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

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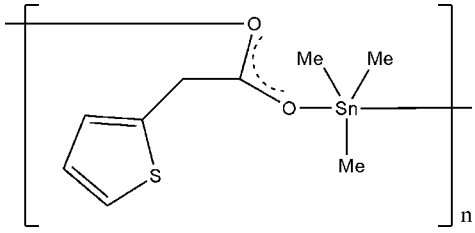
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.014 Å; R factor = 0.037; wR factor = 0.127; data-to-parameter ratio = 18.4.

The title compound, $[Sn(CH_3)_3(C_6H_5O_2S)]_n$, has an infinite chain structure. The SnO_2C_3 centre has a slightly distorted trigonal bipyramidal geometry with the O atoms in the axial positions.

Related literature

For related materials, see Ma *et al.* (2006).



Experimental

Crystal data

$[Sn(CH_3)_3(C_6H_5O_2S)]$
M_r = 304.95
Monoclinic, $P2_1/c$
a = 9.5179 (13) Å
b = 10.1177 (14) Å
c = 13.2038 (18) Å
β = 104.039 (2)°
V = 1233.5 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.21 mm^{-1}
T = 298 (2) K
0.54 × 0.39 × 0.37 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.381, T_{max} = 0.495
(expected range = 0.340–0.441)
4898 measured reflections
2168 independent reflections
1622 reflections with $I > 2\sigma(I)$
R_{int} = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.127
S = 1.00
2168 reflections
118 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.10 e Å^{-3}
$\Delta\rho_{min}$ = −0.63 e Å^{-3}

Table 1
Selected bond lengths (Å).

Sn1—C8	2.113 (8)	Sn1—O1	2.200 (5)
Sn1—C9	2.120 (7)	Sn1—O2^{i}	2.353 (5)
Sn1—C7	2.121 (7)		

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

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2631).

References

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supplementary materials

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

H. Wang, H. Yin and D. Wang

Comment

The title compound, (I) (Fig. 1), possesses an infinite one-dimensional chain structure arising from Sn—O bridges to the ligand. The Sn—O distances in (I) (Table 1) are similar to those in related organotin carboxylates (Ma *et al.*, 2006). The Sn atom has distorted trigonal-bipyramidal geometry, with the O atoms in axial positions [O1—Sn1—$O2^{i}$ = 173.28 (17) °] and the C atoms of the three methyl groups in equatorial positions. The sum of the equatorial C—Sn—C angles is 359.4 °, indicating near coplanarity for these atoms.

Experimental

The reaction was carried out under a nitrogen atmosphere. 2-Thiopheneacetic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to 30 ml of benzene in a Schlenk flask and stirred for 0.5 h. Trimethyltin chloride (1 mmol) was then added to the reactor and the reaction mixture was stirred for 12 h at 313 K·The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/methanol (1:1 *v*/*v*) to yield colourless blocks of (I). Yield 80%; m.p. 452 K. Analysis calculated (%) for $C_9H_{14}O_2SSn$: C 35.44; H 4.63%. found: C 35.37; H 4.71%.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

Figures

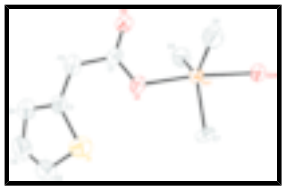

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity. Atom O2A is generated by the symmetry operation (1 − *x*, 1/2 + *y*, 3/2 − *z*).

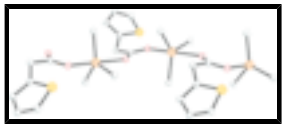

Fig. 2. Part of the chain structure of (I), H atoms have been omitted for clarity.

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

Crystal data

$[Sn(CH_3)_3(C_6H_5O_2S)]$ F_{000} = 600

M_r = 304.95	D_x = 1.642 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2389 reflections
a = 9.5179 (13) Å	θ = 2.6–25.8º
b = 10.1177 (14) Å	μ = 2.21 mm^{-1}
c = 13.2038 (18) Å	T = 298 (2) K
β = 104.039 (2)º	Block, colourless
V = 1233.5 (3) Å^3	0.54 × 0.39 × 0.37 mm
Z = 4	

Data collection

Siemens SMART CCD diffractometer	2168 independent reflections
Radiation source: fine-focus sealed tube	1622 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.032
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −11→11
T_{min} = 0.381, T_{max} = 0.495	k = −11→12
4898 measured reflections	l = −15→13

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.037	H-atom parameters constrained
$wR(F^2)$ = 0.127	$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 1.6901P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.001
2168 reflections	$\Delta\rho_{max}$ = 1.10 e Å^{-3}
118 parameters	$\Delta\rho_{min}$ = −0.62 e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.56253 (5)	1.10603 (4)	0.72279 (3)	0.0566 (2)
O1	0.7129 (5)	0.9441 (5)	0.7131 (5)	0.0843 (15)
O2	0.5752 (5)	0.7961 (5)	0.7658 (4)	0.0794 (14)
S1	0.9638 (3)	0.8817 (2)	0.6287 (2)	0.1037 (8)
C1	0.6853 (9)	0.8260 (7)	0.7362 (6)	0.0735 (19)

C2	0.7962 (9)	0.7225 (8)	0.7295 (7)	0.093 (3)
H2A	0.7478	0.6374	0.7194	0.112*
H2B	0.8667	0.7193	0.7962	0.112*
C3	0.8771 (7)	0.7394 (7)	0.6452 (6)	0.0703 (18)
C4	0.8965 (11)	0.6402 (9)	0.5751 (9)	0.103 (3)
H4	0.8577	0.5554	0.5706	0.123*
C5	0.9859 (13)	0.6919 (12)	0.5122 (10)	0.125 (3)
H5	1.0093	0.6439	0.4585	0.150*
C6	1.0323 (11)	0.8122 (11)	0.5361 (9)	0.115 (3)
H6	1.0972	0.8550	0.5047	0.138*
C7	0.7008 (9)	1.2365 (8)	0.6666 (7)	0.086 (2)
H7A	0.6764	1.2347	0.5917	0.129*
H7B	0.7996	1.2092	0.6925	0.129*
H7C	0.6889	1.3246	0.6901	0.129*
C8	0.5859 (11)	1.0867 (8)	0.8854 (6)	0.090 (3)
H8A	0.6722	1.1315	0.9219	0.136*
H8B	0.5926	0.9947	0.9039	0.136*
H8C	0.5034	1.1250	0.9041	0.136*
C9	0.3859 (8)	1.0250 (9)	0.6101 (6)	0.087 (2)
H9A	0.3962	1.0458	0.5414	0.130*
H9B	0.2970	1.0617	0.6196	0.130*
H9C	0.3847	0.9308	0.6185	0.130*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0716 (3)	0.0419 (3)	0.0623 (3)	−0.0046 (2)	0.0279 (2)	−0.00282 (19)
O1	0.090 (3)	0.044 (3)	0.133 (5)	0.005 (3)	0.055 (3)	0.007 (3)
O2	0.090 (4)	0.052 (3)	0.109 (4)	−0.003 (3)	0.049 (3)	0.003 (3)
S1	0.0950 (16)	0.0907 (17)	0.129 (2)	−0.0182 (13)	0.0331 (15)	0.0003 (14)
C1	0.088 (5)	0.045 (4)	0.093 (5)	−0.001 (4)	0.033 (4)	0.004 (4)
C2	0.102 (6)	0.062 (5)	0.127 (7)	0.018 (4)	0.051 (5)	0.011 (5)
C3	0.058 (4)	0.054 (4)	0.100 (5)	0.012 (3)	0.020 (4)	0.006 (4)
C4	0.110 (6)	0.073 (5)	0.140 (6)	0.008 (4)	0.058 (5)	−0.001 (5)
C5	0.140 (6)	0.104 (6)	0.149 (6)	0.034 (6)	0.072 (5)	−0.001 (6)
C6	0.110 (5)	0.105 (6)	0.148 (6)	0.018 (5)	0.067 (5)	0.015 (6)
C7	0.108 (6)	0.050 (4)	0.112 (6)	−0.019 (4)	0.053 (5)	0.012 (4)
C8	0.128 (7)	0.080 (6)	0.064 (4)	0.001 (5)	0.024 (5)	−0.002 (4)
C9	0.096 (5)	0.089 (6)	0.074 (5)	−0.011 (5)	0.019 (4)	−0.018 (4)

Geometric parameters (Å, °)

Sn1—C8	2.113 (8)	C4—C5	1.425 (14)
Sn1—C9	2.120 (7)	C4—H4	0.9300
Sn1—C7	2.121 (7)	C5—C6	1.307 (14)
Sn1—O1	2.200 (5)	C5—H5	0.9300
Sn1—O2^{i}	2.353 (5)	C6—H6	0.9300
O1—C1	1.276 (9)	C7—H7A	0.9600

O2—C1	1.242 (8)	C7—H7B	0.9600
O2—Sn1^{ii}	2.353 (5)	C7—H7C	0.9600
S1—C6	1.674 (10)	C8—H8A	0.9600
S1—C3	1.699 (8)	C8—H8B	0.9600
C1—C2	1.505 (10)	C8—H8C	0.9600
C2—C3	1.509 (10)	C9—H9A	0.9600
C2—H2A	0.9700	C9—H9B	0.9600
C2—H2B	0.9700	C9—H9C	0.9600
C3—C4	1.408 (12)		
C8—Sn1—C9	123.2 (4)	C3—C4—H4	125.9
C8—Sn1—C7	119.5 (4)	C5—C4—H4	125.9
C9—Sn1—C7	116.7 (3)	C6—C5—C4	114.6 (10)
C8—Sn1—O1	94.6 (3)	C6—C5—H5	122.7
C9—Sn1—O1	95.0 (3)	C4—C5—H5	122.7
C7—Sn1—O1	88.6 (3)	C5—C6—S1	113.5 (8)
C8—Sn1—O2^{i}	86.2 (3)	C5—C6—H6	123.3
C9—Sn1—O2^{i}	90.1 (3)	S1—C6—H6	123.3
C7—Sn1—O2^{i}	85.2 (3)	Sn1—C7—H7A	109.5
O1—Sn1—O2^{i}	173.28 (17)	Sn1—C7—H7B	109.5
C1—O1—Sn1	120.6 (4)	H7A—C7—H7B	109.5
C1—O2—Sn1^{ii}	138.2 (5)	Sn1—C7—H7C	109.5
C6—S1—C3	91.4 (5)	H7A—C7—H7C	109.5
O2—C1—O1	122.8 (7)	H7B—C7—H7C	109.5
O2—C1—C2	120.4 (7)	Sn1—C8—H8A	109.5
O1—C1—C2	116.8 (7)	Sn1—C8—H8B	109.5
C1—C2—C3	117.0 (7)	H8A—C8—H8B	109.5
C1—C2—H2A	108.0	Sn1—C8—H8C	109.5
C3—C2—H2A	108.0	H8A—C8—H8C	109.5
C1—C2—H2B	108.0	H8B—C8—H8C	109.5
C3—C2—H2B	108.0	Sn1—C9—H9A	109.5
H2A—C2—H2B	107.3	Sn1—C9—H9B	109.5
C4—C3—C2	125.1 (7)	H9A—C9—H9B	109.5
C4—C3—S1	112.0 (6)	Sn1—C9—H9C	109.5
C2—C3—S1	122.8 (6)	H9A—C9—H9C	109.5
C3—C4—C5	108.3 (9)	H9B—C9—H9C	109.5

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

Fig. 1

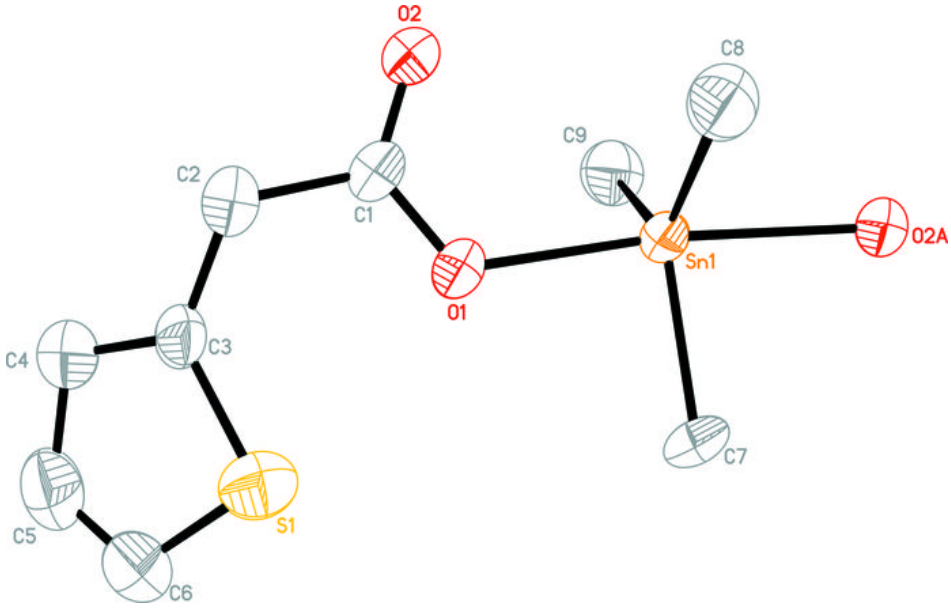

Fig. 2