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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$
Disorder in main residue
R factor = 0.020
wR factor = 0.051
Data-to-parameter ratio = 14.1

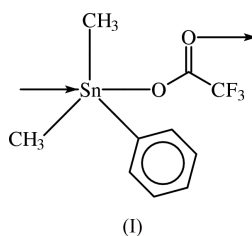
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

catena-Poly[μ -trifluoroacetato-O:O'-dimethylphenyltin(IV)]

catena-Poly[dimethylphenyltin(IV)- μ -trifluoroacetato-O:O'], $[(\text{CH}_3)_2(\text{C}_6\text{H}_5)\text{SnOC}(\text{O})\text{CF}_3]_n$, adopts a helical carboxylate-bridged chain structure, in which the Sn atom shows *trans*- C_3SnO_2 trigonal-bipyramidal coordination, with unequal Sn—O distances of 2.181 (2) and 2.580 (2) Å.

Comment

Triorganotin carboxylates commonly self-assemble as linear chains, whose repeat units involve bridging carboxylate groups (Ng *et al.*, 1988; Haiduc & Edelman, 1999). When the repeat units are propagated by a glide plane in the crystal structure, a zigzag polymeric chain is formed whereas when these are propagated by screw-axis symmetry transformations, a helical polymeric chain results. The repeat distance is generally insensitive to the nature of the groups bonded to the Sn atom and the substituent of the carboxylate group. The dative Sn—O distance generally exceeds the covalent Sn—O distance in these five-coordinate *trans*- C_3SnO_2 trigonal bipyramidal compounds (Tiekink, 1991; Tiekink, 1994), though an exception has been noted (Ng, Kumar Das & Syed, 1989). The triorganotin carboxylates reported in the literature are rarely of the $R'_2R''\text{SnO}_2\text{CR}'''$ type, as the synthesis of the mixed $R'_2R''\text{SnX}$ ($X = \text{halide}$) starting reagent is not trivial.



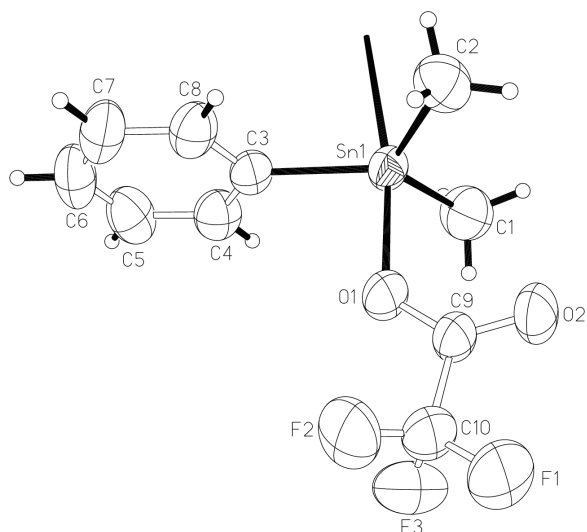
An earlier study has detailed the synthesis and crystal structure of dimethylphenyltin acetate (Amini *et al.*, 1989). The compound exists as a helical, carboxylate-bridged polymer, a structure also adopted by the trifluoroacetate, as determined in the present study (Figs. 1 and 2). In the title compound, (I), the Sn atom is displaced out of the equatorial plane by 0.149 (3) Å in the direction of the covalently bonded O atom O1 [Sn1—O1 = 2.181 (2), Sn1—O2ⁱ = 2.580 (2) Å; symmetry code (i): $1 - x, \frac{1}{2} + y, \frac{3}{2} - z$]. The equatorial plane is almost coplanar with the phenyl ring, the dihedral angle between the planes being 4.2 (2)°. The trifluoromethyl group is disordered, which is quite common for trifluoroacetate structures (Ng *et al.*, 1999).

In contrast to dimethylphenyltin acetate and trifluoroacetate, trimethyltin trifluoroacetate adopts a zigzag conformation (Chih & Penfold, 1973). The mode of propagation of these polymers can be deduced from variable-

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**Figure 1**

ORTEP (Johnson, 1976) plot of the repeat unit of the helical chain of dimethylphenyltin trifluoroacetate; displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii; the minor component of the disordered trifluoromethyl group is omitted.

temperature tin-119m Mössbauer measurements; a zigzag polymer, being more rigid, gives a smaller slope compared with a helical polymer such as triphenyltin chloroacetate (Ng, Chin *et al.*, 1989).

Experimental

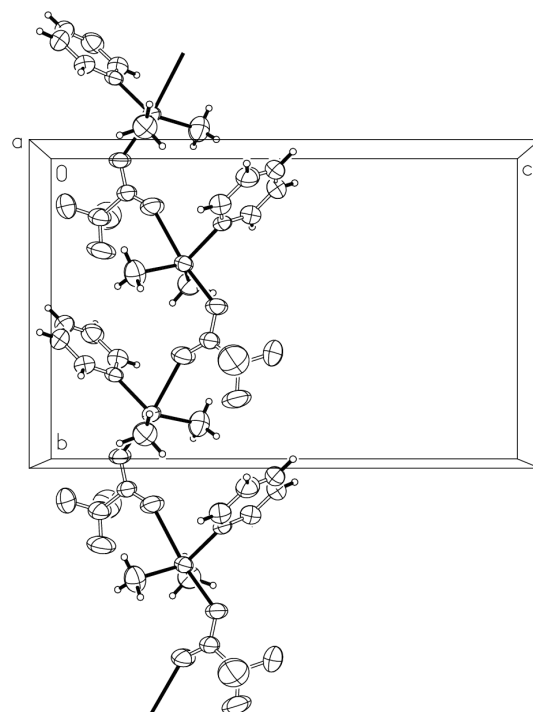
Equimolar quantities of dimethylphenyltin iodide (0.71 g, 2 mmol), which was obtained by the iodine cleavage of dimethyldiphenyltin (Davison & Rakita, 1970; Amini *et al.*, 1989), and silver trifluoroacetate (0.45 g, 2 mmol) were dissolved in ethanol to afford a precipitate of silver iodide. The precipitate was removed by filtration and the solvent evaporated off to yield the crude title compound. Crystals, m.p. 395–396 K, were obtained by recrystallization from carbon tetrachloride. In the ^1H NMR spectrum in CDCl_3 , the two-bond tin-methyl coupling constant was 58 Hz. In the IR spectrum, the tin-methyl bands appeared at 575 and 540 cm^{-1} .

Crystal data

$[\text{Sn}(\text{C}_2\text{F}_3\text{O}_2)(\text{C}_6\text{H}_5)(\text{CH}_3)_2]$	Mo $K\alpha$ radiation
$M_r = 338.88$	Cell parameters from 5881 reflections
Orthorhombic, $P2_12_12_1$	$\theta = 2.2\text{--}26.0^\circ$
$a = 6.6552$ (3) Å	$\mu = 2.07$ mm^{-1}
$b = 10.9949$ (5) Å	$T = 293$ (2) K
$c = 17.0794$ (7) Å	Prism, colorless
$V = 1249.8$ (1) Å ³	$0.24 \times 0.16 \times 0.05$ mm
$Z = 4$	
$D_x = 1.801$ Mg m^{-3}	

Data collection

Bruker AXS CCD area-detector diffractometer	2465 independent reflections
ω scans	2364 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{\text{int}} = 0.026$
$T_{\text{min}} = 0.637$, $T_{\text{max}} = 0.904$	$\theta_{\text{max}} = 26.0^\circ$
10949 measured reflections	$h = -8 \rightarrow 8$
	$k = -13 \rightarrow 13$
	$l = -21 \rightarrow 21$

**Figure 2**

ORTEP (Johnson, 1976) plot of the helical chain of dimethylphenyltin trifluoroacetate; displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii; the minor component of the disordered trifluoromethyl group is omitted.

Refinement

Refinement on F^2	$(\Delta/\sigma)_{\text{max}} < 0.001$
$R[F^2 > 2\sigma(F^2)] = 0.020$	$\Delta\rho_{\text{max}} = 0.27$ e \AA^{-3}
$wR(F^2) = 0.051$	$\Delta\rho_{\text{min}} = -0.43$ e \AA^{-3}
$S = 0.99$	Absolute structure: Flack & Schwarzenbach (1988)
2465 reflections	Flack parameter = 0.04(3);
175 parameters	1197 Friedel pairs
H-atom parameters constrained	
$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2]$	
where $P = (F_o^2 + 2F_c^2)/3$	

Table 1

Selected geometric parameters (Å, °).

Sn1—O1	2.181 (2)	Sn1—C2	2.111 (4)
Sn1—O2 ⁱ	2.580 (2)	Sn1—C3	2.113 (3)
Sn1—C1	2.099 (4)		
O1—Sn1—O2 ⁱ	170.7 (1)	C3—Sn1—O1	90.3 (1)
C1—Sn1—O1	95.6 (2)	C3—Sn1—O2 ⁱ	80.7 (1)
C1—Sn1—O2 ⁱ	87.2 (2)	C1—Sn1—C2	120.6 (2)
C2—Sn1—O1	96.2 (2)	C1—Sn1—C3	121.2 (2)
C2—Sn1—O2 ⁱ	89.9 (2)	C2—Sn1—C3	116.6 (2)

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

The trifluoromethyl group is disordered over two positions; their occupancy ratio was refined to 61 (2):39 (2). The six C—F distances were restrained to be approximately equal; additionally, the F··F interactions were restrained. The temperature factors of the CF_3 group were restrained to be approximately isotropic. H atoms were placed in calculated positions and were allowed to ride on their parent C-atoms; $U(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for the aromatic C atoms and $U(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for the methyl C atoms.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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