



catena-Poly[μ -trifluoroacetato-*O*:*O'*-dimethyl-4-fluorophenyltin(IV)]

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Key indicators

Single-crystal X-ray study

$T = 298$ K

Mean $\sigma(\text{C}-\text{C}) = 0.007$ Å

R factor = 0.030

wR factor = 0.061

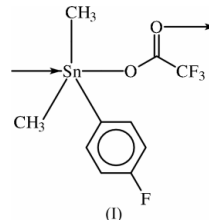
Data-to-parameter ratio = 18.8

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

catena-Poly[μ -trifluoroacetato-*O*:*O'*-dimethyl-4-fluorophenyltin(IV)], $[(\text{CH}_3)_2(4\text{-FC}_6\text{H}_4)\text{SnOC}(\text{O})\text{CF}_3]_n$, exists as a helical carboxylate-bridged chain in which the Sn atom shows $\text{-C}_3\text{SnO}_2$ trigonal bipyramidal coordination [Sn—O 2.194 (3) and Sn \leftarrow O 2.531 (3) Å].

Comment

An earlier study had documented the crystal structure of dimethylphenyltin trifluoroacetate (Amini *et al.*, 2002), a member of the $R_2R''\text{SnO}_2\text{CR}'''$ class of carboxylate-bridged compounds, whose synthesis is non-trivial owing to the difficulty of obtaining the $R_2R''\text{SnX}$ ($X = \text{halide}$) reagent in a pure form. The compound adopts a helical motif as the repeat unit propagates by 2_1 screw axial translations along the b -axis of the orthorhombic cell. The 4-fluoro-substituted derivative, (I), (Fig. 1) is isomorphous with this compound, whose structure has already been discussed in detail.



Experimental

Dimethyl(4-fluorophenyl)tin iodide was synthesized using iodine to cleave the tin–aryl bond of dimethyldi(4-fluorophenyl)tin (Davison & Rakita, 1970). The iodide (0.37 g, 1 mmol) and silver trifluoroacetate (0.22 g, 1 mmol) when reacted in ethanol gave a precipitate of silver iodide, which was removed by filtration. Evaporation of the solvent gave an oily material, which was purified by crystallization from a 1/1 $\text{CHCl}_3/\text{CCl}_4$ mixture to furnish colorless crystals, m.p. 403–404 K. In the ^1H NMR in CDCl_3 , the tin–methyl coupling constant was 57 Hz; the ^{119}Sn NMR signal appeared at 140 p.p.m.. IR (KBr): 1639 (CO_2), 1573 (CO_2), 562 and 535 (Sn—C) cm^{-1} .

Crystal data

$[\text{Sn}(\text{C}_2\text{F}_3\text{O}_2)(\text{C}_6\text{H}_4\text{F})(\text{CH}_3)_2]$

$M_r = 356.87$

Orthorhombic, $P2_12_12_1$

$a = 7.0005$ (3) Å

$b = 10.8221$ (4) Å

$c = 16.7241$ (6) Å

$V = 1267.02$ (8) Å³

$Z = 4$

$D_x = 1.871$ Mg m⁻³

Mo $K\alpha$ radiation

Cell parameters from 9210

reflections

$\theta = 2.3\text{--}28.3^\circ$

$\mu = 2.05$ mm⁻¹

$T = 298$ (2) K

Parallelepiped, colorless

$0.37 \times 0.34 \times 0.31$ mm

Data collection

Bruker SMART APEX area-detector diffractometer

 φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\min} = 0.438$, $T_{\max} = 0.529$

10861 measured reflections

2931 independent reflections

 2772 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\max} = 28.3^\circ$
 $h = -9 \rightarrow 9$
 $k = -14 \rightarrow 14$
 $l = -21 \rightarrow 21$

Refinement

 Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.030$
 $wR(F^2) = 0.061$
 $S = 0.92$

2931 reflections

156 parameters

H-atom parameters constrained

 $w = 1/[\sigma^2(F_o^2) + (0.0343P)^2]$

 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.40 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.60 \text{ e } \text{\AA}^{-3}$

Absolute structure: Flack parameter (Flack & Schwarzenbach, 1988) from 1181 Friedel pairs

 Flack parameter = $-0.03(3)$
Table 1

 Selected geometric parameters (\AA , $^\circ$).

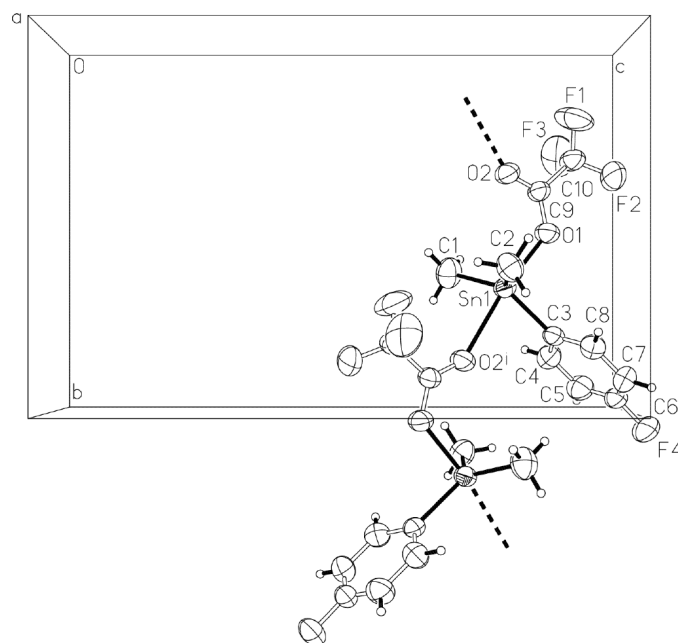
Sn1—O1	2.194 (3)	Sn1—C2	2.109 (5)
Sn1—O2 ⁱ	2.531 (3)	Sn1—C3	2.115 (4)
Sn1—C1	2.103 (5)		
O1—Sn1—O2 ⁱ	171.5 (1)	O2 ⁱ —Sn1—C2	87.4 (1)
O1—Sn1—C1	93.9 (2)	O2 ⁱ —Sn1—C3	82.3 (1)
O1—Sn1—C2	97.7 (2)	C1—Sn1—C2	123.5 (2)
O1—Sn1—C3	89.4 (1)	C1—Sn1—C3	119.8 (2)
O2 ⁱ —Sn1—C1	88.8 (2)	C2—Sn1—C3	115.4 (2)

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

The structure was solved by using the atomic coordinates of the dimethylphenyltin trifluoroacetate structure.

The H atoms were placed at calculated position and were allowed to ride on their parent C-atoms [$C-H$ 0.93 \AA and $U(H) = 1.2U_{\text{eq}}(C)$ for the aromatic H atoms; $C-H$ 0.96 \AA and $U(H) = 1.5U_{\text{eq}}(C)$ for the methyl H atoms]. The torsional angles were refined for the methyl groups.

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT; program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.


Figure 1

ORTEP (Johnson, 1976) plot of the helical chain of dimethyl-4-fluorophenyltin trifluoroacetate; displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$.]

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