metal-organic papers

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## catena-Poly[[diphenylethyltin(IV)]-μ-chloroacetato-κ²O:O′]

The polymeric title compound, $[Sn(C_2H_5)(C_6H_5)_2(C_2H_4ClO_2)]_n$, adopts a carboxylate-bridged zigzag motif. The Sn center exhibits a *trans*-C_3SnO_2 trigonal–bipyramidal coordination.

Comment

The solid-state structures of a large number of triorganotin carboxylates are known, the majority of which are symmetrical R_3SnO_2CR' systems; mixed organic groups on tin present severe difficulties in their synthesis, and only a few have been reported. The mixed aryl/alkyl carboxylates are limited to the diphenylmethyltin (Amini *et al.*, 2002) and diphenylcyclopentyltin (Teo *et al.*, 2004) systems only. These adopt carboxylate-bridged motifs (Ng *et al.*, 1988), as does diphenylethyltin chloroacetate (Fig. 1).

(I)
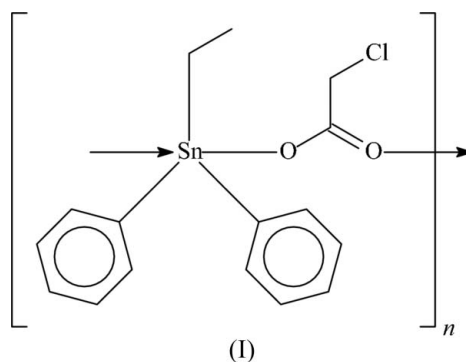
The title compound, (I), exists as a zigzag polymer, whereas others generally adopt a helical chain motif.

In (I), the Sn center shows a *trans*-C_3SnO_2 trigonal bipyramidal coordination, one axial Sn—O (dative) bond being much longer than the other axial Sn—O (covalent) bond (Table 1). The repeat distance, i.e. half the *c*-axial length, is similar to those reported earlier (Ng *et al.*, 1988).

Experimental

Triphenylethyltin was prepared by using a conventional Grignard synthesis with triphenyltin chloride and ethylmagnesium bromide. The reagent was then treated with elemental iodine in order to cleave one of the three aromatic groups to afford diphenylethytin iodide (Davison & Rakita, 1970). Diphenylethytin iodide (0.43 g, 1 mmol) and silver monochloroacetate (0.20 g, 1 mmol) when reacted in ethanol (20 ml) gave a precipitate of silver iodide, which was removed by filtration. Evaporation of solvent gave a white solid, which was purified by crystallization from a CH_2Cl_2/C_6H_{14} (4:1 v/v) mixture to furnish colorless crystals (m.p. 394–395 K).

Crystal data

$[Sn(C_2H_5)(C_6H_5)_2(C_2H_4ClO_2)]$
$M_r = 395.44$
Monoclinic, Cc
$a = 12.265 (3)$ Å
$b = 12.542 (2)$ Å
$c = 10.980 (2)$ Å
$\beta = 93.59 (2)°$
$V = 1685.8 (6)$ Å^3

$Z = 4$
$D_x = 1.558$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.67$ mm^{-1}
$T = 298 (2)$ K
Prism, colorless
$0.30 \times 0.10 \times 0.06$ mm

Data collection

Stoe IPDS-II Imaging Plate
  diffractometer
ω scans
Absorption correction: analytical
  (*X-SHAPE*; Stoe & Cie, 2005)
  $T_{min} = 0.763$, $T_{max} = 0.820$

6300 measured reflections
3368 independent reflections
3242 reflections with $I > 2\sigma(I)$
$R_{int} = 0.020$
$\theta_{max} = 26.7°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.024$
$wR(F^2) = 0.061$
$S = 1.05$
3368 reflections
157 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0348P)^2 + 1.4346P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}
Absolute structure: Flack (1983),
  1590 Friedel pairs
Flack parameter: 0.00 (3)

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.134 (2)	Sn1—O1	2.171 (3)
Sn1—C7	2.127 (2)	Sn1—O2^i	2.522 (3)
Sn1—C13	2.128 (5)		
C1—Sn1—C7	115.2 (1)	C7—Sn1—O1	94.4 (1)
C1—Sn1—C13	117.3 (2)	C7—Sn1—O2^i	85.2 (1)
C1—Sn1—O1	89.9 (1)	C13—Sn1—O1	102.2 (2)
C1—Sn1—O2^i	83.6 (1)	C13—Sn1—O2^i	84.0 (2)
C7—Sn1—C13	124.5 (2)	O1—Sn1—O2^i	172.6 (1)

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

The two phenyl rings were refined as rigid hexagons with edge lengths of 1.39 Å. The H atoms were placed at calculated positions (C—H = 0.93–0.98 Å) and included in the refinement in the riding-model approximation, with their displacement parameters set at 1.2 or 1.5 (methyl) times U_{eq} of the parent atom.

Data collection: *X-AREA* (Stoe & Cie, 2003); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s)
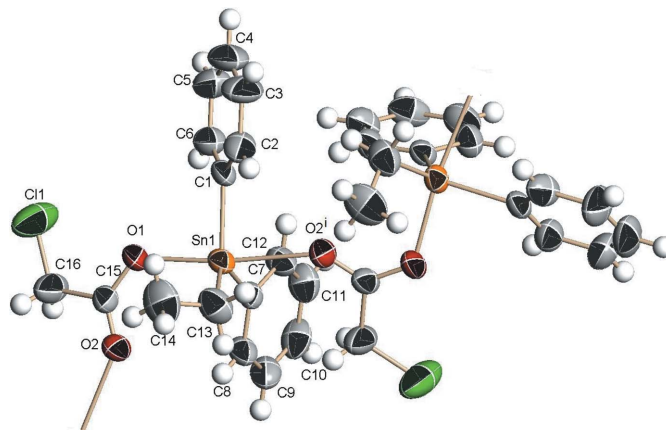

Figure 1
A portion of the polymeric chain in (I), showing the atom-labeling scheme; displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) x, 1-y, $\frac{1}{2} + z$.]

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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