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catena-Poly[[trimethyltin(IV)]-μ-3-(4-chlorophenyl)-2-phenylpropenoato-κ^2O:O']

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.079
Data-to-parameter ratio = 20.1

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

The crystal structure of the title compound, $[Sn(CH_3)_3(C_{15}H_{10}ClO_2)]_n$, contains polymeric chains along the *b* axis. The geometry around the Sn atom is distorted trigonal bipyramidal, wherein three methyl groups are bonded to the Sn atom at equatorial positions with essentially identical bond distances [mean Sn—C = 2.119 (6) Å] and two O atoms of the carboxylate ligand are bonded asymmetrically with significantly different Sn—O distances of 2.159 (2) and 2.351 (2) Å.

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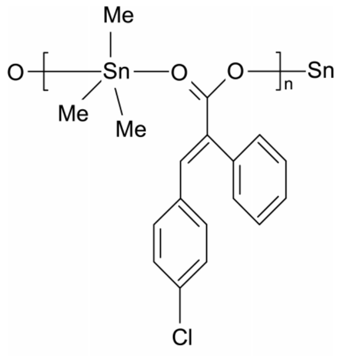
Comment

Organotin compounds are of current interest due to their dramatic increase of industrial, agricultural and biological applications (Xie *et al.*, 1996; Nath *et al.*, 2001). Organotin carboxylates are also employed as catalysts in some reactions, such as reduction of aldehydes to alcohols by 1-butanol in the presence of triphenyltin formate (Wuest & Zacharie, 1984). The solution equilibrium studies of organotin and biologically important ligands have gained importance due to potential pharmaceutical applications of organotin compounds. Today, a number of dialkyltin carboxylate derivatives are known as efficient antitumor and anticancer agents (Crowe, 1989; Gielen, 1996, 2002; Gielen *et al.*, 1994; 2000; de Vos *et al.*, 1998). We have reported the synthesis, spectroscopic characterization and biological applications of several compounds in this area (Badshah *et al.*, 1994; Danish *et al.*, 1995; Bhatti *et al.*, 2000). In continuation of our studies on the structural aspects of organotin carboxylates (Parvez, Ali, Mazhar, Bhatti & Khokhar, 1999; Parvez, Ali, Bhatti *et al.*, 1999; Parvez, Ali, Mazhar, Bhatti & Choudhary, 1999; Parvez *et al.*, 2000, 2002; Sadiq-ur-Rehman, Shouldice *et al.*, 2004; Sadiq-ur-Rehman, Abdelrahman *et al.*, 2004), we have now prepared *catena*-poly[[trimethyltin(IV)]-μ-2-phenyl-3-(4-chlorophenyl)propenoato-κ^2O:O'], (I), the structure of which is reported here.



(I)

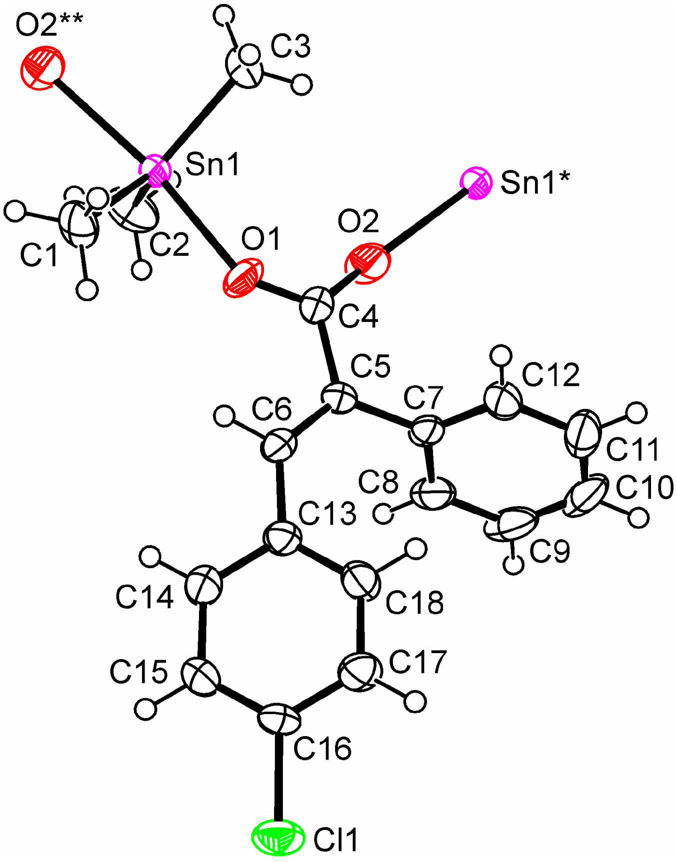


Figure 1
*ORTEP*II (Johnson, 1976) drawing of (I) with displacement ellipsoids plotted at the 50% probability level. [Symmetry codes: (*) $x, y - \frac{1}{2}, \frac{1}{2} - z$; (**) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$]

The structure of (I) (Fig. 1) is composed of polymeric chains (Fig. 2) lying along the *b* axis, wherein both O atoms of the carboxylate ligand are bonded asymmetrically to Sn atoms with significantly different Sn—O distances [Sn1—O1 = 2.159 (2) Å and Sn1—O2** = 2.351 (2) Å; symmetry code: (**) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$]. The geometry around the Sn atom is distorted trigonal bipyramidal. Three methyl groups are bonded to the Sn atom at equatorial positions with essentially identical bond distances [mean Sn—C = 2.119 (6) Å]. The Sn atom lies 0.065 (2) Å out of the equatorial plane formed by the three methyl C atoms, towards the more strongly bonded atom O1. The O—Sn—O angle is approximately linear [171.21 (9)°] and the C—Sn—C and O—Sn—C angles are within the expected range of values [C—Sn—C = 119.24 (15)–120.62 (15)° and O—Sn—C = 84.47 (12)–97.24 (12)°], as observed in similar Sn complexes (Gibson *et al.*, 1997; Parvez *et al.*, 1997, 2000; Hans *et al.*, 2002; Sadiq-ur-Rehman, Shouldice *et al.*, 2004; Sadiq-ur-Rehman, Abdelrahman *et al.*, 2004; Stocco *et al.*, 1996; Gielen *et al.*, 1998; Ramirez *et al.*, 2002).

The molecular dimensions in the ligand are comparable to those reported previously for derivatives of 2,3-diphenylpropenoic acid (Sadiq-ur-Rehman, Shouldice *et al.*, 2004; Sadiq-ur-Rehman, Abdelrahman *et al.*, 2004). The bond distances O2—C4 and O1—C4 [1.214 (4) and 1.260 (4) Å, respectively] indicate that these are double and single bonds, respectively. The propenoate moiety (O1/O2/C4/C5/C6) is planar with a maximum deviation of 0.026 (3) Å for atom C5 and the benzene rings C7–C12 and C13–C18 are inclined at 69.73 (10) and 31.76 (13)°, respectively, to the mean plane of the propenoate moiety. Benzene rings C7–C12 and C13–C18 are inclined at 62.63 (11)° with respect to each other.

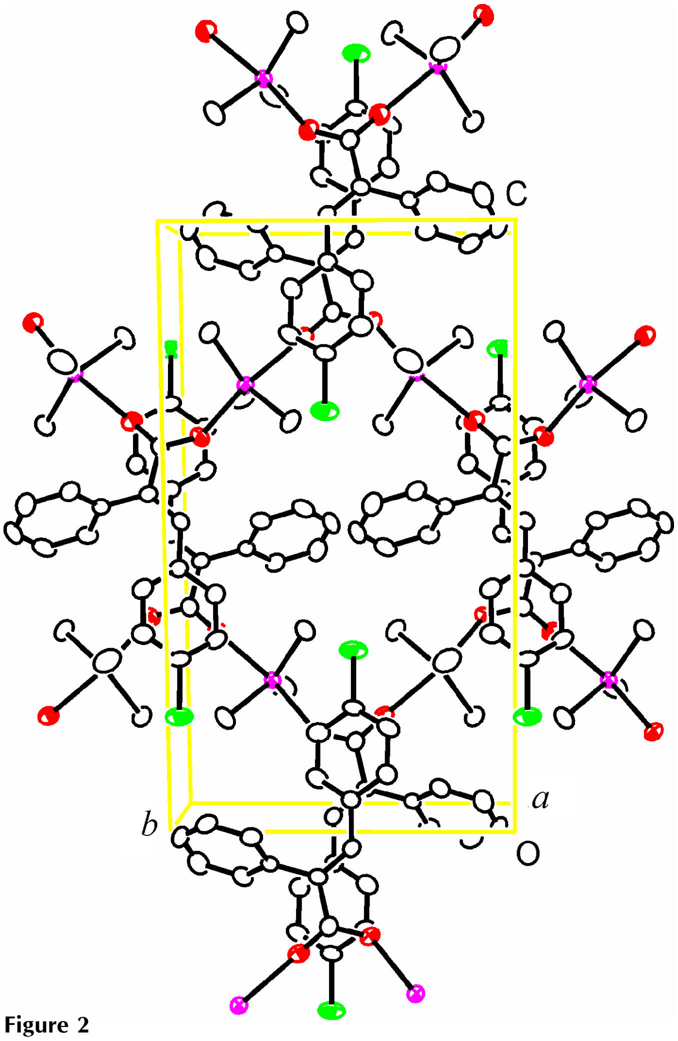


Figure 2
*ORTEP*II (Johnson, 1976) drawing of the contents of the unit cell. H atoms have been omitted.

Experimental

3-(4-Chlorophenyl)-2-phenylpropenoic acid was prepared by a reported method (Nodiff *et al.*, 1971). The sodium salt of the acid was prepared by dissolving 4.0 g (0.016 mol) of acid in ethanol (150 ml), followed by the addition of 1.299 g (0.016 mol) sodium bicarbonate in aqueous solution. The mixture was stirred for 2 h at room temperature and then evaporated on a rotary evaporator. The resultant solid was dried in air (m.p. 596–599 K). The sodium salt of the acid (2.0 g, 0.007 mol) and trimethyltin chloride (1.42 g, 0.007 mol) were suspended in dry toluene (80 ml). The reaction mixture was refluxed for 10 h, filtered at room temperature and the solvent was evaporated under reduced pressure. Compound (I) was recrystallized from a solution of chloroform–*n*-hexane (2:1) by slow evaporation at room temperature (m.p. 389–391 K).

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Crystal data

$[Sn(CH_3)_3(C_{15}H_{10}ClO_2)]$
$M_r = 421.47$
Monoclinic, $P2_1/c$
$a = 9.350$ (3) Å
$b = 10.454$ (3) Å
$c = 18.902$ (7) Å
$\beta = 103.764$ (14)°
$V = 1794.5$ (10) Å^3
$Z = 4$
$D_x = 1.560$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6771 reflections
$\theta = 3.0$–27.5°
$\mu = 1.58$ mm^{-1}
$T = 173$ (2) K
Block, colorless
0.20 × 0.17 × 0.12 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
$T_{\min} = 0.743$, $T_{\max} = 0.833$
6771 measured reflections
4051 independent reflections
3038 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.034$
$\theta_{\max} = 27.5°$
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 11$
$l = -24 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.079$
$S = 1.01$
4051 reflections
202 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0297P)^2 + 0.4273P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.61$ e Å^{-3}
$\Delta\rho_{\min} = -0.69$ e Å^{-3}

Table 1

Selected geometric parameters (Å, °).

Sn1—C2	2.110 (4)	Sn1—O2^{i}	2.351 (2)
Sn1—C1	2.123 (3)	Cl1—C16	1.741 (3)
Sn1—C3	2.123 (3)	O1—C4	1.260 (4)
Sn1—O1	2.159 (2)	O2—C4	1.214 (4)
C2—Sn1—C1	120.62 (15)	C2—Sn1—O2^{i}	87.59 (15)
C2—Sn1—C3	119.85 (14)	C1—Sn1—O2^{i}	87.43 (12)
C1—Sn1—C3	119.24 (14)	C3—Sn1—O2^{i}	89.69 (12)
C2—Sn1—O1	93.60 (16)	O1—Sn1—O2^{i}	171.21 (9)
C1—Sn1—O1	84.47 (12)	C4—O1—Sn1	141.7 (2)
C3—Sn1—O1	97.24 (12)	C4—O2—Sn1^{ii}	178.0 (3)

Symmetry codes: (i) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.

The H atoms were located in difference Fourier syntheses and were included in the refinement at geometrically idealized positions, with C—H = 0.95 and 0.98 Å, and $U_{\rm iso}$ = 1.5 (methyl) and 1.2 (the rest) times $U_{\rm eq}$ of the atoms to which they were bonded. The final difference map was free of any chemically significant features.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *HKL DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI*91 (Fan, 1991); 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.

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