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Key indicators

Single-crystal X-ray study

$T = 173$ K

Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å

R factor = 0.030

wR factor = 0.075

Data-to-parameter ratio = 19.5

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

catena-Poly[[trimethyltin(IV)]- μ -2-(4-chlorophenyl)-3-(4-methoxyphenyl)propenoato- $\kappa^2\text{O}:\text{O}'$]

The title compound, $[\text{Sn}(\text{CH}_3)_3(\text{C}_{16}\text{H}_{12}\text{ClO}_3)]_n$, forms polymeric chains incorporating both O atoms of the propenoate ligand. The coordination geometry around the Sn atom is distorted trigonal bipyramidal. The three methyl C atoms occupy the equatorial positions with almost identical Sn—C distances [2.115 (3)–2.120 (3) Å] and O atoms from two symmetry-related ligands are in the axial positions with significantly different Sn—O distances [2.150 (2) and 2.430 (2) Å].

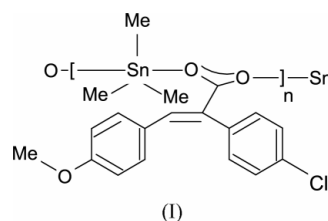
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Comment

The structural chemistry of organotin compounds that have a coordination number greater than four has been widely studied because of the biological activity, enhanced reactivity and stereochemical non-rigidity of these compounds (Mehring *et al.*, 1998). The synthesis and biocidal applications of a number of organotin compounds have been reported (Magos, 1986; Ronconi *et al.*, 2002). Continuing our interest to further our understanding of the structural aspects of organotin carboxylates (Parvez *et al.*, 1999; Parvez, Ali, Bhatti *et al.*, 1999; Parvez, Ali, Mazhar, Bhatti & Choudhary, 1999; Parvez *et al.*, 2000, 2002; Sadiq-ur-Rehman *et al.*, 2004), we now report the structure of *catena*-poly[[trimethyltin(IV)]- μ -2-(4-chlorophenyl)-3-(4-methoxyphenyl)propenoato- $\kappa^2\text{O}:\text{O}'$], (I).



The structure of (I) (Fig. 1) consists of polymeric chains (Fig. 2) incorporating both O atoms of the substituted propenoate, with significantly different Sn—O distances [$\text{Sn}1-\text{O}1 = 2.150$ (2) Å and $\text{Sn}1-\text{O}2^i = 2.430$ (2) Å; symmetry code: (i) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$]. The geometry around the Sn atom is distorted trigonal bipyramidal, with the three methyl groups occupying the positions in the equatorial plane. The Sn—C distances are identical within 3σ limits [mean Sn—C = 2.117 (2) Å]. The Sn atom in (I) is displaced from the equatorial plane formed by the three methyl C atoms by 0.129 (2) Å, towards the more strongly bonded atom O1. The O—Sn—O angle is approximately linear [170.85 (7)°], the C—Sn—C angles are between 118.20 (11) and 121.97 (12)°, deviating very little from the ideal value of 120°, and the O—Sn—C angles are in the range 85.91 (9)–100.23 (9)°. These

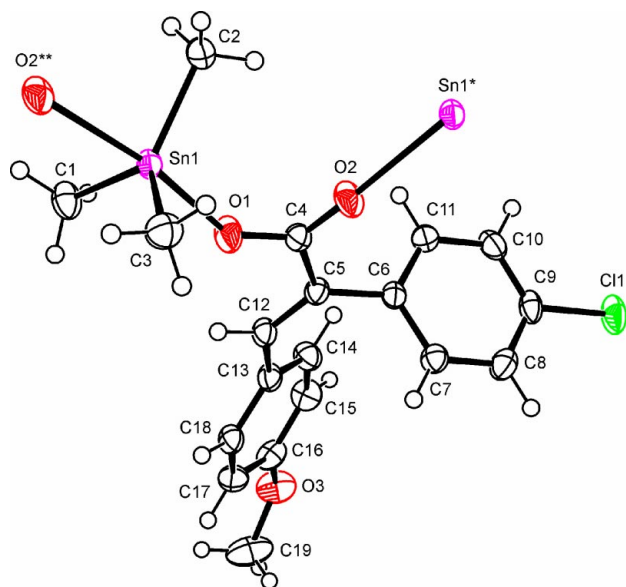


Figure 1
ORTEPII (Johnson, 1976) drawing of (I), with displacement ellipsoids plotted at the 50% probability level. [Symmetry codes: (*) $1 - x, \frac{1}{2} + y, \frac{1}{2} - z$; (**) $1 - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

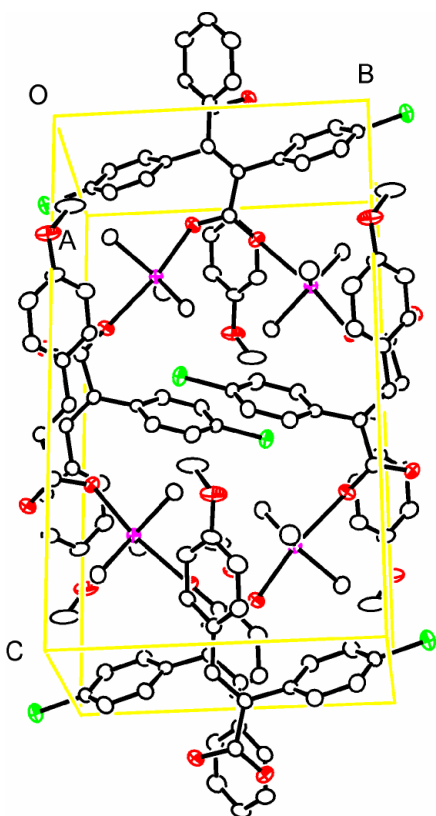


Figure 2
ORTEPII (Johnson, 1976) drawing of the contents of the unit cell, showing the polymeric chains of (I). H atoms have been omitted.

molecular dimensions are in agreement with the corresponding values reported for similar Sn complexes in the Cambridge Structural Database (Version 5.25, 2003 release; Allen, 2002). The molecular dimensions in the ligand are normal. The bond distances O1—C4 and O2—C4 of 1.270 (3)

and 1.227 (3) Å, respectively, clearly indicate that the former is a single bond and the latter is a double bond. Both the phenyl rings are individually planar, as expected, and are inclined at 66.74 (9)° to each other. The propenoate moiety, O1/O2/C4/C5/C12, is essentially planar [maximum deviation for C5 of 0.027 (2) Å] and the mean planes of phenyl rings C6—C11 and C13—C18 form angles of 67.92 (9) and 44.87 (10)°, respectively, with the propenoate group.

Experimental

The silver salt of (*E*)-3-(4-methoxyphenyl)-2-(4-chlorophenyl)-propenoic acid (2.5 g, 6.32 mmol) was suspended in dry chloroform (50 ml) contained in a 250 ml two-necked round-bottomed flask, equipped with all accessories. Trimethyltin chloride (1.36 g, 6.32 mmol) dissolved in dry chloroform (30 ml) was added dropwise with constant stirring to this suspension. The reaction mixture was refluxed for 6–8 h and allowed to stand overnight at room temperature. The silver chloride which settled was filtered off and the solvent was evaporated under reduced pressure. The solid obtained was recrystallized from chloroform–*n*-hexane (4:1) (yield = 90%, m.p. = 399–401 K).

Crystal data

[Sn(CH₃)₃(C₁₆H₁₂ClO₃)]
M_r = 451.50
 Monoclinic, *P*2₁/*c*
a = 9.512 (2) Å
b = 10.424 (2) Å
c = 19.421 (4) Å
 β = 101.118 (14)°
V = 1889.5 (7) Å³
Z = 4

D_x = 1.587 Mg m⁻³
 Mo K α radiation
 Cell parameters from 7498 reflections
 θ = 3.3–27.5°
 μ = 1.51 mm⁻¹
T = 173 (2) K
 Block, colorless
 0.14 × 0.14 × 0.09 mm

Data collection

Nonius KappaCCD diffractometer
 ω and φ scans
 Absorption correction: multi-scan (SORTAV; Blessing, 1997)
T_{min} = 0.817, *T_{max}* = 0.876
 7498 measured reflections
 4314 independent reflections

3546 reflections with *I* > 2 σ (*I*)
R_{int} = 0.027
 θ_{\max} = 27.5°
h = -12 → 12
k = -13 → 13
l = -25 → 25

Refinement

Refinement on *F*²
R [*F*² > 2 σ (*F*²)] = 0.030
wR(*F*²) = 0.075
S = 1.03
 4314 reflections
 221 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0378P)^2 + 0.4627P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.04 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.76 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Sn1—C3	2.115 (3)	Cl1—C9	1.751 (3)
Sn1—C1	2.117 (3)	O1—C4	1.270 (3)
Sn1—C2	2.120 (3)	O2—C4	1.227 (3)
Sn1—O1	2.150 (2)	O3—C16	1.377 (3)
Sn1—O2 ⁱ	2.430 (2)	O3—C19	1.418 (4)
C3—Sn1—C1	118.73 (12)	Cl1—Sn1—O2 ⁱ	85.91 (9)
C3—Sn1—C2	121.97 (12)	C2—Sn1—O2 ⁱ	87.52 (9)
C1—Sn1—C2	118.20 (11)	O1—Sn1—O2 ⁱ	170.85 (7)
C3—Sn1—O1	93.83 (11)	C4—O1—Sn1	139.0 (2)
C1—Sn1—O1	86.13 (10)	C4—O2—Sn1 ⁱⁱ	176.0 (2)
C2—Sn1—O1	100.23 (9)	C16—O3—C19	117.3 (2)
C3—Sn1—O2 ⁱ	86.05 (10)		

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

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 $U_{\text{iso}}(\text{H}) = 1.5$ (methyl) and 1.2 (aromatic) times U_{eq} of the atoms to which they were bonded. The largest peak in the difference map is close to Sn with no chemical significance, and may be attributed to residual effects caused by deficiencies in the absorption correction procedures.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *HKL DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALE-PACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI91* (Fan, 1991); 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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