Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[trimethyltin(IV)]-μ-2,3-bis(4-chlorophenyl)propenoato-κ^2O:O']

Sadiq-ur-Rehman,[a] Stephen R. Shouldice,[b] Saqib Ali,[a] Amin Badshah[a] and Masood Parvez[c]*

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, [b]Department of Microbiology and Infectious Disease, The University of Calgary, 3300 Hospital Drive NW, Calgary, Alberta, Canada T2N 4N1, and [c]Department of Chemistry, The University of Calgary, 2500 University Drive NW, Calgary, Alberta, Canada T2N 1N4

Correspondence e-mail: parvez@ucalgary.ca

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.029
wR factor = 0.073
Data-to-parameter ratio = 21.5

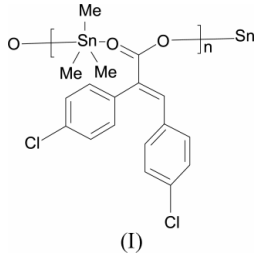
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 14 April 2004
Accepted 20 April 2004
Online 30 April 2004

The title compound, $[Sn(CH_3)_3(C_{15}H_9Cl_2O_2)]_n$, forms polymeric chains involving both O atoms of the carboxylate group. The coordination geometry around the Sn atom is distorted trigonal–bipyramidal. The three methyl C atoms occupy the equatorial positions, with Sn—C distances of 2.113 (3)–2.124 (2) Å, and two O atoms, including one from a symmetry-related molecule, are at the axial positions, with Sn—O distances of 2.152 (2) and 2.454 (2) Å.

Comment

There has been widespread success of platinum compounds in the clinical treatment of tumors since the 1960s (Köpf-Maier, 1994). However, the toxic side effects and frequent development of drug resistance in patients has directed the search for other metal complexes able to offer improved antitumor activity and a more acceptable level of toxicity (Respondek & Engel, 1996). Numerous organotin compounds which exhibit a variety of biocidal properties have been synthesized and described in the literature (Magos, 1986; Ronconi *et al.*, 2002). Even though their mode of action remains unclear within the body, several organotin compounds have been shown to exhibit important cytotoxic effects and are actively investigated as possible antitumor compounds (Penninks, 1990; Crowe, 1987). In order to further our understanding of organotin complexes in general and organotin carboxylates in particular there has been a focus in recent years on determining and analyzing the structures of these very important compounds. The structural aspects of these biologically active ligands have been reviewed by several investigators (Nath *et al.*, 2001; Chandrasekhar *et al.*, 2002). Continuing our interest in the structural aspects of organotin carboxylates (Parvez, Ali, Mazhar, Bhatti & Khokhar, 1999; Parvez, Ali, Bhatti *et al.*, 1999; Parvez, Ali, Mazhar, Bhatti & Choudhary, 1999; Parvez *et al.*, 2000, 2002), we report the structure of the title compound, (I), in this paper.



(I)

The structure of (I) (Fig. 1) consists of polymeric chains (Fig. 2) incorporating both O atoms of the carboxylate group, with significantly different Sn—O distances [Sn1—O1 = 2.152 (2) Å and Sn—O2^{i} = 2.454 (2) Å; symmetry code as in

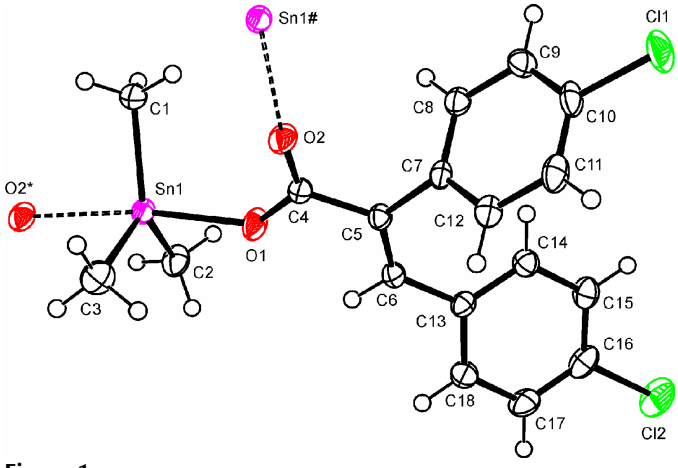


Figure 1
*ORTEP*II (Johnson, 1976) drawing of (I), with displacement ellipsoids drawn at the 50% probability level. The symbols * and # correspond to symmetry codes (i) and (ii), respectively, in Table 1.

Table 1], indicating that the Sn—O bonds are asymmetric. 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].

A search for complexes with a similar coordination geometry around the Sn atom in the Cambridge Structural Database (CSD; Version 1.6, 2003 release; Allen, 2002) revealed numerous compounds with similar dimensions. The bond distances for Sn—O ranged from 2.107 (4) to 2.514 (3) Å, in compounds from the database with refcodes HIQCUF, HIQDAM, HIQDEQ, HIQDIU, HIQDOA, KOFBOW and RESCOH; all of these complexes had phenyl groups bonded to the Sn atoms. The Sn—C distances ranged from 2.117 (11) to 2.130 (9) Å for compounds with refcodes BALZAP, BEQPES, CIBQUZ and HIGWOJ.

The Sn atom in (I) is pulled out of the equatorial plane formed by the three methyl C atoms by 0.135 (2) Å, towards the more strongly bonded atom O1. The O—Sn—O angle is approximately linear [170.69 (6)°], the C—Sn—C angles lie between 118.44 (11) and 121.11 (11)°, deviating very little from the ideal value of 120°, and the O—Sn—C angles are in the range 85.50 (9)–92.87 (10)°, again very close to the ideal 90° value. These dimensions are in agreement with the corresponding values reported for similar Sn complexes in the CSD. The molecular dimensions of the ligand are normal. The O1—C4 bond distance of 1.277 (3) Å indicates that this is a single bond, whereas the O2—C4 bond distance of 1.233 (3) Å reveals that this is a double bond. Both benzene rings are individually planar as expected and are inclined at 64.11 (7)° to each other. Atoms Cl1 and Cl2 lie 0.095 (3) and 0.050 (3) Å, respectively, from the mean planes of the benzene rings to which they are bonded. The propionate moiety, O1/O2/C4/C5/C6, is essentially planar [maximum deviation for C5 of 0.049 (2) Å] and the mean planes of benzene rings C7–C12 and C13–C18 form angles of 66.19 (6) and 35.83 (10)°, respectively, with the propionate group.

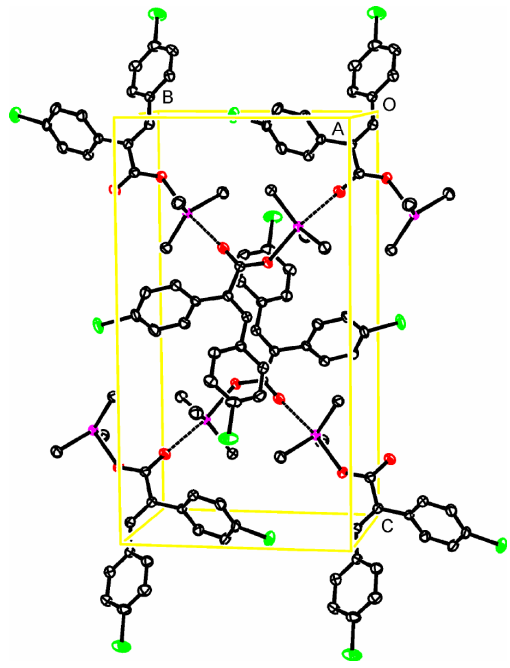


Figure 2
*ORTEP*II (Johnson, 1976) drawing of the contents of the unit cell, showing polymeric chains of (I) running parallel to the *b* axis.

Experimental

The title compound, (I), was prepared by the reaction of a stoichiometric amount of the silver salt of 2,3-bis(4-chlorophenyl)propionic acid (2.5 g, 6.25 mmol) with trimethyltin chloride (1.25 g, 6.25 mmol) in dry chloroform (60 ml). The reaction mixture was refluxed for 6–8 h in a two-necked round-bottomed flask (250 ml), fitted with a magnetic stirrer and condenser. It was allowed to stand overnight at room temperature. The resulting silver salt was removed by filtration and the solvent was evaporated under reduced pressure. The solid material obtained was recrystallized from a mixture of chloroform–*n*-hexane (80:20), giving fine crystals suitable for single-crystal X-ray crystallography (yield 85%, m.p. 423–425 K).

Crystal data

$[Sn(CH_3)_3(C_{15}H_9Cl_2O_2)]$
M_r = 455.91
Monoclinic, $P2_1/c$
a = 9.238 (2) Å
b = 10.435 (2) Å
c = 19.120 (4) Å
β = 91.456 (11)°
V = 1842.5 (7) Å^3
Z = 4
D_x = 1.644 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 15 524 reflections
θ = 2.9–28.3°
μ = 1.68 mm^{-1}
T = 173 (2) K
Prism, colorless
0.20 × 0.20 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.723, T_{max} = 0.767
15 524 measured reflections
4528 independent reflections
4032 reflections with $I > 2\sigma(I)$
R_{int} = 0.041
θ_{max} = 28.3°
$h = -12 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -25 \rightarrow 24$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 1.52P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.029$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.073$	$\Delta\rho_{max} = 0.58$ e Å^{-3}
$S = 1.05$	$\Delta\rho_{min} = -0.87$ e Å^{-3}
4528 reflections	
211 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—C3	2.113 (3)	Cl1—C10	1.745 (2)
Sn1—C2	2.118 (2)	Cl2—C16	1.745 (2)
Sn1—C1	2.124 (2)	O1—C4	1.277 (3)
Sn1—O1	2.152 (2)	O2—C4	1.233 (3)
Sn1—O2^{i}	2.454 (2)		
C3—Sn1—C2	119.25 (11)	C3—Sn1—O2^{i}	85.50 (9)
C3—Sn1—C1	121.11 (11)	C2—Sn1—O2^{i}	85.56 (8)
C2—Sn1—C1	118.44 (11)	C1—Sn1—O2^{i}	88.01 (8)
C3—Sn1—O1	92.87 (10)	O1—Sn1—O2^{i}	170.69 (6)
C2—Sn1—O1	87.25 (9)	C4—O1—Sn1	136.32 (15)
C1—Sn1—O1	100.64 (8)	C4—O2—Sn1^{ii}	173.24 (17)

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_{iso} = 1.5 (methyl) and 1.2 (aromatic) times U_{eq} of the atoms to which they were bonded. The final difference map was free of any chemically significant features.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *HKL DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SAPI*91 (Fan, 1991); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1997). *J. Appl. Cryst.* **30**, 421–426.
Chandrasekhar, V., Nagendran, S. & Baskar, V. (2002). *Coord. Chem. Rev.* **235**, 1–52.
Crowe, A. J. (1987). *Drugs Future*, **12**, 255–275.
Fan, H.-F. (1991). *SAPI*91. Rigaku Corporation, Tokyo, Japan.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Köpf-Maier, P. (1994). *Eur. J. Clin. Pharmacol.* **47**, 1–16.
Magos, L. (1986). *Handbook on the Toxicology of Metals*, edited by L. Friberg, G. F. Nordberg and V. B. Vouk, pp. 569–593. Amsterdam: Elsevier.
Nath, M., Pokharia, S. & Yadav, R. (2001). *Coord. Chem. Rev.* **215**, 99–149.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Parvez, M., Ali, S., Ahmad, S., Bhatti, M. H. & Mazhar, M. (2002). *Acta Cryst.* C**58**, m334–m335.
Parvez, M., Ali, S., Bhatti, M. H., Khokhar, M. N. Mazhar, M. & Qureshi, S. I. (1999). *Acta Cryst.* C**55**, 1427–1429.
Parvez, M., Ali, S., Mazhar, M., Bhatti, M. H. & Choudhary, M. A. (1999). *Acta Cryst.* C**55**, 1429–1431.
Parvez, M., Ali, S., Mazhar, M., Bhatti, M. H. & Khokhar, M. N. (1999). *Acta Cryst.* C**55**, 1280–1282.
Parvez, M., Bhatti, M. H., Ali, S., Mazhar, M. & Qureshi, S. I. (2000). *Acta Cryst.* C**56**, 327–328.
Penninks, A. H. (1990). *Tin-Based Antitumor Drugs*, edited by M. Gielen, pp. 169–190. Berlin: Springer.
Respondek, J. & Engel, J. (1996). *Drugs Future*, **21**, 391–408.
Ronconi, L., Marzano, C., Russo, U., Sitran, S., Graziani, R. & Fregona, D. (2002). *J. Inorg. Biochem.* **91**, 413–420.
Sheldrick, G. M. (1997). *SHELXL*97. University of Göttingen, Germany.