Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

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

Mostafa M. Amini,[a] Shabnam Hossein Abadi,[a] Mahdi Mirzaee,[a] Shi-Yao Yang[b] and Seik Weng Ng[c]*

[a]Department of Chemistry, Shahid Beheshti University, Tehran, Iran, [b]Department of Chemistry, Xiamen University, Xiamen 361005, People's Republic of China, and [c]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Received 29 August 2003
Accepted 1 September 2003
Online 5 September 2003

catena-Poly[μ-trifluoroacetato-*O:O*′-dimethyl-4-fluorophenyltin(IV)], $[(CH_3)_2(4\text{–}FC_6H_4)SnOC(O)CF_3]_n$, exists as a helical carboxylate-bridged chain in which the Sn atom shows $–C_3SnO_2$ trigonal bipyramidal coordination [Sn—O 2.194 (3) and Sn←O 2.531 (3) Å].

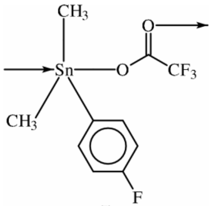
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–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.

Comment

An earlier study had documented the crystal structure of dimethylphenyltin trifluoroacetate (Amini *et al.*, 2002), a member of the $R'_2R''SnO_2CR'''$ class of carboxylate-bridged compounds, whose synthesis is non-trivial owing to the difficulty of obtaining the $R'_2R''SnX$ (X = 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.



(I)

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 $CHCl_3/CCl_4$ 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

$[Sn(C_2F_3O_2)(C_6H_4F)(CH_3)_2]$
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) Å^3
Z = 4
D_x = 1.871 Mg m^{-3}

Mo *Kα* radiation
Cell parameters from 9210 reflections
θ = 2.3–28.3°
μ = 2.05 mm^{-1}
T = 298 (2) K
Parallelepiped, colorless
0.37 × 0.34 × 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 $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\max} = 28.3°$
$h = -9 \rightarrow 9$
$k = -14 \rightarrow 14$
$l = -21 \rightarrow 21$

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 $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.40$ e Å^{-3}
$\Delta\rho_{\min} = -0.60$ e Å^{-3}
Absolute structure: Flack parameter (Flack & Schwarzenbach, 1988) from 1181 Friedel pairs
Flack parameter = −0.03 (3)

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.194 (3)	Sn1—C2	2.109 (5)
Sn1—O2$^{\rm i}$	2.531 (3)	Sn1—C3	2.115 (4)
Sn1—C1	2.103 (5)		
O1—Sn1—O2$^{\rm i}$	171.5 (1)	O2$^{\rm i}$—Sn1—C2	87.4 (1)
O1—Sn1—C1	93.9 (2)	O2$^{\rm i}$—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$^{\rm i}$—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 Å and U(H) = $1.2U_{\rm eq}$(C) for the aromatic H atoms; C—H 0.96 Å and U(H) = $1.5U_{\rm eq}$(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: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

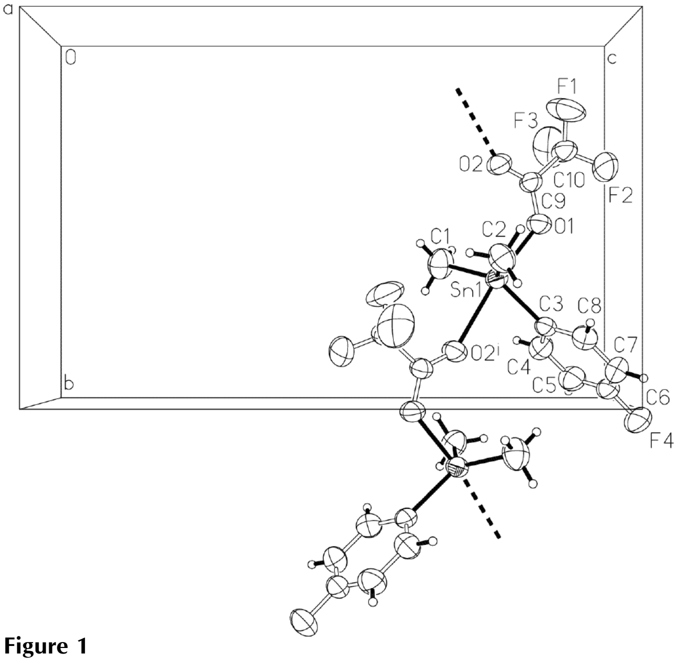


Figure 1
ORTEP (Johnson, 1976) plot of the helical chain of dimethyl-4-fluorophenyltin trifluoroacetate; displacement ellipsoids are drawn at the 50% probability level and H atoms are drawn as spheres of arbitrary radii. [Symmetry code: (i) $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$.]

The authors thank the Vice President's Office of Research Affairs of Shahid Beheshti University, Xiamen University and the University of Malaya for supporting this work.

References

Amini, M. M., Abadi, S. H., Mirzaee, M., Lügger, T., Hahn, F. E. & Ng, S. W. (2002). *Acta Cryst.* E**58**, m650–m652.
Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Davison, A. & Rakita, P. E. (1970). *J. Organomet. Chem.* **23**, 407–436.
Flack, H. D. & Schwarzenbach, D. (1988). *Acta Cryst.* A**44**, 499–506.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Oak Ridge, Tennessee, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.

m848 Mostafa M. Amini *et al.* • $[{\rm Sn(C_2F_3O_2)(C_6H_4F)(CH_3)_2}]$ *Acta Cryst.* (2003). E**59**, m847–m848