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catena-Poly[[trimethyltin(IV)]-μ-3,5-difluorobenzoato-κ^2O:O']

Hong Liu and Handong Yin*

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

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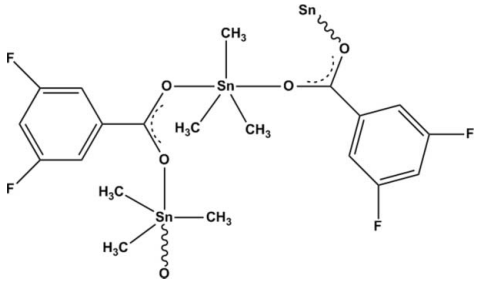
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.032; wR factor = 0.073; data-to-parameter ratio = 15.5.

In the title compound, $[Sn(CH_3)_3(C_7H_3F_2O_2)]_n$, the central Sn atom is coordinated by two O atoms from the anion and three methyl C atoms in a polymeric fashion owing to the presence of bidentate bridging carboxylate ligands. The five-coordinate Sn atom exists in a distorted trigonal–bipyramidal geometry with the molecules connected by weak C—H···F intermoleclar interactions, forming supramolecular chains parallel to [010].

Related literature

For industrial applications and the biological activity of organotin compounds, see: Duboy & Roy (2003). For related trimethyl carboxylates with similar structures, see: Tiekink, (1994).



Experimental

Crystal data

$[Sn(CH_3)_3(C_7H_3F_2O_2)]$
M_r = 320.89
Monoclinic, $C2/c$
a = 13.1371 (12) Å
b = 10.0847 (11) Å
c = 18.9643 (19) Å
β = 101.864 (1)°
V = 2458.8 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.08 mm^{-1}
T = 298 K
0.50 × 0.42 × 0.40 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.422, T_{max} = 0.490
5945 measured reflections
2165 independent reflections
1725 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.073
S = 1.17
2165 reflections
140 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.76 e Å^{-3}
$\Delta\rho_{min}$ = −0.69 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9C···F1^{i}	0.96	2.62	3.470 (7)	148

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 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: JJ2092).

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supporting information

Acta Cryst. (2011). E**67**, m1030 [doi:10.1107/S1600536811025608]

catena-Poly[[trimethyltin(IV)]-μ-3,5-difluorobenzoato-κ^2O:O']

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S1. Comment

In recent years, organotin compounds have attracted increasing attention owing to their wide industrial applications and biological activities (Duboy and Roy, 2003). In continuation of our work in this area, we present the crystal structure of a new compound, (I), $C_{10}H_{12}F_2O_2Sn$. Similar structures for related trimethyl carboxylates have been reported. (Tiekink, 1994).

In the title compound, (I), the central Sn atom is coordinated by two oxygen atoms from the ligand and three carbon methyl atoms in a polymeric fashion owing to the presence of bidentate bridging carboxylate ligands (Fig. 1). The Sn(1)—O(1) and Sn(1)—O(2)#1 (#1 = -*x* + 1/2,*y* - 1/2,-*z* + 1/2) distances are 2.137 (3)Å and 2.540 (4) Å, respectively. The angle of the axial O(1)—Sn(1)—O(2)#1 is 175.92 (13)°, which deviates slightly from linearity. The five-coordinate Sn atom exists in a distorted trigonal bipyramidal geometry with the molecules connected by weak C—H···F intermoleclar interactions, forming one-dimensional supramolecular chains along the (101) plane (Fig. 2).

S2. Experimental

3,5-difluorobenzoic acid (0.4 mmol) was added to a methanol solution of sodium ethoxide (0.4 mmol) and heated at reflux for 0.5 h. To this solution was added trimethyltin chloride (0.8 mmol) in benzene and the mixture was refluxed for 8 h, cooled and filtered. The filtrate was evaporated *in vacuo*. The obtained solid was recrystallized from dichloro-methane-petroleum ether. Anal. Calcd (%) for $C_{10}H_{12}F_2O_2Sn$ (Mr = 320.89): C, 37.43; H, 3.77; Found (%): C, 38.21; H, 3.92.

S3. Refinement

The H atoms were positioned geometrically and refined using the riding model with C–H = 0.93 Å, for aromatic H, 0.96 Å for methyl H atoms. The U_{iso} parameters for H atoms were constraned to be $1.5U_{eq}$ of the carrier atom for the methyl H atoms and $1.2U_{eq}$ of the carrier atom for the remaining H atoms

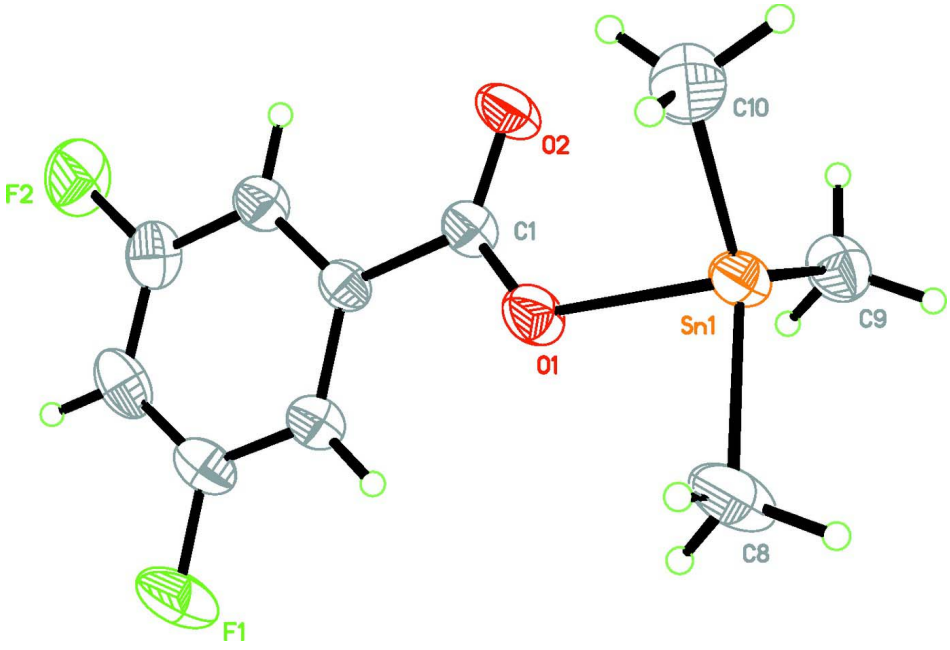

Figure 1

ORTEP diagram of the title compound, with 50% probability displacement ellipsoids.

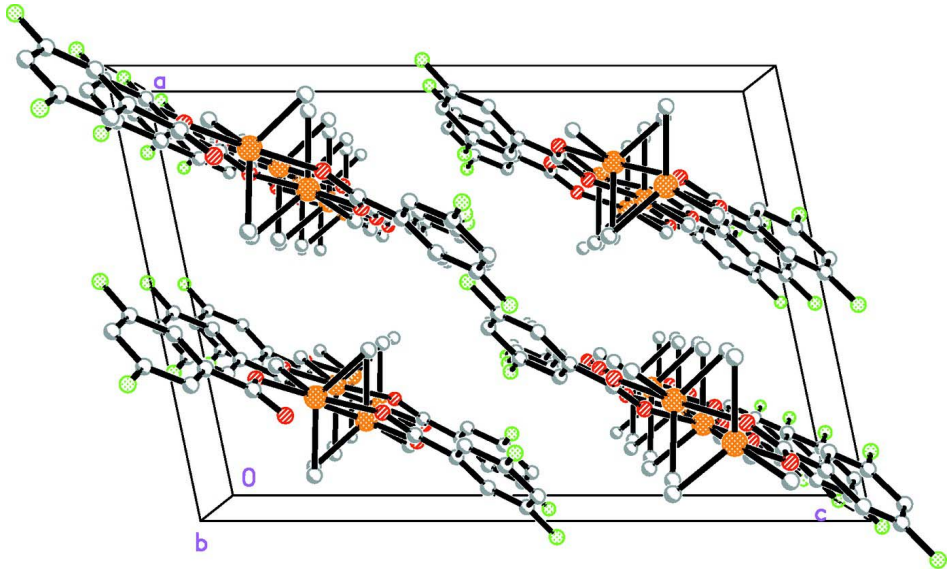

Figure 2

The crystal packing of the title compound, viewed along the *b* axis. H atoms have been omitted for clarity.

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Crystal data

$[Sn(CH_3)_3(C_7H_3F_2O_2)]$
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Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
a = 13.1371 (12) Å
b = 10.0847 (11) Å
c = 18.9643 (19) Å
β = 101.864 (1)°
V = 2458.8 (4) Å^3
Z = 8

$F(000) = 1248$
$D_x = 1.734$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3905 reflections
$\theta = 2.7$–$26.3°$
$\mu = 2.08$ mm^{-1}
$T = 298$ K
Block, colorless
0.50 × 0.42 × 0.40 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.422$, $T_{max} = 0.490$
5945 measured reflections
2165 independent reflections
1725 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.7°$
$h = -14 \rightarrow 15$
$k = -9 \rightarrow 12$
$l = -22 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.073$
$S = 1.17$
2165 reflections
140 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
$w = 1/[\sigma^2(F_o^2) + (0.0148P)^2 + 7.4343P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.008$
$\Delta\rho_{max} = 0.76$ e Å^{-3}
$\Delta\rho_{min} = -0.69$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00219 (15)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.21709 (3)	−0.11988 (3)	0.275296 (18)	0.04976 (17)
O1	0.1757 (3)	0.0218 (3)	0.34840 (19)	0.0620 (10)
O2	0.2446 (3)	0.2018 (4)	0.3102 (2)	0.0664 (10)
F1	−0.0238 (3)	0.1709 (4)	0.5259 (2)	0.0939 (12)
F2	0.1732 (3)	0.5409 (3)	0.4910 (2)	0.0944 (12)
C1	0.1945 (4)	0.1461 (5)	0.3495 (3)	0.0483 (12)
C2	0.1503 (3)	0.2219 (5)	0.4043 (2)	0.0431 (11)
C3	0.0816 (4)	0.1598 (5)	0.4403 (3)	0.0523 (12)
H3	0.0613	0.0724	0.4300	0.063*
C4	0.0443 (4)	0.2301 (6)	0.4913 (3)	0.0587 (14)
C5	0.0744 (4)	0.3574 (6)	0.5100 (3)	0.0658 (15)
H5	0.0497	0.4024	0.5459	0.079*
C6	0.1422 (5)	0.4153 (5)	0.4736 (3)	0.0623 (15)
C7	0.1796 (4)	0.3514 (5)	0.4209 (3)	0.0539 (13)
H7	0.2243	0.3947	0.3964	0.065*
C8	0.1543 (6)	−0.2738 (6)	0.3291 (4)	0.094 (2)
H8A	0.1335	−0.3461	0.2964	0.141*
H8B	0.0949	−0.2412	0.3459	0.141*
H8C	0.2059	−0.3039	0.3693	0.141*

C9	0.1173 (4)	−0.0367 (6)	0.1847 (3)	0.0685 (16)
H9A	0.1543	0.0292	0.1635	0.103*
H9B	0.0587	0.0036	0.1994	0.103*
H9C	0.0933	−0.1051	0.1501	0.103*
C10	0.3794 (4)	−0.0930 (6)	0.2996 (3)	0.0766 (18)
H10A	0.4073	−0.1137	0.2580	0.115*
H10B	0.4098	−0.1505	0.3386	0.115*
H10C	0.3951	−0.0025	0.3134	0.115*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0557 (2)	0.0429 (2)	0.0565 (2)	0.00350 (16)	0.02496 (16)	0.00374 (17)
O1	0.085 (3)	0.044 (2)	0.068 (2)	0.0015 (18)	0.040 (2)	−0.0038 (17)
O2	0.087 (3)	0.059 (2)	0.066 (2)	−0.0043 (19)	0.046 (2)	0.0052 (19)
F1	0.101 (3)	0.099 (3)	0.102 (3)	0.009 (2)	0.070 (2)	0.014 (2)
F2	0.130 (3)	0.058 (2)	0.100 (3)	0.002 (2)	0.033 (2)	−0.0238 (19)
C1	0.055 (3)	0.044 (3)	0.048 (3)	0.007 (2)	0.017 (2)	0.004 (2)
C2	0.042 (3)	0.047 (3)	0.042 (3)	0.007 (2)	0.013 (2)	0.004 (2)
C3	0.056 (3)	0.051 (3)	0.053 (3)	0.004 (2)	0.018 (2)	0.006 (2)
C4	0.058 (3)	0.067 (4)	0.056 (3)	0.013 (3)	0.025 (3)	0.013 (3)
C5	0.077 (4)	0.073 (4)	0.052 (3)	0.031 (3)	0.023 (3)	0.004 (3)
C6	0.075 (4)	0.048 (3)	0.062 (3)	0.016 (3)	0.011 (3)	−0.006 (3)
C7	0.060 (3)	0.051 (3)	0.054 (3)	0.004 (2)	0.018 (2)	0.003 (2)
C8	0.145 (6)	0.049 (3)	0.118 (5)	0.007 (4)	0.097 (5)	0.008 (4)
C9	0.056 (3)	0.083 (4)	0.066 (4)	0.011 (3)	0.013 (3)	−0.002 (3)
C10	0.058 (3)	0.091 (5)	0.078 (4)	0.011 (3)	0.007 (3)	−0.007 (3)

Geometric parameters (Å, º)

Sn1—C10	2.104 (5)	C4—C5	1.368 (7)
Sn1—C9	2.109 (5)	C5—C6	1.365 (8)
Sn1—C8	2.115 (6)	C5—H5	0.9300
Sn1—O1	2.137 (3)	C6—C7	1.363 (7)
Sn1—O2^{i}	2.540 (4)	C7—H7	0.9300
O1—C1	1.278 (6)	C8—H8A	0.9600
O2—C1	1.227 (6)	C8—H8B	0.9600
O2—Sn1^{ii}	2.540 (4)	C8—H8C	0.9600
F1—C4	1.353 (6)	C9—H9A	0.9600
F2—C6	1.351 (6)	C9—H9B	0.9600
C1—C2	1.500 (6)	C9—H9C	0.9600
C2—C7	1.379 (6)	C10—H10A	0.9600
C2—C3	1.389 (6)	C10—H10B	0.9600
C3—C4	1.368 (7)	C10—H10C	0.9600
C3—H3	0.9300		
C10—Sn1—C9	124.0 (2)	C4—C5—H5	121.5
C10—Sn1—C8	117.8 (3)	F2—C6—C7	119.1 (6)

C9—Sn1—C8	116.5 (3)	F2—C6—C5	118.3 (5)
C10—Sn1—O1	98.80 (19)	C7—C6—C5	122.7 (5)
C9—Sn1—O1	93.67 (19)	C6—C7—C2	119.3 (5)
C8—Sn1—O1	90.07 (19)	C6—C7—H7	120.3
C10—Sn1—O2^{i}	84.63 (19)	C2—C7—H7	120.3
C9—Sn1—O2^{i}	86.19 (18)	Sn1—C8—H8A	109.5
C8—Sn1—O2^{i}	86.33 (19)	Sn1—C8—H8B	109.5
O1—Sn1—O2^{i}	175.91 (13)	H8A—C8—H8B	109.5
C1—O1—Sn1	126.3 (3)	Sn1—C8—H8C	109.5
C1—O2—Sn1^{ii}	155.9 (3)	H8A—C8—H8C	109.5
O2—C1—O1	124.4 (5)	H8B—C8—H8C	109.5
O2—C1—C2	121.4 (4)	Sn1—C9—H9A	109.5
O1—C1—C2	114.2 (4)	Sn1—C9—H9B	109.5
C7—C2—C3	119.5 (5)	H9A—C9—H9B	109.5
C7—C2—C1	120.8 (4)	Sn1—C9—H9C	109.5
C3—C2—C1	119.7 (4)	H9A—C9—H9C	109.5
C4—C3—C2	118.5 (5)	H9B—C9—H9C	109.5
C4—C3—H3	120.7	Sn1—C10—H10A	109.5
C2—C3—H3	120.7	Sn1—C10—H10B	109.5
F1—C4—C3	118.9 (5)	H10A—C10—H10B	109.5
F1—C4—C5	118.2 (5)	Sn1—C10—H10C	109.5
C3—C4—C5	122.9 (5)	H10A—C10—H10C	109.5
C6—C5—C4	117.0 (5)	H10B—C10—H10C	109.5
C6—C5—H5	121.5		

C10—Sn1—O1—C1	59.5 (4)	C1—C2—C3—C4	178.5 (4)
C9—Sn1—O1—C1	−65.8 (4)	C2—C3—C4—F1	179.1 (4)
C8—Sn1—O1—C1	177.7 (4)	C2—C3—C4—C5	−2.2 (8)
Sn1^{ii}—O2—C1—O1	133.6 (7)	F1—C4—C5—C6	−179.2 (5)
Sn1^{ii}—O2—C1—C2	−46.9 (11)	C3—C4—C5—C6	2.0 (8)
Sn1—O1—C1—O2	−4.0 (7)	C4—C5—C6—F2	180.0 (5)
Sn1—O1—C1—C2	176.5 (3)	C4—C5—C6—C7	−0.1 (8)
O2—C1—C2—C7	−11.4 (7)	F2—C6—C7—C2	178.3 (4)
O1—C1—C2—C7	168.2 (4)	C5—C6—C7—C2	−1.6 (8)
O2—C1—C2—C3	170.6 (5)	C3—C2—C7—C6	1.5 (7)
O1—C1—C2—C3	−9.9 (6)	C1—C2—C7—C6	−176.6 (4)
C7—C2—C3—C4	0.4 (7)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9*C*···F1^{iii}	0.96	2.62	3.470 (7)	148

Symmetry code: (iii) *x*, −*y*, *z*−1/2.