15.6.

The title complex, $[Sn(CH_3)_2(C_8H_{10}O_4)]_n$, was synthesized from *cis*-cyclohexane-1,2-dicarboxylic acid and dimethyltin dichloride. The complex has a bridging bis-bidentate carboxylate group resulting in a zig-zag chain structure parallel to [001]. The Sn atom is six-coordinated and displays a distorted octahedral geometry.

Related literature

For background to organotin complexes, see: Gielen (2002); Han *et al.* (2007). For related structures, see: Swisher *et al.* (1984).



Experimental

Crystal data

$[Sn(CH_3)_2(C_8H_{10}O_4)]$
M_r = 318.92
Monoclinic, $P2_1/c$
a = 10.0880 (16) Å
b = 10.430 (2) Å
c = 11.592 (2) Å
β = 99.041 (2)°
V = 1204.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.11 mm^{-1}
T = 298 (2) K
0.32 × 0.19 × 0.17 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.551, T_{max} = 0.715
6188 measured reflections
2117 independent reflections
1822 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.062
S = 1.19
2117 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O3	2.089 (3)	Sn1—O1	2.102 (3)
Sn1—C9	2.089 (4)	Sn1—O4	2.570 (3)
Sn1—C10	2.098 (4)	Sn1—O2	2.660 (3)
C9—Sn1—C10	137.14 (18)		

Data collection: *SMART* (Bruker, 1996); cell refinement: *SAINT* (Bruker, 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2192).

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supplementary materials

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catena-Poly[[dimethyltin(IV)]-μ-*cis*-cyclohexane-1,2-dicarboxylato]

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Comment

Recently, organotin complexes have been attracting increasing attention partly owing to their determinately or potentially pharmic value, which have been reported many before (Gielen, 2002), and also for the versatile molecular structure and supramolecular architecture exhibited by these complexes (Han *et al.*, 2007). In order to explore the relationships between the properties and structures, we report here the structure of the title complex. Fig. 1 the structure of (I) showing one-dimensional extended polymeric network, and the one-dimensional chain along [001] direction of complex is shown in Fig. 2. Sn atom is six coordinated and displays a octahedral distorted geometry.

Experimental

The reaction was carried out under nitrogen atmoshpere. *cis*-cyclohexane-1,2-dicarboxylic acid (0.173 g, 1 mmol) was added to the solution of benzene(30 ml) with sodium ethoxide (0.136 g, 2 mmol) in a Schlenk flask. After stirring for 10 min, dimethyltin dichloride (0.220 g, 1 mmol) was added to the mixture. The mixture was kept at 328 K for 12 h. After cooling down to the room temperature, the solution was filtered. The solvent of the filtrate was gradually removed by evaporation under vacuum until a solid product was obtained. The solid was then recrystallized from aether. Colorless single crystals of the title complex were obtained after one week. Yield, 86%. Analysis calculated for $C_{10}H_{16}O_4Sn$: C 48.76, H 6.55; found: C 48.66, H 6.68. The elemental analyses were performed with PERKIN ELMER MODEL 2400 SERIES II.

Refinement

All H atoms were placed in geometrically idealized positions methyl (C—H = 0.96 Å), methylene (C—H = 0.97 Å), (C—H = 0.98 Å) and treated as riding on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(CH_3), U_{iso}(H) = 1.2U_{eq}(CH_2), U_{iso}(H) = 1.2U_{eq}(CH).

Figures

Fig. 1. Part of the structure of (I) showing one-dimensional extended polymeric network, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms have been omitted for clarity. [Symmetry codes: (*a*) *x*, 1/2 - *y*, -1/2 + *z*; (*b*) *x*, 1/2 - *x*, 1/2 + *z*]

Fig. 2. The one-dimensional zigzag chain of the title complex

catena-Poly[[dimethyltin(IV)]-μ-*cis*-cyclohexane-1,2- dicarboxylato]

Crystal data

$[Sn(CH_3)_2(C_8H_{10}O_4)]$	$F_{000} = 632$
$M_r = 318.92$	$D_x = 1.759$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 4238 reflections
$a = 10.0880$ (16) Å	$\theta = 2.7$–28.3º
$b = 10.430$ (2) Å	$\mu = 2.11$ mm^{-1}
$c = 11.592$ (2) Å	$T = 298$ K
$\beta = 99.041$ (2)º	Block, colourless
$V = 1204.5$ (4) Å^3	0.32 × 0.19 × 0.17 mm
$Z = 4$	

Data collection

Bruker SMART CCD area-detector diffractometer	2117 independent reflections
Radiation source: fine-focus sealed tube	1822 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.022$
$T = 298$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 2.0$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 12$
$T_{min} = 0.551$, $T_{max} = 0.715$	$k = -11 \rightarrow 12$
6188 measured reflections	$l = -11 \rightarrow 13$

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
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0181P)^2 + 1.262P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.19$	$(\Delta/\sigma)_{max} = 0.001$
2117 reflections	$\Delta\rho_{max} = 0.52$ e Å^{-3}
136 parameters	$\Delta\rho_{min} = -0.43$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.67183 (3)	0.15366 (3)	0.10133 (2)	0.03534 (10)
O1	0.8345 (3)	0.2746 (3)	0.1623 (2)	0.0437 (7)
O2	0.6720 (3)	0.3482 (3)	0.2497 (3)	0.0459 (7)
O3	0.8140 (3)	0.0831 (3)	0.0045 (2)	0.0427 (7)
O4	0.6338 (3)	−0.0337 (3)	−0.0441 (2)	0.0448 (7)
C1	0.8867 (4)	0.4597 (4)	0.2822 (3)	0.0333 (9)
H1	0.9542	0.4175	0.3399	0.040*
C2	0.8184 (4)	0.5633 (3)	0.3471 (3)	0.0330 (9)
H2	0.8906	0.6163	0.3888	0.040*
C3	0.7305 (4)	0.6523 (4)	0.2649 (4)	0.0413 (10)
H3A	0.6967	0.7202	0.3095	0.050*
H3B	0.6542	0.6049	0.2246	0.050*
C4	0.8092 (5)	0.7109 (4)	0.1751 (4)	0.0493 (11)
H4A	0.7495	0.7637	0.1209	0.059*
H4B	0.8797	0.7655	0.2149	0.059*
C5	0.8706 (5)	0.6077 (5)	0.1080 (4)	0.0548 (12)
H5A	0.7998	0.5575	0.0630	0.066*
H5B	0.9224	0.6475	0.0539	0.066*
C6	0.9609 (4)	0.5204 (4)	0.1905 (4)	0.0459 (11)
H6A	1.0366	0.5694	0.2296	0.055*
H6B	0.9956	0.4531	0.1457	0.055*
C7	0.7883 (4)	0.3568 (4)	0.2295 (3)	0.0366 (9)
C8	0.7475 (4)	−0.0040 (3)	−0.0606 (3)	0.0344 (9)
C9	0.5448 (4)	0.2734 (4)	−0.0107 (4)	0.0503 (11)
H9A	0.4773	0.3083	0.0302	0.075*
H9B	0.5026	0.2249	−0.0768	0.075*
H9C	0.5962	0.3419	−0.0369	0.075*
C10	0.6548 (5)	0.0271 (4)	0.2389 (4)	0.0476 (11)
H10A	0.5894	0.0594	0.2834	0.071*
H10B	0.7401	0.0197	0.2885	0.071*
H10C	0.6271	−0.0556	0.2077	0.071*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03871 (17)	0.03394 (16)	0.03343 (16)	0.00183 (14)	0.00588 (11)	0.00006 (13)
O1	0.0425 (16)	0.0383 (17)	0.0494 (18)	0.0012 (14)	0.0043 (14)	−0.0157 (14)
O2	0.0424 (17)	0.0444 (17)	0.0523 (18)	−0.0088 (14)	0.0116 (14)	−0.0093 (14)
O3	0.0429 (16)	0.0443 (17)	0.0414 (16)	−0.0032 (14)	0.0083 (13)	−0.0124 (13)
O4	0.0463 (17)	0.0475 (17)	0.0436 (17)	−0.0052 (14)	0.0167 (14)	0.0006 (13)
C1	0.031 (2)	0.030 (2)	0.038 (2)	0.0017 (17)	0.0040 (17)	−0.0027 (17)
C2	0.035 (2)	0.027 (2)	0.036 (2)	−0.0024 (16)	0.0042 (17)	0.0000 (16)
C3	0.042 (2)	0.035 (2)	0.048 (2)	0.003 (2)	0.0098 (19)	0.0068 (19)
C4	0.051 (3)	0.044 (3)	0.054 (3)	−0.003 (2)	0.011 (2)	0.016 (2)
C5	0.065 (3)	0.058 (3)	0.044 (3)	−0.011 (2)	0.018 (2)	0.006 (2)
C6	0.042 (2)	0.049 (3)	0.050 (3)	−0.009 (2)	0.018 (2)	−0.009 (2)
C7	0.042 (2)	0.034 (2)	0.032 (2)	0.0055 (19)	0.0026 (18)	0.0016 (18)
C8	0.046 (2)	0.025 (2)	0.031 (2)	0.0025 (18)	0.0038 (18)	0.0057 (16)
C9	0.047 (3)	0.051 (3)	0.052 (3)	0.002 (2)	0.003 (2)	0.011 (2)
C10	0.058 (3)	0.045 (3)	0.041 (2)	0.004 (2)	0.009 (2)	0.007 (2)

Geometric parameters (Å, °)

Sn1—O3	2.089 (3)	C3—H3A	0.9700
Sn1—C9	2.089 (4)	C3—H3B	0.9700
Sn1—C10	2.098 (4)	C4—C5	1.516 (6)
Sn1—O1	2.102 (3)	C4—H4A	0.9700
Sn1—O4	2.570 (3)	C4—H4B	0.9700
Sn1—O2	2.660 (3)	C5—C6	1.517 (6)
O1—C7	1.294 (4)	C5—H5A	0.9700
O2—C7	1.235 (5)	C5—H5B	0.9700
O3—C8	1.298 (4)	C6—H6A	0.9700
O4—C8	1.232 (5)	C6—H6B	0.9700
C1—C7	1.523 (5)	C8—C2^{ii}	1.509 (5)
C1—C6	1.530 (5)	C9—H9A	0.9600
C1—C2	1.540 (5)	C9—H9B	0.9600
C1—H1	0.9800	C9—H9C	0.9600
C2—C8^{i}	1.509 (5)	C10—H10A	0.9600
C2—C3	1.514 (5)	C10—H10B	0.9600
C2—H2	0.9800	C10—H10C	0.9600
C3—C4	1.532 (6)		
O3—Sn1—C9	106.41 (15)	C5—C4—C3	111.2 (4)
O3—Sn1—C10	109.39 (15)	C5—C4—H4A	109.4
C9—Sn1—C10	137.14 (18)	C3—C4—H4A	109.4
O3—Sn1—O1	80.02 (10)	C5—C4—H4B	109.4
C9—Sn1—O1	102.72 (15)	C3—C4—H4B	109.4
C10—Sn1—O1	105.95 (15)	H4A—C4—H4B	108.0
O3—Sn1—O4	54.83 (10)	C6—C5—C4	110.9 (4)
C9—Sn1—O4	91.89 (15)	C6—C5—H5A	109.5

C10—Sn1—O4	89.93 (14)	C4—C5—H5A	109.5
O1—Sn1—O4	134.84 (9)	C6—C5—H5B	109.5
O3—Sn1—O2	133.28 (9)	C4—C5—H5B	109.5
C9—Sn1—O2	83.34 (15)	H5A—C5—H5B	108.1
C10—Sn1—O2	88.85 (14)	C5—C6—C1	112.1 (3)
O1—Sn1—O2	53.39 (9)	C5—C6—H6A	109.2
O4—Sn1—O2	171.54 (9)	C1—C6—H6A	109.2
C7—O1—Sn1	105.3 (2)	C5—C6—H6B	109.2
C7—O2—Sn1	80.6 (2)	C1—C6—H6B	109.2
C8—O3—Sn1	102.9 (2)	H6A—C6—H6B	107.9
C8—O4—Sn1	82.2 (2)	O2—C7—O1	120.5 (4)
C7—C1—C6	111.9 (3)	O2—C7—C1	123.7 (4)
C7—C1—C2	112.1 (3)	O1—C7—C1	115.8 (3)
C6—C1—C2	110.8 (3)	O4—C8—O3	119.6 (4)
C7—C1—H1	107.3	O4—C8—C2^{ii}	124.3 (3)
C6—C1—H1	107.3	O3—C8—C2^{ii}	116.1 (3)
C2—C1—H1	107.3	Sn1—C9—H9A	109.5
C8^{i}—C2—C3	113.7 (3)	Sn1—C9—H9B	109.5
C8^{i}—C2—C1	110.9 (3)	H9A—C9—H9B	109.5
C3—C2—C1	112.7 (3)	Sn1—C9—H9C	109.5
C8^{i}—C2—H2	106.3	H9A—C9—H9C	109.5
C3—C2—H2	106.3	H9B—C9—H9C	109.5
C1—C2—H2	106.3	Sn1—C10—H10A	109.5
C2—C3—C4	111.0 (3)	Sn1—C10—H10B	109.5
C2—C3—H3A	109.4	H10A—C10—H10B	109.5
C4—C3—H3A	109.4	Sn1—C10—H10C	109.5
C2—C3—H3B	109.4	H10A—C10—H10C	109.5
C4—C3—H3B	109.4	H10B—C10—H10C	109.5
H3A—C3—H3B	108.0		

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

Fig. 1

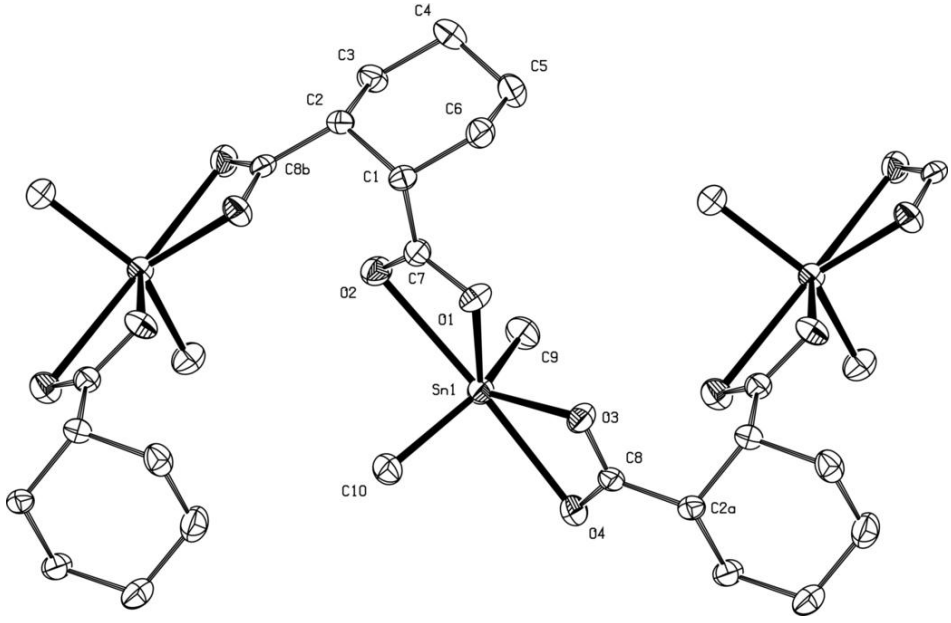

Fig. 2