IUCrData

ISSN 2414-3146

catena-Poly[[trimethyltin(IV)]-μ-methylphenylphosphinato-$\kappa^2O:O'$]

Chunhua Fu,[a] Rufen Zhang[b]* and Shaoliang Zhang[b]

[a]Department of Pharmacy, Shandong Medical College, Jinan 250000, People's Republic of China, and [b]School of Chemistry and Chemical Engineering, Liaocheng University, Liaocheng 252059, People's Republic of China. *Correspondence e-mail: zhangrf856@163.com

Received 24 September 2017
Accepted 6 October 2017

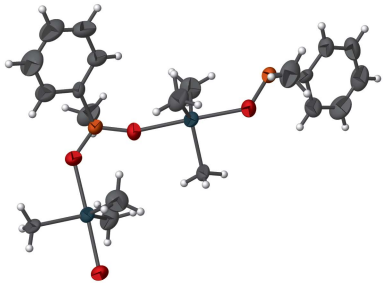
Edited by J. Simpson, University of Otago, New Zealand

Keywords: crystal structure; organotin; methylphenylphosphinic acid; trimethyltin(IV); coordination compound; polymeric chain.

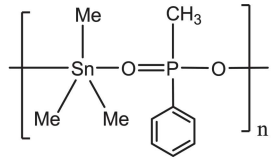
Structural data: full structural data are available from iucrdata.iucr.org

A new trimethyltin(IV) coordination polymer, $[Sn(CH_3)_3(C_7H_8O_2P)]$, has been prepared by treatment of methylphenylphosphinic acid and trimethyltin chloride with sodium ethoxide in methanol. In the solid state, the title compound adopts an infinite one-dimensional polymeric chain structure with each Sn^{IV} atom adopting a distorted trigonal–bipyramidal geometry.

3D view



Chemical scheme



Structure description

In recent years, organotin complexes have been attracting more and more attention due to their significant number of industrial applications and their biological activity (Dubey & Roy, 2003; Gielen, 2002). As a part of our ongoing investigations in this field (Ma *et al.*, 2008), we have synthesized the title compound and present its crystal structure here. As can been seen from Fig. 1, the asymmetric unit of the title compound consists of one $[(CH_3)_3Sn]$ group and a deprotonated methylphenylphosphinic acid. Each Sn^{IV} atom adopts a distorted trigonal–bipyramidal geometry where the two oxygen atoms from the bridging methylphenylphosphinate ligands occupy the axial positions [O1—Sn1—O2($\frac{3}{2}-x$, $\frac{3}{2}+y$, $\frac{1}{2}-z$) = 178.6 (3)°]. The three C atoms of the $[Me_3Sn]^+$ group are equatorial with the three trigonal C—Sn1—C angles summing to 359.9°. Hence atoms Sn1, C8, C9 and C10 are almost coplanar with an r.m.s. deviation of 0.0128 Å from the best fit plane through these atoms. Two P(=O)O– units of the deprotonated methylphenylphosphinic acid ligand link adjacent $[Me_3Sn]^+$ atoms into a one-dimensional zigzag chain structure along the *b*-axis direction (Fig. 2).

Synthesis and crystallization

The reaction was carried out under a nitrogen atmosphere using standard Schlenk techniques. The compound was synthesized by dissolving methylphenylphosphinic acid

Table 1
Experimental details.

Crystal data	
Chemical formula	$[Sn(CH_3)_3(C_7H_8O_2P)]$
M_r	318.89
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	298
a, b, c (Å)	10.8051 (11), 10.3376 (13), 12.4466 (15)
β (°)	103.485 (1)
V (Å^3)	1351.9 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.99
Crystal size (mm)	0.48 × 0.45 × 0.33
Data collection	
Diffractometer	Bruker APEXIII CCD area detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.449, 0.560
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5890, 2371, 1581
R_{int}	0.120
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.085, 0.266, 1.05
No. of reflections	2371
No. of parameters	131
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.75, −2.29

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

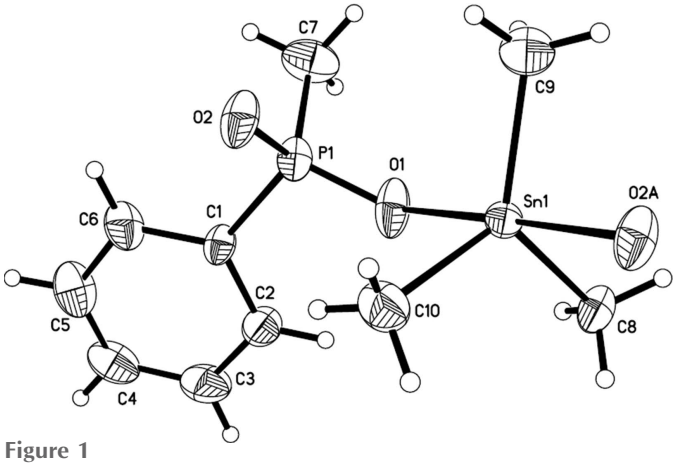


Figure 1
The asymmetric unit of the title compound, showing 30% probability displacement ellipsoids.

(0.156 g, 1.0 mmol), sodium ethoxide (0.068 g, 1.0 mmol) in methanol (30 ml) and stirring for 30 min. Trimethyltin chloride (0.199 g, 1.0 mmol) was then added and stirred for further 12 h at 318 K. The reaction mixture was filtered and the solvent was gradually evaporated under vacuum until a white solid product was obtained. The resulting product was recrystallized from diethyl ether to give transparent colourless crystals of the title compound (yield 88%, m.p. 428–430 K). Analysis calculated for $C_{10}H_{17}O_2PSn$: C 37.66, H 5.37%; found: C 37.43, H 5.48%.

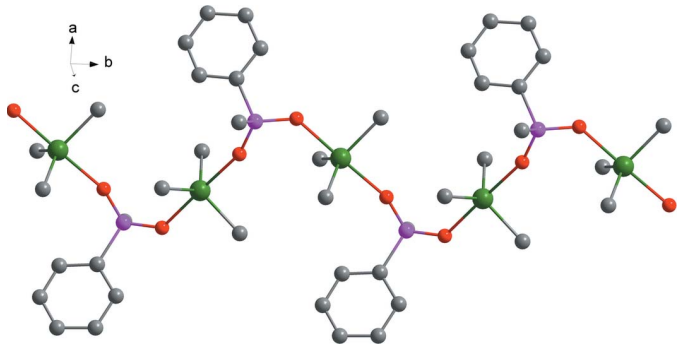


Figure 2
View of the one-dimensional zigzag chain structure running parallel to the *b* axis in the title compound. H atoms have been omitted for clarity.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1.

Funding information

We thank the National Natural Science Foundation of China (21371087) for financial support.

References

Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Dubey, S. K. & Roy, U. (2003). *Appl. Organomet. Chem.* **17**, 3–8.
Gielen, M. (2002). *Appl. Organomet. Chem.* **16**, 481–494.
Ma, C. L., Yang, M. Q., Zhang, R. F. & Du, L. Y. (2008). *Inorg. Chim. Acta*, **361**, 2979–2984.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

full crystallographic data

IUCrData (2017). **2**, x171442 [https://doi.org/10.1107/S2414314617014420]

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

Chunhua Fu, Rufen Zhang and Shaoliang Zhang

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

Crystal data

$[Sn(CH_3)_3(C_7H_8O_2P)]$
M_r = 318.89
Monoclinic, $P2_1/n$
a = 10.8051 (11) Å
b = 10.3376 (13) Å
c = 12.4466 (15) Å
β = 103.485 (1)°
V = 1351.9 (3) Å^3
Z = 4
$F(000)$ = 632
D_x = 1.567 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2834 reflections
θ = 2.3–27.2°
μ = 1.99 mm^{-1}
T = 298 K
Block, colorless
0.48 × 0.45 × 0.33 mm

Data collection

Bruker APEXIII CCD area detector diffractometer
Radiation source: fine-focus sealed tube
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.449, T_{max} = 0.560
5890 measured reflections
2371 independent reflections
1581 reflections with $I > 2\sigma(I)$
R_{int} = 0.120
θ_{max} = 25.0°, θ_{min} = 2.3°
h = −12→12
k = −12→9
l = −13→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.266
S = 1.05
2371 reflections
131 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1668P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 2.75 e Å^{-3}
$\Delta\rho_{min}$ = −2.29 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.79793 (7)	0.62599 (8)	0.22275 (6)	0.0396 (4)
P1	0.8534 (4)	0.3397 (3)	0.1053 (3)	0.0471 (9)
O1	0.8773 (10)	0.4803 (8)	0.1248 (8)	0.067 (3)
O2	0.7787 (10)	0.2766 (9)	0.1787 (8)	0.066 (3)
C1	1.0072 (12)	0.2600 (11)	0.1224 (10)	0.044 (3)
C2	1.1181 (14)	0.3355 (15)	0.1300 (13)	0.064 (4)
H2	1.1134	0.4253	0.1277	0.077*
C3	1.2345 (15)	0.273 (2)	0.1408 (14)	0.085 (5)
H3	1.3083	0.3213	0.1458	0.102*
C4	1.2404 (18)	0.1382 (18)	0.1441 (15)	0.081 (5)
H4	1.3180	0.0964	0.1503	0.097*
C5	1.1335 (18)	0.0686 (18)	0.1384 (13)	0.078 (5)
H5	1.1388	−0.0211	0.1432	0.094*
C6	1.0176 (16)	0.1269 (13)	0.1256 (13)	0.061 (4)
H6	0.9450	0.0765	0.1190	0.073*
C7	0.7727 (16)	0.3131 (19)	−0.0378 (12)	0.080 (5)
H7A	0.7518	0.2231	−0.0490	0.119*
H7B	0.8275	0.3384	−0.0847	0.119*
H7C	0.6961	0.3637	−0.0554	0.119*
C8	0.9178 (13)	0.7666 (12)	0.1790 (12)	0.055 (3)
H8A	0.9294	0.8363	0.2314	0.082*
H8B	0.8799	0.7994	0.1066	0.082*
H8C	0.9988	0.7285	0.1789	0.082*
C9	0.6111 (15)	0.6020 (15)	0.1233 (12)	0.067 (4)
H9A	0.5694	0.5328	0.1523	0.100*
H9B	0.6155	0.5818	0.0490	0.100*
H9C	0.5639	0.6806	0.1236	0.100*
C10	0.8716 (15)	0.5208 (15)	0.3710 (11)	0.070 (4)
H10A	0.8054	0.5079	0.4096	0.104*
H10B	0.9401	0.5687	0.4169	0.104*
H10C	0.9026	0.4384	0.3532	0.104*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0286 (6)	0.0407 (6)	0.0522 (6)	0.0003 (3)	0.0145 (4)	0.0010 (3)
P1	0.051 (2)	0.0397 (18)	0.060 (2)	0.0044 (15)	0.0310 (17)	0.0035 (15)
O1	0.080 (7)	0.042 (5)	0.096 (7)	0.015 (5)	0.058 (6)	0.009 (5)
O2	0.078 (7)	0.043 (5)	0.094 (7)	0.001 (5)	0.057 (6)	0.012 (5)
C1	0.043 (7)	0.040 (7)	0.056 (7)	0.000 (6)	0.029 (6)	0.008 (6)
C2	0.049 (9)	0.059 (9)	0.088 (11)	0.001 (7)	0.024 (8)	−0.010 (8)
C3	0.038 (9)	0.113 (15)	0.103 (13)	−0.003 (9)	0.016 (9)	0.001 (11)
C4	0.054 (11)	0.109 (16)	0.080 (11)	0.028 (10)	0.020 (9)	0.007 (9)
C5	0.088 (14)	0.062 (10)	0.095 (12)	0.025 (10)	0.040 (10)	−0.003 (9)
C6	0.058 (10)	0.057 (9)	0.076 (10)	0.015 (7)	0.030 (8)	0.002 (7)

C7	0.066 (11)	0.113 (13)	0.060 (9)	−0.001 (10)	0.017 (8)	−0.021 (9)
C8	0.037 (8)	0.044 (7)	0.095 (10)	0.002 (6)	0.040 (7)	−0.006 (7)
C9	0.050 (9)	0.090 (12)	0.064 (9)	0.004 (8)	0.019 (7)	0.006 (8)
C10	0.068 (11)	0.073 (10)	0.064 (9)	0.010 (8)	0.008 (8)	0.008 (7)

Geometric parameters (Å, º)

Sn1—C8	2.101 (13)	C4—H4	0.9300
Sn1—C9	2.122 (15)	C5—C6	1.36 (2)
Sn1—C10	2.129 (13)	C5—H5	0.9300
Sn1—O1	2.231 (9)	C6—H6	0.9300
Sn1—O2^{i}	2.255 (8)	C7—H7A	0.9600
P1—O1	1.486 (9)	C7—H7B	0.9600
P1—O2	1.502 (9)	C7—H7C	0.9600
P1—C7	1.812 (15)	C8—H8A	0.9600
P1—C1	1.822 (13)	C8—H8B	0.9600
O2—Sn1^{ii}	2.255 (8)	C8—H8C	0.9600
C1—C6	1.380 (16)	C9—H9A	0.9600
C1—C2	1.415 (18)	C9—H9B	0.9600
C2—C3	1.39 (2)	C9—H9C	0.9600
C2—H2	0.9300	C10—H10A	0.9600
C3—C4	1.40 (2)	C10—H10B	0.9600
C3—H3	0.9300	C10—H10C	0.9600
C4—C5	1.35 (2)		
C8—Sn1—C9	119.3 (6)	C4—C5—C6	121.4 (17)
C8—Sn1—C10	116.7 (6)	C4—C5—H5	119.3
C9—Sn1—C10	123.9 (6)	C6—C5—H5	119.3
C8—Sn1—O1	89.3 (4)	C5—C6—C1	120.7 (16)
C9—Sn1—O1	92.1 (5)	C5—C6—H6	119.7
C10—Sn1—O1	90.9 (5)	C1—C6—H6	119.7
C8—Sn1—O2^{i}	89.4 (4)	P1—C7—H7A	109.5
C9—Sn1—O2^{i}	88.7 (5)	P1—C7—H7B	109.5
C10—Sn1—O2^{i}	89.5 (5)	H7A—C7—H7B	109.5
O1—Sn1—O2^{i}	178.6 (3)	P1—C7—H7C	109.5
O1—P1—O2	115.0 (5)	H7A—C7—H7C	109.5
O1—P1—C7	109.5 (8)	H7B—C7—H7C	109.5
O2—P1—C7	109.2 (7)	Sn1—C8—H8A	109.5
O1—P1—C1	107.7 (6)	Sn1—C8—H8B	109.5
O2—P1—C1	109.7 (5)	H8A—C8—H8B	109.5
C7—P1—C1	105.3 (7)	Sn1—C8—H8C	109.5
P1—O1—Sn1	132.5 (6)	H8A—C8—H8C	109.5
P1—O2—Sn1^{ii}	161.4 (6)	H8B—C8—H8C	109.5
C6—C1—C2	119.1 (13)	Sn1—C9—H9A	109.5
C6—C1—P1	121.3 (11)	Sn1—C9—H9B	109.5
C2—C1—P1	119.6 (10)	H9A—C9—H9B	109.5
C3—C2—C1	118.9 (15)	Sn1—C9—H9C	109.5
C3—C2—H2	120.6	H9A—C9—H9C	109.5

C1—C2—H2	120.6	H9B—C9—H9C	109.5
C2—C3—C4	120.0 (16)	Sn1—C10—H10A	109.5
C2—C3—H3	120.0	Sn1—C10—H10B	109.5
C4—C3—H3	120.0	H10A—C10—H10B	109.5
C5—C4—C3	119.9 (17)	Sn1—C10—H10C	109.5
C5—C4—H4	120.1	H10A—C10—H10C	109.5
C3—C4—H4	120.1	H10B—C10—H10C	109.5

Symmetry codes: (i) $-x+3/2, y+1/2, -z+1/2$; (ii) $-x+3/2, y-1/2, -z+1/2$.