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catena-Poly[[cyclohexyldiphenyltin(IV)]-μ-hydroxido-κ^2O:O]

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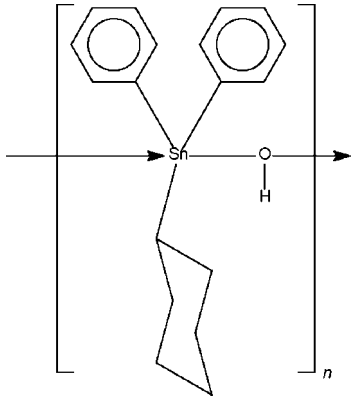
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.005 Å; R factor = 0.018; wR factor = 0.072; data-to-parameter ratio = 17.6.

The title polymeric mixed-organyl tin hydroxide, $[Sn(C_6H_5)_2(C_6H_{11})(OH)]_n$, hass a hydroxide-bridged chain structure; the tin center shows *trans*-C_3SnO_2 trigonal bipyramidal coordination. The Sn atom lies on a special position of site symmetry *m*; the symmetry element relates one phenyl ring to the other and also relates one half of the cyclohexyl ring to the other half.

Related literature

For background literature on mixed alkyl/diaryltin(IV) compounds, see: Koshy *et al.* (2001). For the synthesis of cyclohexyldiphenyltin hydroxide, see: Teo *et al.* (2007). For the structure of triethyltin hydroxide, see: Deacon *et al.* (1993). For the structure of tribenzyltin hydroxide, see: Chen *et al.* (2005); Reuter (2004). For the structure of triphenyltin hydroxide, see: Fu *et al.* (2003); Glidewell & Liles (1978); Glidewell *et al.* (2002). For the structure of the mixed organyl compound, benzyldimethyltin hydroxide, see: Wannagat *et al.* (1993).



Experimental

Crystal data

$[Sn(C_6H_5)_2(C_6H_{11})(OH)]$
M_r = 373.05
Orthorhombic, $Cmc2_1$
a = 18.3830 (2) Å
b = 10.2801 (1) Å
c = 8.1762 (1) Å
V = 1545.13 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.65 mm^{-1}
T = 100 (2) K
0.22 × 0.09 × 0.08 mm

Data collection

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.771, T_{max} = 0.880
9651 measured reflections
1711 independent reflections
1637 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.017
$wR(F^2)$ = 0.071
S = 1.28
1711 reflections
97 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.57 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 650 Friedel pairs
Flack parameter: 0.02 (4)

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.201 (4)	Sn1—C5	2.139 (3)
Sn1—C1	2.159 (4)		
C1—Sn1—C5	118.4 (1)	C5—Sn1—O1	90.7 (1)
C1—Sn1—O1	94.1 (2)	C5—Sn1—O1^{i}	87.5 (1)
C1—Sn1—O1^{i}	89.8 (2)	O1—Sn1—O1^{i}	176.1 (1)
C5—Sn1—C5^{ii}	122.9 (2)	Sn1—O1—Sn1^{iii}	133.7 (2)

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2257).

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supplementary materials

Acta Cryst. (2008). E**64**, m724-m725 [**doi:10.1107/S1600536808011100**]

catena-Poly[[cyclohexyldiphenyltin(IV)]-μ-hydroxido-$\kappa^2 O{:}O$]

K. M. Lo and S. W. Ng

Comment

Mixed alkyl/diaryltin compounds possess much more useful activity against plant pathogens than the symmetrical triorganotin homologs, particularly if one of the alkyl substituent is a cyclic unit (Koshy *et al.*, 2001). The title compound (I) is the starting reactant for the synthesis of mixed organotin carboxylates.

The compound adopts a zigzag chain motif that propagates along the *c*-axis of the orthorhombic unit cell; the tin center shows *trans*-C_3SnO_2 trigonal bipyramidal coordination (Figs 1 and 2 & Table 1).

Experimental

The compound was synthesized as described previously (Teo *et al.*, 2007). Crystals were obtained by recrystallization from ethanol.

Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U_{eq}(C). The hydroxo H atom (O–H 0.84 Å) was similarly treated.

Figures

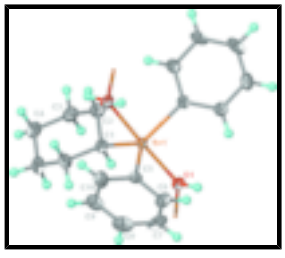

Fig. 1. 70% Probability thermal ellipsoid plot of the asymmetric unit in $Sn(C_6H_{11})(C_6H_5)_2(OH)$ (I) extended to show the *trans*-C_3SnO_2 trigonal bipyramidal coordination geometry. Hydrogen atoms are drawn as spheres of arbitrary radius; symmetry-related atoms are not labeled.

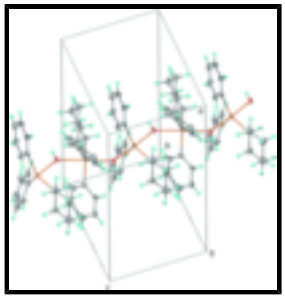

Fig. 2. Hydroxo-bridged chain motif in (I).

catena-Poly[[cyclohexyldiphenyltin(IV)]-μ-hydroxido- $\kappa^2 O{:}O$]

Crystal data

$[Sn(C_6H_5)_2(C_6H_{11})(OH)]$	F_{000} = 752
M_r = 373.05	D_x = 1.604 Mg m^{-3}
Orthorhombic, $Cmc2_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: C 2c -2	Cell parameters from 8850 reflections
a = 18.3830 (2) Å	θ = 2.2–28.3º
b = 10.2801 (1) Å	μ = 1.65 mm^{-1}
c = 8.1762 (1) Å	T = 100 (2) K
V = 1545.13 (3) Å^3	Prism, colorless
Z = 4	0.22 × 0.09 × 0.08 mm

Data collection

Bruker SMART APEXII diffractometer	1711 independent reflections
Radiation source: fine-focus sealed tube	1637 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.024
T = 100(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −23→23
T_{min} = 0.771, T_{max} = 0.880	k = −13→13
9651 measured reflections	l = −9→10

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.017	$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2 + 0.0692P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.071	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.28	$\Delta\rho_{max}$ = 0.57 e Å^{-3}
1711 reflections	$\Delta\rho_{min}$ = −0.31 e Å^{-3}
97 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 650 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.02 (4)
Secondary atom site location: difference Fourier map	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.5000	0.494121 (18)	0.50000 (18)	0.01298 (10)
O1	0.5000	0.5850 (3)	0.2563 (4)	0.0165 (6)
H1O	0.5000	0.6666	0.2598	0.025*
C1	0.5000	0.2980 (4)	0.4053 (6)	0.0189 (9)
H1	0.5000	0.3071	0.2836	0.023*
C2	0.43184 (16)	0.2226 (3)	0.4465 (5)	0.0234 (7)
H2A	0.3888	0.2721	0.4084	0.028*
H2B	0.4281	0.2132	0.5667	0.028*
C3	0.4313 (2)	0.0883 (3)	0.3681 (5)	0.0260 (8)
H3A	0.3885	0.0392	0.4078	0.031*
H3B	0.4268	0.0977	0.2480	0.031*
C4	0.5000	0.0125 (4)	0.4074 (8)	0.0248 (13)
H4A	0.5000	−0.0102	0.5251	0.030*
H4B	0.5000	−0.0696	0.3442	0.030*
C5	0.60222 (16)	0.5831 (3)	0.5558 (4)	0.0170 (6)
C6	0.62261 (15)	0.7060 (2)	0.5004 (5)	0.0227 (6)
H6	0.5897	0.7548	0.4352	0.027*
C7	0.69028 (19)	0.7587 (3)	0.5387 (4)	0.0296 (8)
H7	0.7023	0.8441	0.5036	0.036*
C8	0.74004 (18)	0.6867 (4)	0.6280 (5)	0.0308 (8)
H8	0.7867	0.7216	0.6514	0.037*
C9	0.72163 (17)	0.5644 (4)	0.6826 (5)	0.0256 (7)
H9	0.7553	0.5149	0.7449	0.031*
C10	0.6529 (3)	0.5133 (3)	0.6458 (7)	0.0247 (9)
H10	0.6407	0.4287	0.6836	0.030*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01281 (14)	0.01401 (14)	0.01211 (16)	0.000	0.000	0.0003 (2)
O1	0.0227 (14)	0.0168 (15)	0.0101 (15)	0.000	0.000	−0.0008 (11)
C1	0.022 (2)	0.0167 (19)	0.018 (2)	0.000	0.000	0.0005 (17)
C2	0.0200 (15)	0.0215 (14)	0.0288 (19)	−0.0023 (11)	0.0003 (13)	−0.0006 (12)
C3	0.0306 (19)	0.0193 (15)	0.028 (2)	−0.0044 (13)	0.0033 (14)	0.0001 (14)
C4	0.038 (4)	0.019 (2)	0.017 (3)	0.000	0.000	−0.0032 (17)
C5	0.0168 (13)	0.0194 (13)	0.0147 (15)	−0.0006 (12)	0.0029 (11)	−0.0018 (11)
C6	0.0268 (14)	0.0242 (12)	0.0171 (16)	−0.0042 (10)	−0.0025 (17)	0.001 (2)
C7	0.0366 (18)	0.0302 (16)	0.022 (2)	−0.0150 (14)	0.0004 (14)	0.0036 (13)
C8	0.0213 (16)	0.043 (2)	0.028 (2)	−0.0107 (14)	−0.0009 (15)	−0.0088 (16)
C9	0.0174 (15)	0.0343 (19)	0.0250 (18)	0.0007 (13)	−0.0047 (13)	−0.0072 (15)
C10	0.023 (2)	0.0195 (17)	0.032 (3)	−0.0007 (11)	−0.0051 (18)	−0.0014 (14)

Geometric parameters (Å, °)

Sn1—O1	2.201 (4)	C8—C9	1.377 (5)

Sn1—C1	2.159 (4)	C9—C10	1.400 (5)
Sn1—C5	2.139 (3)	O1—H1O	0.8400
Sn1—C5^{i}	2.139 (3)	C1—H1	1.0000
Sn1—O1^{ii}	2.248 (4)	C2—H2A	0.9900
O1—Sn1^{iii}	2.248 (4)	C2—H2B	0.9900
C1—C2	1.511 (4)	C3—H3A	0.9900
C1—C2^{i}	1.511 (4)	C3—H3B	0.9900
C2—C3	1.522 (4)	C4—H4A	0.9900
C3—C4	1.518 (4)	C4—H4B	0.9900
C4—C3^{i}	1.518 (4)	C6—H6	0.9500
C5—C10	1.388 (6)	C7—H7	0.9500
C5—C6	1.394 (4)	C8—H8	0.9500
C6—C7	1.393 (4)	C9—H9	0.9500
C7—C8	1.385 (5)	C10—H10	0.9500
C1—Sn1—C5	118.4 (1)	C2—C1—H1	105.6
C1—Sn1—O1	94.1 (2)	Sn1—C1—H1	105.6
C1—Sn1—O1^{ii}	89.8 (2)	C1—C2—H2A	109.2
C5—Sn1—C5^{i}	122.9 (2)	C3—C2—H2A	109.2
C5—Sn1—O1	90.7 (1)	C1—C2—H2B	109.2
C5—Sn1—O1^{ii}	87.5 (1)	C3—C2—H2B	109.2
C5^{i}—Sn1—C1	118.4 (1)	H2A—C2—H2B	107.9
C5^{i}—Sn1—O1	90.7 (1)	C4—C3—H3A	109.3
C5^{i}—Sn1—O1^{ii}	87.5 (1)	C2—C3—H3A	109.3
O1—Sn1—O1^{ii}	176.1 (1)	C4—C3—H3B	109.3
Sn1—O1—Sn1^{iii}	133.7 (2)	C2—C3—H3B	109.3
C2—C1—C2^{i}	112.0 (3)	H3A—C3—H3B	107.9
C2—C1—Sn1	113.5 (2)	C3^{i}—C4—H4A	109.1
C2^{i}—C1—Sn1	113.5 (2)	C3—C4—H4A	109.1
C1—C2—C3	112.1 (3)	C3^{i}—C4—H4B	109.1
C4—C3—C2	111.8 (3)	C3—C4—H4B	109.1
C3^{i}—C4—C3	112.5 (4)	H4A—C4—H4B	107.8
C10—C5—C6	117.4 (3)	C7—C6—H6	119.3
C10—C5—Sn1	118.8 (2)	C5—C6—H6	119.3
C6—C5—Sn1	123.7 (2)	C8—C7—H7	120.0
C7—C6—C5	121.3 (3)	C6—C7—H7	120.0
C8—C7—C6	120.0 (3)	C9—C8—H8	120.1
C9—C8—C7	119.8 (3)	C7—C8—H8	120.1
C8—C9—C10	119.6 (4)	C8—C9—H9	120.2
C5—C10—C9	121.7 (3)	C10—C9—H9	120.2
Sn1—O1—H1O	113.2	C5—C10—H10	119.1
Sn1^{iii}—O1—H1O	113.2	C9—C10—H10	119.1
C5—Sn1—O1—Sn1^{iii}	118.53 (8)	C1—Sn1—C5—C10	−47.4 (4)
C5^{i}—Sn1—O1—Sn1^{iii}	−118.53 (8)	O1—Sn1—C5—C10	−142.4 (3)
C1—Sn1—O1—Sn1^{iii}	0.0	O1^{ii}—Sn1—C5—C10	41.0 (3)

C5—Sn1—C1—C2	151.7 (2)	C5^{i}—Sn1—C5—C6	−56.7 (4)
C5^{i}—Sn1—C1—C2	−22.3 (3)	C1—Sn1—C5—C6	129.6 (3)
O1—Sn1—C1—C2	−115.3 (3)	O1—Sn1—C5—C6	34.5 (3)
O1^{ii}—Sn1—C1—C2	64.7 (3)	O1^{ii}—Sn1—C5—C6	−142.0 (3)
C5—Sn1—C1—C2^{i}	22.3 (3)	C10—C5—C6—C7	−2.2 (5)
C5^{i}—Sn1—C1—C2^{i}	−151.7 (2)	Sn1—C5—C6—C7	−179.2 (3)
O1—Sn1—C1—C2^{i}	115.3 (3)	C5—C6—C7—C8	2.6 (5)
O1^{ii}—Sn1—C1—C2^{i}	−64.7 (3)	C6—C7—C8—C9	−1.8 (6)
C2^{i}—C1—C2—C3	−53.8 (5)	C7—C8—C9—C10	0.7 (6)
Sn1—C1—C2—C3	176.0 (3)	C6—C5—C10—C9	1.0 (6)
C1—C2—C3—C4	52.9 (5)	Sn1—C5—C10—C9	178.2 (3)
C2—C3—C4—C3^{i}	−52.3 (6)	C8—C9—C10—C5	−0.3 (7)
C5^{i}—Sn1—C5—C10	126.3 (3)		

Symmetry codes: (i) −*x*+1, *y*, *z*; (ii) −*x*+1, −*y*+1, *z*+1/2; (iii) −*x*+1, −*y*+1, *z*−1/2.

Fig. 1

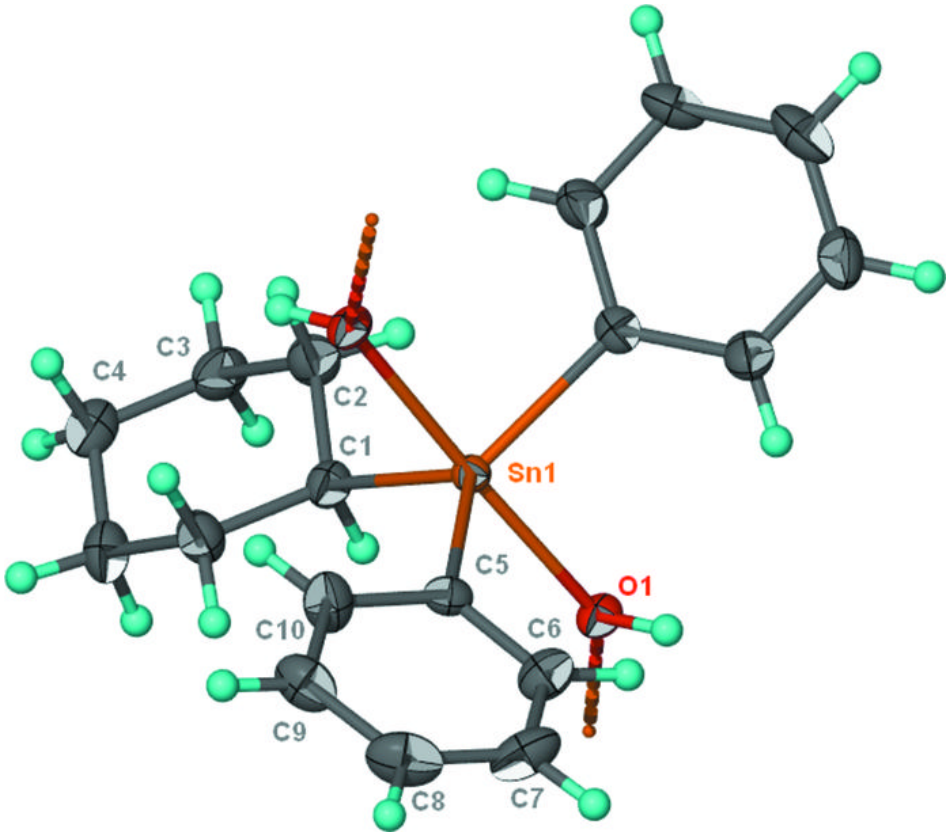

Fig. 2