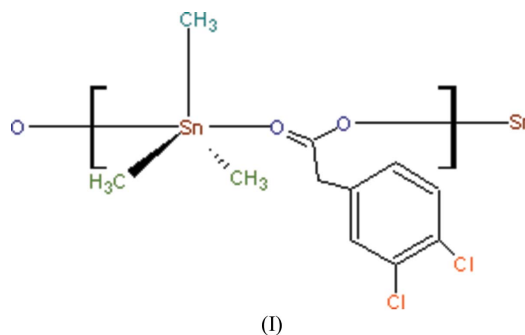


catena-Poly[trimethyltin(IV)- μ -3,4-dichlorophenylacetato]**M. Adeel Saeed,^{a*} D. C. Craig,^b
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adeel_chm@hotmail.com**Key indicators**Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.012$ Å
 R factor = 0.043
 wR factor = 0.055
Data-to-parameter ratio = 13.8For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $[\text{Sn}(\text{CH}_3)_3(\text{C}_8\text{H}_5\text{Cl}_2\text{O}_2)]_n$, forms polymeric chains involving both O atoms of the carboxylate group. The coordination geometry of the Sn atom is slightly distorted trigonal bipyramidal. The three methyl groups occupy the equatorial positions, with Sn—C bond lengths in the range 2.103 (8)–2.118 (7) Å. The two O atoms are situated in the axial positions, with Sn—O distances of 2.189 (4) Å and 2.369 (5) Å.

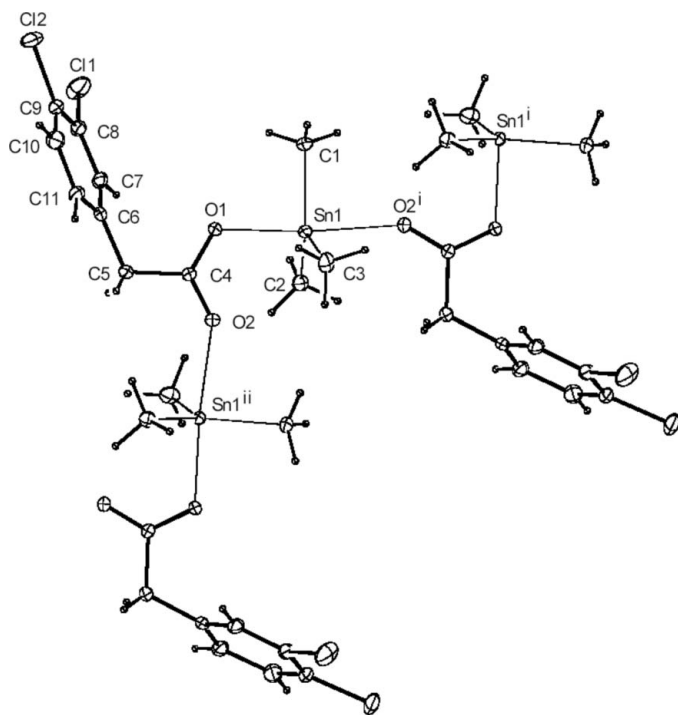
Comment

Tin(IV) organotin halides are utilized to synthesize organotin carboxylates with the use of a suitable solvent, such as acetone or CCl_4 . Tin carboxylates generally exhibit low solubilities in organic solvents because of their polymeric associated structure. This chain polymer structure, involving bridging carboxylate groups and planar or near planar R_3Sn units, has been demonstrated crystallographically for $\text{Me}_3\text{SnOCOMe}$, $\text{Bz}_3\text{SnOCOMe}$ (Chih *et al.*, 1973) and $(\text{CH}_2\text{CH}_3)_3\text{SnOCOCCl}_3$ (Calogero *et al.*, 1979). Organotin complexes of metal carboxylates of the general formula $\text{R}_n\text{Sn}(\text{OCOR})_{4-n}$ have already been reported (Wang & Shreeve, 1972). The biocidal applications of organotin compounds include their implication in acute poisoning in humans (Rudel, 2003; Jiang *et al.*, 2000) and animals (Wester *et al.*, 1990; Martin *et al.*, 1989). Owing to their cytotoxicity, these compounds have been explored as anti-tumour agents (Gielen *et al.*, 2000). Several investigators have studied these biologically active organotin species with coordination number greater than four (Di Stefano *et al.*, 2004; Mehring *et al.*, 1998; Teoh *et al.*, 1999; Carcelli *et al.*, 1995).



Continuing our interest in the structural aspects of organotin carboxylates (Parvez, Ali, Bhatti *et al.*, 1999; Parvez, Ali, Mazhar *et al.*, 1999; Parvez, Ali, Mazhar, Bhatti & Khokhar, 1999; Parvez *et al.*, 2000, 2002; Sadiq-ur-Rehman *et al.*, 2004), we now report the synthesis and crystal structure of the title compound, (I). The structure of (I) consists of poly-

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Figure 1

ORTEP (Johnson, 1976) plot of the title compound, with displacement ellipsoids drawn at the 10% probability level. H atoms are drawn as spheres of arbitrary radius. [Symmetry codes: (i) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (ii) $\frac{1}{2} - x, -\frac{1}{2} + y, 1/2 - z$.]

meric chains, the interaction of both O atoms with the Sn atom having slightly different Sn–O distances [Sn1–O1 = 2.189 (4) Å and Sn1–O2 = 2.369 (5) Å]. The geometry around the Sn atom is distorted trigonal bipyramidal, with the three methyl groups occupying the positions in the equatorial plane. The O–Sn–O angle is approximately linear [174.7 (2)°], the C–Sn–C angles are between 118.1 (4) and 122.8 (3)°, deviating very little from the ideal value of 120°, and the O–Sn–C angles are in the range 85.5 (3)–95.8 (2)°.

Experimental

Trimethyltin(IV) chloride (0.9 g, 0.5 mmol, from Aldrich) and sodium dichlorophenylacetate (1 g, 4.4 mmol from Aldrich) were dissolved in dry toluene (100 ml) in a two-necked round-bottomed flask. The reaction mixture was refluxed for 4 h with continuous stirring. The resulting sodium salt was removed by filtration and the solvent was evaporated under reduced pressure. The solid material obtained was recrystallized from a mixture of acetone–*n*-hexane (80:20), giving fine crystals suitable for single-crystal X-ray diffraction (yield 85%, m.p. 388 K).

Crystal data

[Sn(CH₃)₃(C₈H₅Cl₂O₂)]

M_r = 367.8

Monoclinic, *C*2/*c*

a = 12.660 (3) Å

b = 9.801 (1) Å

c = 23.462 (5) Å

β = 96.01 (1)°

V = 2895 (1) Å³

Z = 8

D_x = 1.69 Mg m^{−3}

Mo *K*α radiation

Cell parameters from 10 reflections

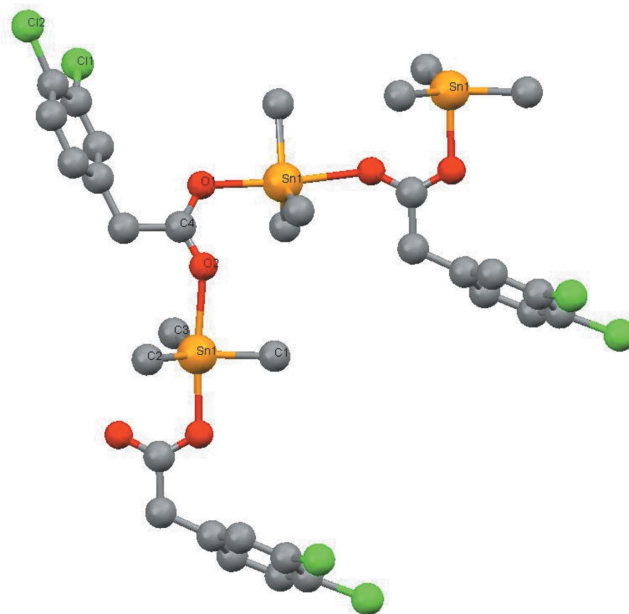
θ = 11–12°

μ = 2.13 mm^{−1}

T = 294 K

Lath, colourless

0.30 × 0.15 × 0.03 mm


Figure 2

The molecular structure of three units of [Sn(CH₃)₃(C₈H₅Cl₂O₂)] with the atom numbering scheme. H atoms have been omitted for clarity.

Data collection

Enraf–Nonius CAD-4

diffractometer

ω–2θ scans

Absorption correction: analytical
(de Meulenaer & Tompa, 1965)

T_{min} = 0.64, *T_{max}* = 0.87

2619 measured reflections

2550 independent reflections

2012 reflections with *I* > 2σ(*I*)

R_{int} = 0.017

θ_{max} = 25°

h = −15 → 15

k = 0 → 11

l = 0 → 27

1 standard reflections

frequency: 30 min

intensity decay: 12%

Refinement

Refinement on *F*

R [*F*² > 2σ(*F*²)] = 0.043

wR(*F*) = 0.055

S = 1.79

2012 reflections

146 parameters

H-atom parameters constrained

w = 1/[σ²(*F*) + 0.0004*F*²]

(Δ/σ)_{max} = 0.011

Δρ_{max} = 0.97 e Å^{−3}

Δρ_{min} = −1.05 e Å^{−3}

H atoms were included in calculated positions (C–H = 1.0 Å) and refined as riding, with *U*_{iso}(H) = *U*_{eq}(C).

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: local program; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *RAELS* (Rae, 1996); molecular graphics: *ORTEP II* (Johnson, 1976); software used to prepare material for publication: local programs.

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