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

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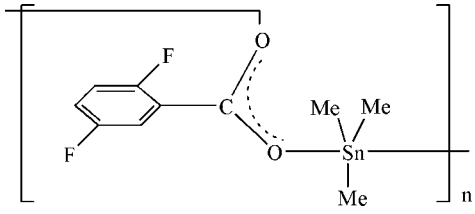
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.014 Å; R factor = 0.036; wR factor = 0.107; data-to-parameter ratio = 15.8.

In the title polymeric coordination compound, $[Sn(CH_3)_3(C_7H_3F_2O_2)]_n$, the Sn atom exhibits a distorted trigonal-bipyramidal coordination geometry with the carboxylate O atoms in the axial positions and the equatorial positions occupied by the methyl groups. The two Sn—O bond lengths are 2.225 (5) and 2.410 (6) Å.

Related literature

For a related structure, see: Wang *et al.* (2007).



Experimental

Crystal data

$[Sn(CH_3)_3(C_7H_3F_2O_2)]$
M_r = 320.91
Tetragonal, $P4_32_12$
a = 9.8857 (9) Å
c = 24.896 (2) Å
V = 2433.0 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 2.11 mm^{-1}
T = 298 (2) K
0.38 × 0.29 × 0.27 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.502, T_{max} = 0.600
(expected range = 0.474–0.566)
10078 measured reflections
2152 independent reflections
1996 reflections with $I > 2\sigma(I)$
R_{int} = 0.034

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.107
S = 1.00
2152 reflections
136 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}
Absolute structure: Flack (1983), 830 Friedel pairs
Flack parameter: −0.01 (8)

Table 1
Selected geometric parameters (Å, °).

Sn1—C9	2.103 (9)	Sn1—O1	2.225 (5)
Sn1—C10	2.110 (8)	Sn1—O2^{i}	2.410 (6)
Sn1—C8	2.118 (7)		
O1—Sn1—O2^{i}	174.15 (19)		

Symmetry code: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+\frac{1}{4}$.

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: GK2177).

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supporting information

Acta Cryst. (2009). E**65**, m29 [doi:10.1107/S1600536808040774]

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S1. Comment

In recent years the organotin derivatives have attracted considerable attention due to a significant antimicrobial properties as well as antitumor activities. Studies on organotin complexes containing carboxylate ligands with an additional donor atom (e.g N, S or F) that is available for coordinating to Sn atom have revealed that new structural types may lead to different activities. We have therefore synthesized the title compound, and present its crystal structure here. The molecular structure of the compound is shown in Fig.1 The Sn atom, assumes a distorted trigonal bipyramidal coordination geometry, provided by three methyl groups at the equatorial positions and two carboxylate groups at the axial positions. The Sn—O bond lengths in the compound (Table 1), are similar to those found in related organotin carboxylates (Wang *et al.*, 2007). In the crystal packing, molecules are linked by intermolecular C—H···F hydrogen bonds (Fig.2, Table 1,)

S2. Experimental

The reaction was carried out under nitrogen atmosphere. 2,5-Difluorobenzoic 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 to the reactor and the reaction mixture was stirred for 12 h at room temperature. The resulting clear solution was evaporated under vacuum. The product was crystallized from dichloromethane/methanol (1:1) to yield colourless block crystals (yield 83%. m.p.393K). Anal. Calcd (%) for $C_{10}H_{12}F_2O_2Sn$(Mr = 320.91): C, 37.43; H, 3.77; F, 11.84; Sn, 36.99. Found (%): C, 37.39; H, 3.86; F, 11.78; Sn, 36.89.

S3. Refinement

The 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, O) or 1.5 U_{eq}(C) for the methyl group.

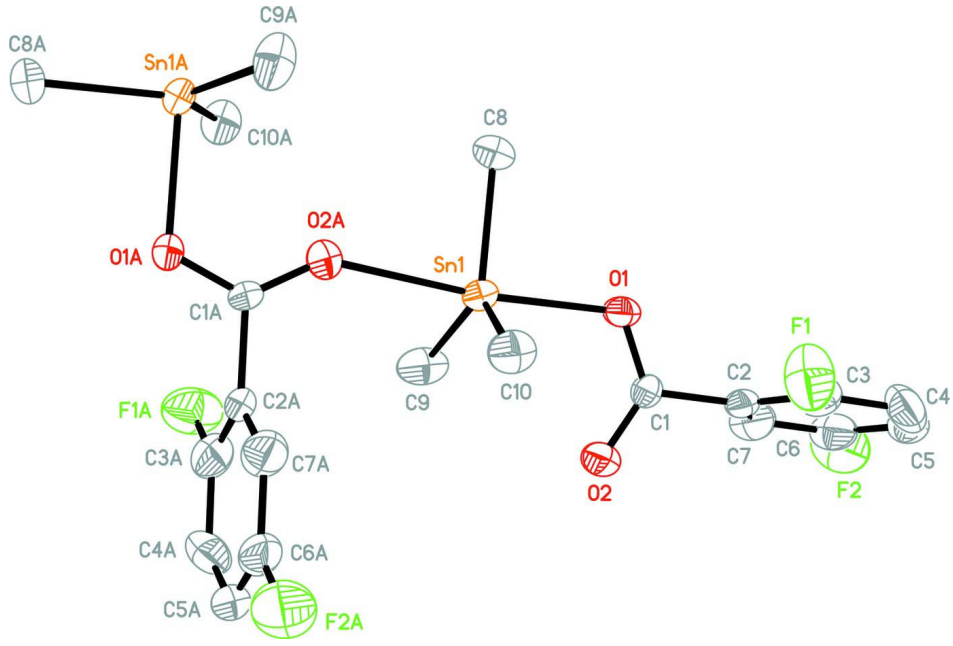

Figure 1

The molecular structure of the compound, showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity. Symmetry codes: (A) = *x* - 1/2,-*y* + 3/2,-*z* + 1/4, (B) = *x* + 1/2,-*y* + 3/2,-*z* + 1/4

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Crystal data

$[Sn(CH_3)_3(C_7H_3F_2O_2)]$
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Hall symbol: P 4nw 2abw
a = 9.8857 (9) Å
c = 24.896 (2) Å
V = 2433.0 (4) Å^3
Z = 8
F(000) = 1248
D_x = 1.752 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 5675 reflections
θ = 2.2–26.4°
μ = 2.11 mm^{-1}
T = 298 K
Block, colourless
0.38 × 0.29 × 0.27 mm

Data collection

Siemens SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.502, T_{max} = 0.600
10078 measured reflections
2152 independent reflections
1996 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −11→11
k = −11→7
l = −16→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.107
S = 1.00
2152 reflections
136 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

$w = 1/[\sigma^2(F_o^2) + (0.066P)^2 + 4.861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.46$ e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: −0.01 (8)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.79786 (5)	0.82634 (5)	0.11522 (2)	0.05163 (18)
F1	1.1717 (7)	1.1333 (7)	0.1597 (3)	0.111 (2)
F2	1.4123 (8)	1.0943 (8)	−0.0335 (3)	0.131 (3)
O1	0.9583 (5)	0.9696 (5)	0.0890 (2)	0.0632 (14)
O2	1.1085 (6)	0.8095 (6)	0.1065 (3)	0.0786 (18)
C1	1.0763 (7)	0.9249 (7)	0.0922 (3)	0.0552 (19)
C2	1.1900 (8)	1.0242 (7)	0.0773 (3)	0.0561 (18)
C3	1.2313 (10)	1.1239 (11)	0.1101 (4)	0.080 (3)
C4	1.3367 (11)	1.2144 (9)	0.0992 (5)	0.089 (3)
H4	1.3649	1.2787	0.1240	0.107*
C5	1.3953 (9)	1.2021 (11)	0.0498 (5)	0.082 (3)
H5	1.4635	1.2615	0.0395	0.098*
C6	1.3539 (10)	1.1028 (11)	0.0153 (4)	0.081 (3)
C7	1.2516 (10)	1.0141 (11)	0.0269 (4)	0.078 (3)
H7	1.2240	0.9495	0.0020	0.093*
C8	0.6502 (9)	0.9694 (8)	0.0912 (3)	0.067 (2)
H8A	0.6849	1.0227	0.0621	0.100*
H8B	0.6287	1.0274	0.1210	0.100*
H8C	0.5700	0.9229	0.0797	0.100*
C9	0.8458 (10)	0.6721 (11)	0.0603 (4)	0.081 (3)
H9A	0.7645	0.6261	0.0497	0.122*
H9B	0.9065	0.6088	0.0769	0.122*
H9C	0.8882	0.7108	0.0292	0.122*
C10	0.8626 (9)	0.8328 (10)	0.1959 (3)	0.070 (2)
H10A	0.9112	0.7514	0.2043	0.105*
H10B	0.7854	0.8405	0.2191	0.105*
H10C	0.9207	0.9095	0.2011	0.105*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0368 (3)	0.0477 (3)	0.0704 (3)	0.0054 (2)	−0.0009 (2)	0.0029 (2)
F1	0.121 (6)	0.108 (5)	0.103 (4)	−0.027 (4)	0.039 (4)	−0.022 (4)
F2	0.138 (6)	0.136 (6)	0.120 (5)	0.010 (5)	0.067 (5)	0.039 (4)
O1	0.040 (3)	0.047 (3)	0.102 (4)	0.009 (2)	0.009 (3)	0.020 (3)
O2	0.054 (3)	0.054 (3)	0.128 (5)	0.005 (3)	−0.001 (3)	0.029 (4)
C1	0.031 (3)	0.047 (4)	0.087 (5)	−0.004 (3)	0.012 (3)	0.014 (4)
C2	0.033 (3)	0.046 (4)	0.089 (5)	0.005 (3)	0.003 (4)	0.015 (4)

C3	0.063 (6)	0.083 (7)	0.094 (7)	0.012 (5)	0.020 (5)	0.004 (6)
C4	0.100 (8)	0.048 (5)	0.119 (8)	−0.007 (5)	0.014 (6)	0.007 (5)
C5	0.046 (5)	0.067 (6)	0.133 (9)	0.001 (5)	0.013 (5)	0.035 (6)
C6	0.058 (5)	0.087 (7)	0.099 (7)	0.012 (5)	0.025 (5)	0.039 (6)
C7	0.067 (6)	0.089 (7)	0.077 (6)	0.006 (5)	0.011 (5)	0.026 (5)
C8	0.062 (5)	0.050 (5)	0.088 (5)	0.013 (4)	−0.004 (4)	0.007 (4)
C9	0.074 (6)	0.092 (7)	0.078 (6)	0.025 (6)	−0.012 (5)	−0.009 (5)
C10	0.068 (5)	0.074 (6)	0.068 (5)	0.008 (4)	−0.003 (4)	−0.004 (4)

Geometric parameters (Å, º)

Sn1—C9	2.103 (9)	C4—H4	0.9300
Sn1—C10	2.110 (8)	C5—C6	1.366 (15)
Sn1—C8	2.118 (7)	C5—H5	0.9300
Sn1—O1	2.225 (5)	C6—C7	1.369 (14)
Sn1—O2^{i}	2.410 (6)	C7—H7	0.9300
F1—C3	1.373 (11)	C8—H8A	0.9600
F2—C6	1.349 (11)	C8—H8B	0.9600
O1—C1	1.250 (9)	C8—H8C	0.9600
O2—C1	1.237 (9)	C9—H9A	0.9600
O2—Sn1^{ii}	2.410 (6)	C9—H9B	0.9600
C1—C2	1.537 (10)	C9—H9C	0.9600
C2—C3	1.344 (13)	C10—H10A	0.9600
C2—C7	1.399 (12)	C10—H10B	0.9600
C3—C4	1.399 (14)	C10—H10C	0.9600
C4—C5	1.365 (14)		
C9—Sn1—C10	125.0 (4)	C6—C5—H5	119.9
C9—Sn1—C8	117.1 (4)	F2—C6—C5	118.8 (10)
C10—Sn1—C8	117.2 (3)	F2—C6—C7	117.7 (11)
C9—Sn1—O1	96.3 (3)	C5—C6—C7	123.4 (10)
C10—Sn1—O1	92.5 (3)	C6—C7—C2	117.7 (11)
C8—Sn1—O1	89.1 (3)	C6—C7—H7	121.2
C9—Sn1—O2^{i}	87.8 (3)	C2—C7—H7	121.2
C10—Sn1—O2^{i}	88.5 (3)	Sn1—C8—H8A	109.5
C8—Sn1—O2^{i}	85.4 (3)	Sn1—C8—H8B	109.5
O1—Sn1—O2^{i}	174.15 (19)	H8A—C8—H8B	109.5
C1—O1—Sn1	114.9 (4)	Sn1—C8—H8C	109.5
C1—O2—Sn1^{ii}	142.9 (5)	H8A—C8—H8C	109.5
O2—C1—O1	125.8 (6)	H8B—C8—H8C	109.5
O2—C1—C2	118.1 (6)	Sn1—C9—H9A	109.5
O1—C1—C2	116.2 (6)	Sn1—C9—H9B	109.5
C3—C2—C7	117.7 (8)	H9A—C9—H9B	109.5
C3—C2—C1	123.0 (8)	Sn1—C9—H9C	109.5
C7—C2—C1	119.3 (8)	H9A—C9—H9C	109.5
C2—C3—F1	117.8 (9)	H9B—C9—H9C	109.5
C2—C3—C4	125.3 (9)	Sn1—C10—H10A	109.5
F1—C3—C4	116.8 (10)	Sn1—C10—H10B	109.5

C5—C4—C3	115.7 (10)	H10A—C10—H10B	109.5
C5—C4—H4	122.1	Sn1—C10—H10C	109.5
C3—C4—H4	122.1	H10A—C10—H10C	109.5
C4—C5—C6	120.1 (9)	H10B—C10—H10C	109.5
C4—C5—H5	119.9		
C9—Sn1—O1—C1	−58.5 (6)	C1—C2—C3—F1	2.4 (13)
C10—Sn1—O1—C1	67.1 (6)	C7—C2—C3—C4	−3.8 (15)
C8—Sn1—O1—C1	−175.6 (7)	C1—C2—C3—C4	178.1 (9)
Sn1^{ii}—O2—C1—O1	−166.0 (7)	C2—C3—C4—C5	3.6 (16)
Sn1^{ii}—O2—C1—C2	13.5 (15)	F1—C3—C4—C5	179.3 (8)
Sn1—O1—C1—O2	2.8 (12)	C3—C4—C5—C6	−2.5 (15)
Sn1—O1—C1—C2	−176.8 (5)	C4—C5—C6—F2	179.0 (9)
O2—C1—C2—C3	−103.1 (10)	C4—C5—C6—C7	2.0 (16)
O1—C1—C2—C3	76.4 (11)	F2—C6—C7—C2	−179.2 (8)
O2—C1—C2—C7	78.8 (11)	C5—C6—C7—C2	−2.1 (15)
O1—C1—C2—C7	−101.7 (9)	C3—C2—C7—C6	2.9 (13)
C7—C2—C3—F1	−179.5 (8)	C1—C2—C7—C6	−178.9 (8)

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*+1/4; (ii) *x*+1/2, −*y*+3/2, −*z*+1/4.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···F1^{iii}	0.93	2.63	3.336 (13)	133

Symmetry code: (iii) *x*+1/2, −*y*+5/2, −*z*+1/4.