Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[dimethyltin(IV)]-μ-benzene-1,4-dicarboxylato]

Ya-Qiong Gong, Rui-Hu Wang, Ben-Yong Lou and Mao-Chun Hong*

State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Fuzhou, Fujian, 350002, People's Republic of China

Correspondence e-mail: hmc@fjirsm.ac.cn

Received 9 May 2005
Accepted 23 May 2005
Online 28 May 2005

In the title compound, [Sn(CH$_3$)$_2$(C$_8$H$_4$O$_4$)], the coordination geometry around the Sn^{IV} centre can be described as highly distorted octahedral. The chelating benzene-1,4-dicarboxylate ligands connect the centres to form an infinite one-dimensional polymeric chain structure.

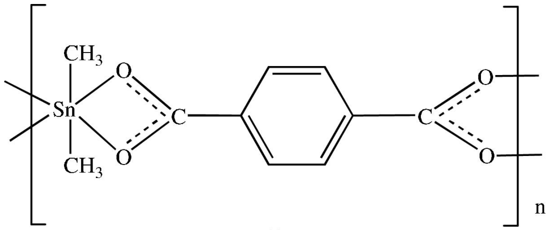
Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.006 Å
R factor = 0.032
wR factor = 0.080
Data-to-parameter ratio = 14.0

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

Comment

Benzenedicarboxylate ligands are interesting ligands because they can exhibit a variety of coordination modes and are capable of forming coordination architectures of diverse shapes (Livage *et al.*, 2001; Ye *et al.*, 2005). Compared with the immense number of transition metal polymers, only a relatively small number of structures with benzenedicarboxylate ligands and the main group elements have been reported so far. It is well known that the solid-state structures of tin(IV) carboxylates can produce some unique frameworks with aesthetic appeal and useful properties, due to their abundant coordination modes (Deák *et al.*, 2001; Wang *et al.*, 2002; García-Zarracino *et al.*, 2003). We report here the synthesis and crystal structure of a new compound, namely *catena*-poly[[dimethyltin(IV)]-μ-benzene-1,4-dicarboxylato], (I).



(I)

Single-crystal X-ray diffraction analysis reveals that the structure of (I) is a neutral one-dimensional chain. The coordination geometry around the Sn^{IV} centre can be described as highly distorted octahedral. Each Sn^{IV} atom is coordinated by four O atoms from two different chelating benzene-1,4-dicarboxylate ligands, which form the equatorial plane [Sn—O = 2.140 (3)–2.507 (3) Å]. The dihedral angles between the benzene rings and the corresponding carboxylate groups

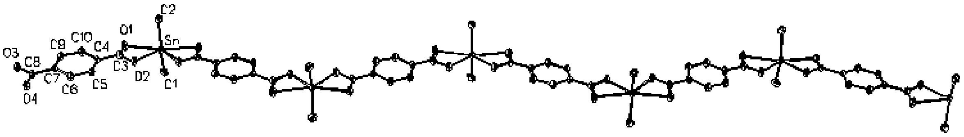


Figure 1
Part of the polymeric chain structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

attached to them are 4.8 (7) and 1.3 (6)°, indicating that the carboxylate groups are approximately coplanar with the benzene rings. Two methyl groups are in the axial positions and prevent the formation of an extended framework. The solid contains one-dimensional chains of Sn^{IV} atoms bridged by chelating benzene-1,4-dicarboxylate ligands, with an Sn···Sn distance of 11.07 (2) Å (Fig. 1).

Experimental

The title complex was hydrothermally synthesized under autogenous pressure. A mixture of benzene-1,4-dicarboxylic acid (0.17 g, 1.0 mmol), Me_3SnCl (0.20 g, 1.0 mmol) and water (15 ml) was neutralized to pH 7.0 with 1 *M* NaOH (2 ml) with continuous stirring and then sealed in a 20 ml Teflon-lined autoclave, which was heated to 433 K for 3 d. After cooling slowly to ambient temperature, a large quantity of crystals suitable for single-crystal X-ray diffraction analysis was obtained (yield 0.18 g, 58%).

Crystal data

$[Sn(CH_3)_2(C_8H_4O_4)]$
$M_r = 312.87$
Monoclinic, $P2_1/c$
$a = 10.0617$ (4) Å
$b = 14.6001$ (6) Å
$c = 7.5491$ (3) Å
$\beta = 98.045$ (1)°
$V = 1098.06$ (8) Å^3
$Z = 4$

$D_x = 1.893$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1335 reflections
$\theta = 2.2$–25.0°
$\mu = 2.32$ mm^{-1}
$T = 173$ (2) K
Block, colourless
0.60 × 0.45 × 0.40 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.241$, $T_{max} = 0.396$
3646 measured reflections

1910 independent reflections
1568 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 25.0°$
$h = -7 \rightarrow 11$
$k = -17 \rightarrow 8$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.080$
$S = 0.98$
1910 reflections
136 parameters

H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.69$ e Å^{-3}
$\Delta\rho_{min} = -1.10$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn—C1	2.087 (5)	Sn—O3^{i}	2.165 (3)
Sn—C2	2.092 (5)	Sn—O4^{i}	2.447 (3)
Sn—O2	2.140 (3)	Sn—O1	2.507 (3)
C1—Sn—C2	151.4 (2)		
C10—C4—C3—O1	−4.8 (7)	C9—C7—C8—O3	−1.3 (6)

Symmetry codes: (i) $x + 1, -y + \frac{3}{2}, z + \frac{1}{2}$.

The H atoms were positioned geometrically at distances of 0.95 (CH) and 0.98 Å (CH_3) from the parent C atoms; a riding model was used during the refinement process. The U_{iso}(H) values were constrained to be 1.2 (1.5 for methyl) times U_{eq} of the carrier atom. The deepest hole is 0.93 Å from the tin(IV) centre.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART* and *SAINT* (Siemens, 1994); data reduction: *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

This work was supported by the Natural Science Foundation of China and the Natural Science Foundation of Fujian Province.

References

Deák, A., Radics, L., Kálmán, A., Párkányi, L. & Haiduc, I. (2001). *Eur. J. Inorg. Chem.* pp. 2849–2856.

García-Zarracino, R., Ramos-Quiñones, J. & Höpfl, H. (2003). *Inorg. Chem.* **42**, 3835–3845.

Livage, C., Guillio, N., Marrot, J. & Férey, G. (2001). *Chem. Mater.* **13**, 4387–4392.

Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.

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

Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wiscosin, USA.

Siemens (1994). *SAINT* and *SHELXTL* (Version 5.0). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

Wang, R.-H., Hong, M.-C., Luo, J.-H., Cao, R. & Weng, J.-B. (2002). *Eur. J. Inorg. Chem.* pp. 2082–2085.

Ye, B.-H., Ding, B.-B, Weng, Y.-Q. & Chen, X.-M. (2005). *Cryst. Growth Des.* **5**, 801–806.

Acta Cryst. (2005). E**61**, m1226–m1227 Gong *et al.* • $[Sn(CH_3)_2(C_8H_4O_4)]$ **1227**