

Mostafa M. Amini,^a Vajihe Alijani,^a Amirreza Azadmehar^a and Seik Weng Ng^{b*}^aDepartment of Chemistry, Shahid Beheshti University, Tehran, Iran, and ^bDepartment of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

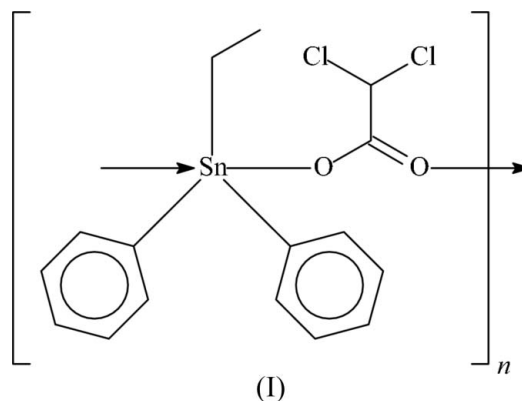
Key indicators

Single-crystal X-ray study
 $T = 173$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.017
 wR factor = 0.059
Data-to-parameter ratio = 14.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.*catena*-Poly[[ethyldiphenyltin(IV)]- μ -dichloroacetato- $\kappa^2\text{O}:\text{O}'$]The title compound, $[\text{Sn}(\text{C}_2\text{HCl}_2\text{O}_2)(\text{C}_2\text{H}_5)(\text{C}_6\text{H}_5)_2]_n$, adopts a carboxylate-bridged zigzag motif that runs along the c axis of the monoclinic unit cell. The metal center shows *trans*- C_3SnO_2 trigonal-bipyramidal coordination.

Received 29 August 2006

Accepted 29 August 2006

Comment

Ethyldiphenyltin(IV) monochloroacetate adopts a carboxylate-bridged zigzag motif in which the tin center shows *trans*- C_3SnO_2 trigonal-bipyramidal coordination, with one axial Sn–O (dative) bond much longer than the other axial Sn–O (covalent) bond [2.522 (3) and 2.171 (3) Å] (Amini *et al.*, 2006). The dichloroacetate analog, (I), crystallizes with matching cell dimensions. In the title compound (Fig. 1), the Sn–O bond lengths are more similar (Table 1).

Experimental

Diphenylethyltin(IV) iodide (0.43 g, 1 mmol) and silver monochloroacetate (0.24 g, 1 mmol) when reacted in ethanol gave a precipitate of silver iodide, which was removed by filtration. Evaporation of the solvent gave a white solid, which was purified by crystallization from a 4:1 (*v/v*) $\text{CH}_3\text{OH}/\text{C}_6\text{H}_{14}$ mixture to furnish colorless crystals.

Crystal data

$[\text{Sn}(\text{C}_2\text{HCl}_2\text{O}_2)(\text{C}_2\text{H}_5)(\text{C}_6\text{H}_5)_2]$
 $M_r = 429.88$
 Monoclinic, Cc
 $a = 12.5470$ (6) Å
 $b = 12.0008$ (5) Å
 $c = 11.2363$ (4) Å
 $\beta = 93.452$ (1)°
 $V = 1688.83$ (12) Å³

$Z = 4$
 $D_x = 1.691$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 1.83$ mm⁻¹
 $T = 173$ (2) K
 Block, colorless
 $0.36 \times 0.18 \times 0.10$ mm

Data collection

Bruker APEX-II CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.648$, $T_{\max} = 0.838$

4353 measured reflections
 2650 independent reflections
 2625 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.015$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.017$
 $wR(F^2) = 0.059$
 $S = 1.20$
 2650 reflections
 188 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0414P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.56 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.81 \text{ e } \text{\AA}^{-3}$
 Absolute structure: Flack (1983),
 743 Friedel pairs
 Flack parameter: $-0.04(2)$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Sn1—C1	2.124 (3)	Sn1—O1	2.201 (2)
Sn1—C7	2.116 (3)	Sn1—O2 ⁱ	2.384 (3)
Sn1—C13	2.129 (4)		
C1—Sn1—C7	115.6 (1)	C7—Sn1—O1	91.3 (1)
C1—Sn1—C13	118.2 (1)	C7—Sn1—O2 ⁱ	88.9 (1)
C1—Sn1—O1	87.2 (1)	C13—Sn1—O1	99.0 (1)
C1—Sn1—O2 ⁱ	84.9 (1)	C13—Sn1—O2 ⁱ	87.9 (1)
C7—Sn1—C13	125.5 (1)	O1—Sn1—O2 ⁱ	171.3 (1)

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

The H atoms were placed at calculated positions ($\text{C—H} = 0.95\text{--}1.00 \text{ \AA}$) and were refined using the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$.

Data collection: *APEXII* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; method used to solve structure: initial atomic coordinates were taken from the structure of the monochloroacetate analog (Amini *et al.*, 2006); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97*.

We thank the Office of the Vice-President's Office for Research Affairs of Shahid Beheshti University and the University of Malaya for supporting this work.

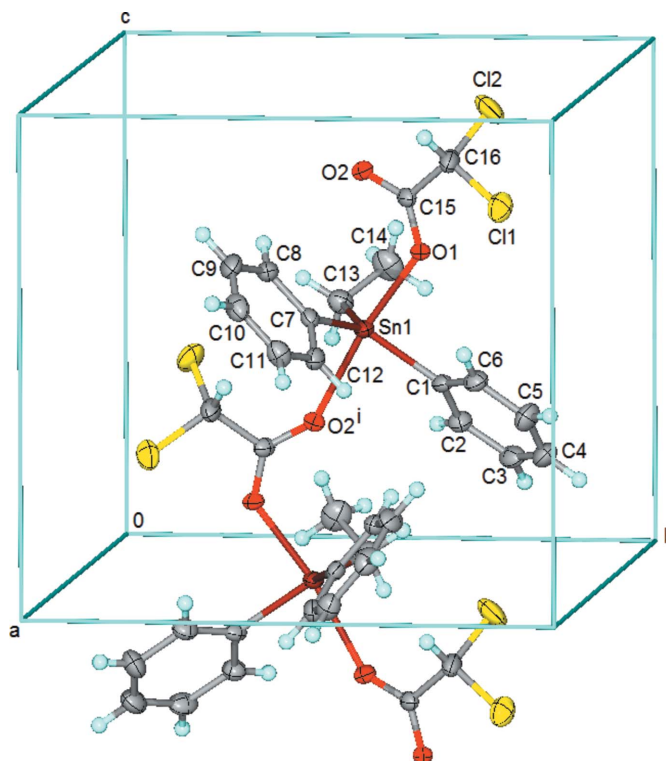


Figure 1

Plot of a portion of the polymeric chain structure of (I); displacement ellipsoids are drawn at the 70% probability level and H atoms as spheres of arbitrary radii. [Symmetry code: (i) $x, 1 - y, -\frac{1}{2} + z$].

References

- Amini, M. M., Azadmeher, A. & Ng, S. W. (2006). *Acta Cryst.* E62, m2293–m2294.
 Barbour, L. J. (2001). *J. Supramol. Chem.* 1, 189–191.
 Bruker (2004). *APEXII* (Version 7.12A) and *SAINT* (Version 7.12A). Bruker AXS Inc., Madison, Wisconsin, USA.
 Flack, H. D. (1983). *Acta Cryst.* A39, 876–881.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.