Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

catena-Poly[[trimethyltin(IV)]-μ-2,2-dicyclohexylacetato-κ^2O:O']

Diop Cheikh Abdoul Khadir,[a]* Touré Assane,[a] Diop Libasse,[a] Bernard Tinant[b] and Bernard Mahieu[c]

[a]Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop Daka, Senegal, [b]Université Catholique de Louvain, Unité de Chimie Structurale et des Mécanismes Réactionnels, 1 Place Louis Pasteur B, 1348 Louvain-la-Neuve, Belgium, and [c]Département de Chimie-Laboratoire de Chimie Inorganique et Nucléaire, Place L. Pasteur 1B, 1348 Louvain-la-Neuve, Belgium

Correspondence e-mail: cakdiop@ucad.sn

Key indicators

Single-crystal X-ray study
T = 110 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.103
Data-to-parameter ratio = 20.6

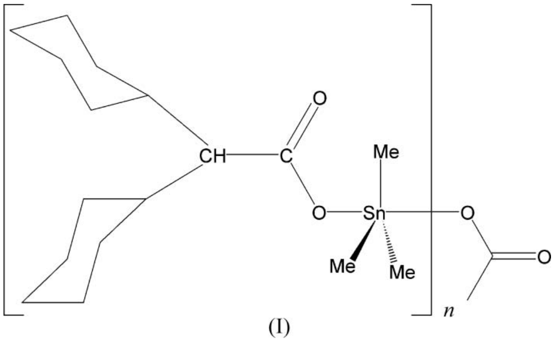
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 5 December 2006
Accepted 12 December 2006

The structure of the title compound, $[Sn(CH_3)_3(C_{14}H_{23}O_2)]_n$, consists of a one-dimensional polymeric chain, containing tin centers in a trigonal–bipyramidal environment and bridging carboxylate anions. The two O atoms of the 2,2-dicyclohexylacetate anion occupy the axial positions, while the three C atoms of the methyl groups are in equatorial sites.

Comment

Organotin(IV) complexes including carboxylate ligands have been studied extensively owing to their biological and pharmaceutical applications in different fields, such as agrochemicals, surface disinfectants, wood preservatives and marine antifouling paints (Davies & Smith, 1982; Gielen, 1996; Kemmer *et al.*, 2000) and, from a chemical point of view, due to the versatile molecular structures and supramolecular architectures exhibited by these complexes even if small changes are made around the central tin atom (Tiekink, 1991, 1994; Willem *et al.*, 1998). Most of the trimethyltin(IV) compounds involving carboxylate ligands are polymeric with a bridging carboxylate anion; the few examples of monomeric compounds are obtained in the case of sterically demanding groups and electron-rich and chelating ligands, *e.g.* Cambridge Structural Database (CSD) (*MOGUL*, Version 1.8, 2006 release; Allen, 2002) refcodes DOZDED (Smith *et al.*, 1986), YOTBUE (Gibson *et al.*, 1995) and TOCHUO (Heinicke *et al.*, 1996). In the scope of our reseach work on the coordination ability of carboxylate ligands towards organotin(IV) derivatives, similar behaviors of carboxylate ligands have also been reported in $(C_6H_{11})_2CHCOOSnPh_3$ (Rénamy *et al.*, 2004), whose structure is discrete and contains monodentate carboxylate ligands with a distorted tetrahedral geometry around the tin center. In the present study, we have synthesized and characterized $[(C_6H_{11})_2CHCOOSnMe_3]_n$, (I).



(I)

In the structure of the title compound, (I) (Fig. 1), the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). The rings *A* (C3–C8) and *B* (C9–C14) are not planar, having total puckering amplitudes, Q_T of 0.576 (3) and 0.576 (4) Å, respectively, and chair conformations [φ = 148.71 (7), θ = 178.06 (3)° and φ = 84.61 (4)°, θ = 4.18 (3)°; Cremer & Pople, 1975]. The structure consists of polymeric chains, in which essentially planar triorganotin units are bridged by carboxylate groups. The nature of this bridging is non-symmetrical; the Sn atom forms one short Sn—O2 [2.173 (3) Å] and one relatively long Sn—O1 [2.453 (3) Å] bond to O atoms. The coordination environment around the tin center is trigonal bipyramidal; the equatorial positions are occupied by the three C atoms of the methyl groups, and the axial positions by the two O atoms of the 2,2-dicyclohexylacetato anion. The sum of the C—Sn—C angles around the tin centre [358.95°] is close to 360°, and the O1—Sn—O2 [177.55 (9)°] angle deviates slightly from linearity. The difference between the geometry around the tin center in (I) and in its triphenyltin homolog (Rénamy *et al.*, 2004) shows that the nature of the radical linked to the tin center also plays an important role in the cordination mode of the carboxylate ligands. Bulky radicals and electron-demanding groups on tin favor monomeric species, *e.g.* CSD refcodes CADKOI (Clarke *et al.*, 2001), DIYNUU (Molloy *et al.*, 1986) and FAXLEW (Tian *et al.*, 2005).

The Mössbauer isomer shift value (1.30 mm/s) is typical of quadrivalent tin in organometallic derivatives while the *QS* value (3.49 mm/s) is consistent with a *trans* O_2SnC_3 stereochemistry about the tin center (Davies *et al.*, 1982). Infrared and Raman spectroscopy indicate the presence of a bidentate carboxylate ligand as $\Delta\nu = \nu_{asym}\mathrm{OCO} - \nu_{sym}\mathrm{OCO} = 199\ \mathrm{cm}^{-1}$ (Ma *et al.*, 2005; Nakamoto, 1997).

Experimental

Trimethyltin(IV) hydroxide, (II), was obtained from the reaction between trimethyltin(IV) chloride (1.0 g, 5 mmol) and potassium hydoxide (0.26 g, 5 mmol) in methanol (5 ml). The mixture was stirred for several hours and the precipitate filtered off. Slow evaporation of the solvent gave colorless crystals. Recrystallization from ethanol (25 ml, 99.99%) gave compound (II). Compound (I) was obtained by reacting an ethanol solution of (II) (99.99%, 50 ml) with dicyclohexylacetic acid (0.705 g, 5 mmol) in a 1:1 ratio. The mixture was stirred for several hours and slow solvent evaporation gave crystals suitable for X-ray analysis.

Crystal data

$[Sn(CH_3)_3(C_{14}H_{23}O_2)]$
M_r = 387.12
Monoclinic, $P2_1/a$
a = 9.488 (4) Å
b = 10.894 (5) Å
c = 17.871 (7) Å
β = 96.03 (2)°
V = 1837.0 (14) Å^3

Z = 4
D_x = 1.400 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.39 mm^{-1}
T = 110 (2) K
Parallelepiped, colorless
0.30 × 0.20 × 0.20 mm

Data collection

Marresearch MAR345 image-plate diffractometer
φ scans
Absorption correction: none
13602 measured reflections

3747 independent reflections
3596 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
$\theta_{\max}$ = 26.4°

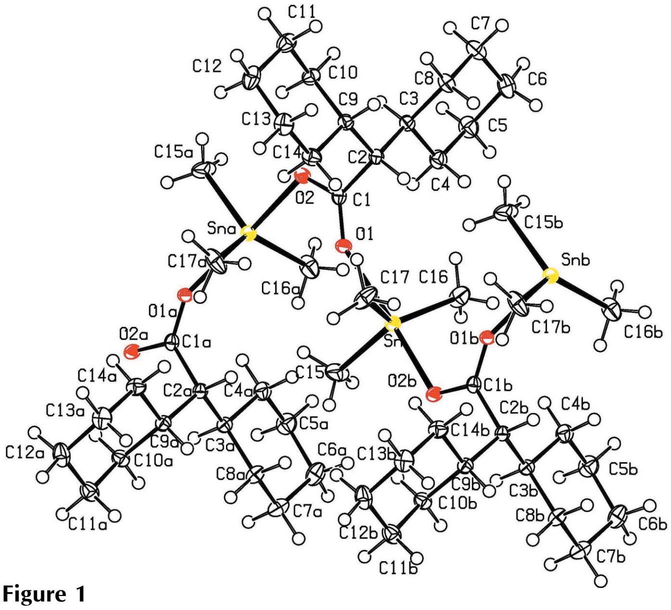


Figure 1
Part of the polymeric structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (a) $x - \frac{1}{2}, \frac{1}{2} - y, z$; (b) $\frac{1}{2} + x, \frac{1}{2} - y, z$.]

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.103
S = 1.25
3747 reflections
182 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 5.4207P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.82 e Å^{-3}
$\Delta\rho_{\min}$ = −0.82 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0241 (13)

Table 1
Selected geometric parameters (Å, °).

Sn—C17	2.112 (4)	Sn—O1	2.453 (3)
Sn—C16	2.113 (4)	O1—C1	1.254 (4)
Sn—C15	2.130 (4)	O2—C1^{i}	1.285 (4)
Sn—O2	2.173 (2)		
C17—Sn—C16	129.87 (18)	C15—Sn—O2	91.24 (14)
C17—Sn—C15	114.3 (2)	C17—Sn—O1	86.56 (13)
C16—Sn—C15	114.8 (2)	C16—Sn—O1	86.86 (13)
C17—Sn—O2	94.67 (13)	C15—Sn—O1	86.33 (14)
C16—Sn—O2	93.95 (13)	O2—Sn—O1	177.56 (8)

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

H atoms were positioned geometrically, with C—H = 1.00, 0.99 and 0.98 Å for aromatic, methylene and methyl H atoms, respectively, and constrained to ride on their parent atoms, with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{C})$.

Data collection: *mar345* (Klein, 1998); cell refinement: *marHKL* (Klein & Bartels, 2000); data reduction: *marHKL*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1998); software used to prepare material for publication: *SHELXL97*.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.

Acta Cryst. (2007). E**63**, m258–m260 Cheikh Abdoul Khadir *et al.* • $[Sn(CH_3)_3(C_{14}H_{23}O_2)]$ **m259**

Clarke, D. J., Dakternieks, D. & Tiekink, E. R. T. (2001). *Main Group Met. Chem.* **24**, 309–310.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Davies, A. G. & Smith, P. J. (1982). *Comprehensive Organometllic Chemistry*, edited by G. Wilkinson, F. Gordon, A. Stone and E. W. Abel, pp. 519–616. New York: Pergamon Press.

Gibson, D. H., Ye, M., Sleadd, B. A., Mehta, J. M., Mbadike, O. P., Richardson, J. F. & Mashuta, M. S. (1995). *Organometallics*, **14**, 1242–1255.

Gielen, M. (1996). *Coord. Chem. Rev.* **151**, 41–51.

Heinicke, J., Kadyrov, R., Kindermann, M. K., Koesling, M. & Jones, P. G. (1996). *Chem. Ber.* **129**, 1547–1560.

Kemmer, M., Dalil, H., Biesemans, M., Martins, J. C., Mahieu, B., Horn, E., de Vos, D., Tiekink, E. R. T., Willem, R. & Gielen, M. (2000). *J. Organomet. Chem.* **608**, 63–70.

Klein, C. (1998). *mar345*. Version 1.1. X-ray Research GmbH, Norderstedt, Germany.

Klein, C. & Bartels, K. (2000). *marHKL*. Version 4.0. X-ray Research GmbH, Norderstedt, Germany.

Ma, C., Zhang, Q., Zhang, R. & Qiu, L. (2005). *J. Organomet. Chem.* **690**, 3033–3043.

Molloy, K. C., Purcell, T. G., Hahn, E., Schumann, H. & Zuckerman, J. J. (1986). *Organometallics*, **5**, 85–89.

Nakamoto, K. (1997). *Infrared and Raman Spectra of Inorganic and Coordination Compounds, Part B, 5th* ed., pp. 57–62. New York: Wiley Interscience.

Rénamy, S. V., Bassène, S., Diop, C. A. K., Sidibé, M., Diop, L., Mahon, M. F. & Molloy, K. C. (2004). *Appl. Organomet. Chem.* **18**, 455–459.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*, University of Göttingen, Germany.

Smith, P. J., Day, R. O., Chandrasekhar, V., Holmes, J. M. & Holmes, R. R. (1986). *Inorg. Chem.* **25**, 2495–2499.

Spek, A. L. (1998). *PLATON*. University of Utrecht, The Netherlands.

Tian, L.-J., Sun, Y.-X., Yang, M. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m74–m75.

Tiekink, E. R. T. (1991). *Appl. Organomet. Chem.* **5**, 1–23.

Tiekink, E. R. T. (1994). *Trends Organomet. Chem.* **1**, 71–116.

Willem, R., Verbruggen, I., Gielen, M., Biesemans, M., Mahieu, B., Basu Baul, T. S. & Tiekink, E. R. T. (1998). *Organometallics*, **17**, 5758–5766.

m260 Cheikh Abdoul Khadir *et al.* • [Sn(CH$_3$)$_3$(C$_{14}$H$_{23}$O$_2$)] *Acta Cryst.* (2007). E**63**, m258–m260