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catena-Poly[[tri-*n*-butyltin(IV)]-μ-2-thiopheneacetato]

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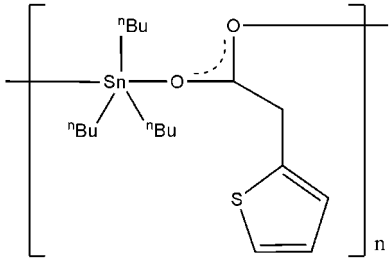
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.019 Å; disorder in main residue; R factor = 0.060; wR factor = 0.197; data-to-parameter ratio = 18.6.

The title compound, $[Sn(C_4H_9)_3(C_6H_5O_2S)]_n$, possesses an infinite chain structure. The SnO_2C_3 centre has a distorted trigonal-bipyramidal geometry (τ = 0.145) with the O atoms in the axial positions. Atoms of the thiophene group S1 and C4 are disordered over two sites The S atom and one C atom, with attached H atom, of the thiophene ring are disordered over two positions; the site occupancy factors are *ca* 0.7 and 0.3.

Related literature

For related literature see: Addison *et al.* (1984); Ma *et al.* (2006).



Experimental

Crystal data

$[Sn(C_4H_9)_3(C_6H_5O_2S)]$
M_r = 431.19
Monoclinic, $P2_1/c$
a = 12.7657 (15) Å
b = 10.6970 (13) Å
c = 16.328 (2) Å
β = 100.435 (2)°
V = 2192.8 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.26 mm^{-1}
T = 298 (2) K
0.46 × 0.21 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.594, T_{max} = 0.863
8428 measured reflections
3715 independent reflections
2104 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.060
$wR(F^2)$ = 0.197
S = 1.10
3715 reflections
200 parameters
483 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.96 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 e Å^{-3}

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: BV2084).

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supporting information

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catena-Poly[[tri-*n*-butyltin(IV)]-μ-2-thiopheneacetato]

Hongyun Wang, Handong Yin and Yuying Sun

S1. Comment

The title compound, (I) (Fig. 1), possesses an infinite one-dimensional chain structure arising from Sn—O bridges to the ligand. The Sn1—O1 distances of 2.183 (6) Å and Sn1—O2A [symmetry code: -*x* + 2,*y* - 1/2,-*z* + 1/2] distance 2.482 (7) Å, are similar to those reported for other organotin carboxylates (Ma *et al.*, 2006). The Sn atom has distorted trigonal-bipyramidal geometry[τ = 0.145; Addison *et al.*,, 1984], with atoms O1 and O2A in axial positions [O1—Sn1—O2A = 171.3 (2) °] and the C atoms of the three butyl groups in equatorial positions. The sum of the equatorial C—Sn—C angles is 358.6 °, indicating approximate coplanarity for these atoms.

S2. Experimental

The reaction was carried out under nitrogen atmosphere. 2-Thiopheneacetic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to the solution of benzene(30 ml) in a Schlenk flask and stirred for 0.5 h. Tri-n-butyltin 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).(yield 80%; m.p. 457 K). Analysis calculated (%) for $C_{18}H_{32}O_2SSn$ (Mr = 431.19): C, 50.14; H, 7.48. found: C, 50.06; H, 7.53.

S3. Refinement

During the refinement atoms S1 and C4 were found to be disordered over two sites, and the ratio of the occupancy factors refined to 0.729 (11):0.271 (11) and 0.271 (11):0.729 (11) for atoms S1:S1'and atoms C4:C4′, respectively. H atoms were positioned geometrically, with C—H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C) where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

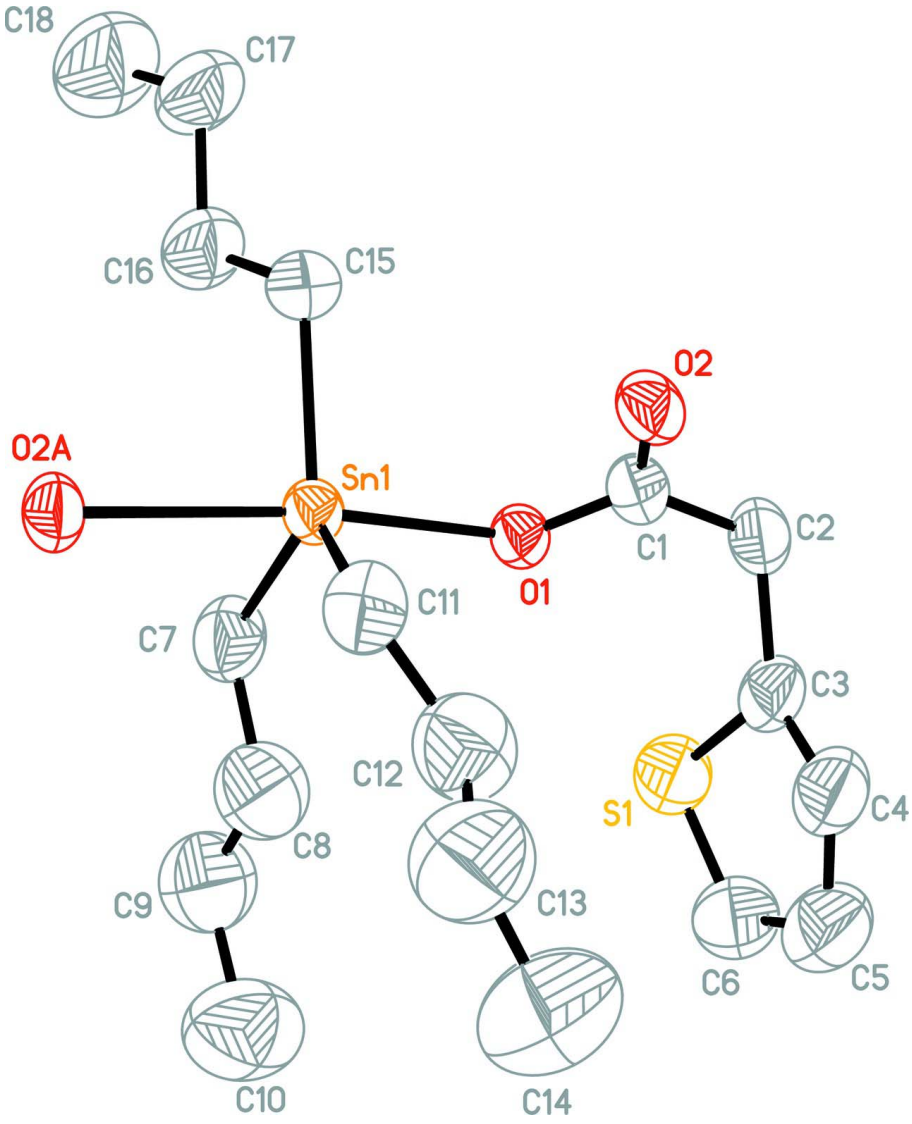

Figure 1

The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

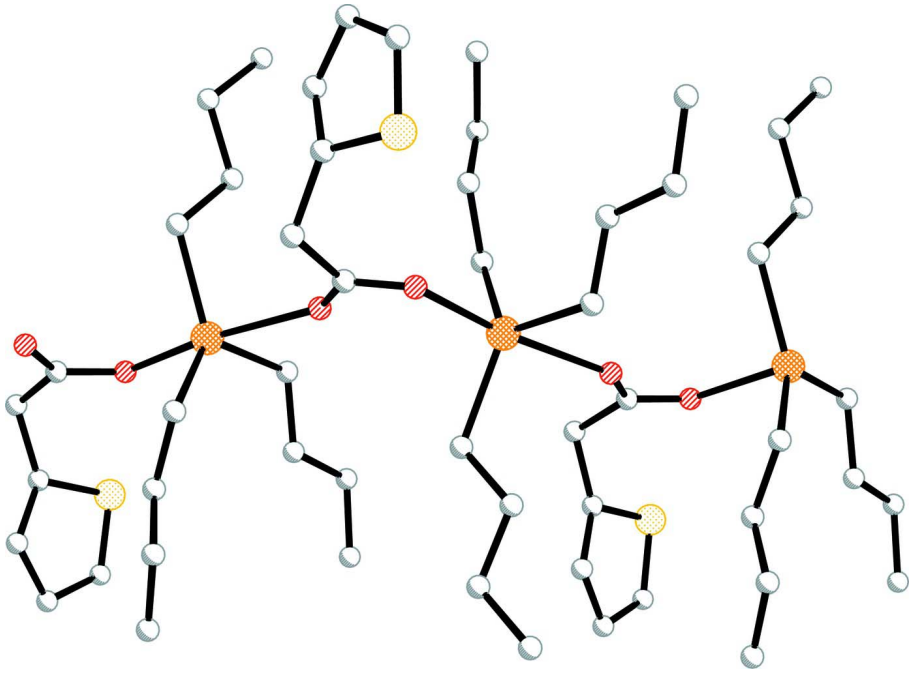

Figure 2

The one-dimensional infinite chain structure of (I), H atoms have been omitted for clarity.

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$b = 10.6970\ (13)$ Å
$c = 16.328\ (2)$ Å
$\beta = 100.435\ (2)°$
$V = 2192.8\ (5)$ Å^3
$Z = 4$
$F(000) = 888$
$D_x = 1.306$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2306 reflections
$\theta = 2.3–22.1°$
$\mu = 1.27$ mm^{-1}
$T = 298$ K
Block, colourless
0.46 × 0.21 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.594$, $T_{max} = 0.863$
8428 measured reflections
3715 independent reflections
2104 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.0°$, $\theta_{min} = 2.3°$
$h = -9\rightarrow15$
$k = -12\rightarrow12$
$l = -19\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.197$
$S = 1.10$
3715 reflections
200 parameters
483 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 4.0018P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.96$ e Å^{-3}
	$\Delta\rho_{min} = -0.51$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.99480 (5)	0.76650 (6)	0.29167 (4)	0.0663 (3)	
O1	0.9550 (5)	0.9174 (5)	0.3707 (4)	0.0663 (3)	
O2	0.9708 (5)	1.0734 (6)	0.2834 (5)	0.0845 (19)	
S1	0.7850 (4)	0.9564 (5)	0.4888 (4)	0.1199 (19)	0.729 (11)
C4′	0.7695 (14)	1.001 (5)	0.494 (2)	0.1199 (19)	0.271 (11)
H4′	0.8167	0.9802	0.5426	0.144*	0.271 (11)
C1	0.9465 (8)	1.0331 (9)	0.3486 (8)	0.085 (2)	
C2	0.9043 (8)	1.1152 (9)	0.4098 (7)	0.091 (3)	
H2A	0.8984	1.2001	0.3886	0.109*	
H2B	0.9548	1.1157	0.4619	0.109*	
C3	0.7953 (6)	1.0734 (9)	0.4269 (7)	0.096 (3)	
C4	0.6941 (9)	1.094 (2)	0.3728 (9)	0.120 (3)	0.729 (11)
H4	0.6844	1.1329	0.3210	0.144*	0.729 (11)
S1′	0.6898 (9)	1.1447 (13)	0.3827 (10)	0.120 (3)	0.271 (11)
C5	0.6121 (8)	1.0451 (13)	0.4115 (9)	0.141 (4)	
H5	0.5398	1.0630	0.3972	0.169*	
C6	0.6597 (8)	0.9649 (12)	0.4754 (9)	0.132 (4)	
H6	0.6200	0.9197	0.5077	0.158*	
C7	0.9691 (9)	0.6340 (11)	0.3839 (9)	0.111 (3)	
H7A	1.0023	0.5550	0.3745	0.133*	
H7B	1.0010	0.6640	0.4388	0.133*	
C8	0.8496 (10)	0.6152 (15)	0.3792 (10)	0.152 (4)	
H8A	0.8180	0.6950	0.3891	0.182*	
H8B	0.8186	0.5890	0.3231	0.182*	
C9	0.8204 (12)	0.5212 (15)	0.4396 (10)	0.174 (6)	
H9A	0.8505	0.5469	0.4959	0.209*	
H9B	0.8508	0.4407	0.4296	0.209*	
C10	0.7012 (12)	0.5082 (19)	0.4313 (12)	0.219 (9)	
H10A	0.6792	0.4285	0.4072	0.329*	
H10B	0.6666	0.5736	0.3961	0.329*	
H10C	0.6819	0.5144	0.4853	0.329*	
C11	0.8709 (9)	0.8019 (12)	0.1866 (9)	0.117 (3)	
H11A	0.8916	0.8710	0.1545	0.140*	
H11B	0.8613	0.7287	0.1509	0.140*	
C12	0.7657 (10)	0.8333 (16)	0.2144 (9)	0.155 (4)	
H12A	0.7578	0.7793	0.2606	0.186*	
H12B	0.7691	0.9188	0.2345	0.186*	
C13	0.6690 (12)	0.820 (2)	0.1477 (11)	0.207 (7)	
H13A	0.6709	0.7394	0.1202	0.249*	

H13B	0.6685	0.8848	0.1063	0.249*
C14	0.5677 (14)	0.829 (3)	0.1860 (15)	0.252 (10)
H14A	0.5511	0.7479	0.2059	0.379*
H14B	0.5095	0.8571	0.1445	0.379*
H14C	0.5793	0.8868	0.2316	0.379*
C15	1.1571 (7)	0.8270 (10)	0.2960 (8)	0.096 (3)
H15A	1.1707	0.8312	0.2395	0.116*
H15B	1.1648	0.9107	0.3190	0.116*
C16	1.2406 (7)	0.7433 (11)	0.3470 (10)	0.125 (4)
H16A	1.2330	0.6590	0.3249	0.150*
H16B	1.2292	0.7408	0.4041	0.150*
C17	1.3543 (8)	0.7906 (14)	0.3454 (11)	0.146 (5)
H17A	1.3663	0.7918	0.2885	0.175*
H17B	1.3619	0.8753	0.3668	0.175*
C18	1.4368 (12)	0.7064 (18)	0.3981 (14)	0.209 (8)
H18A	1.4031	0.6308	0.4115	0.313*
H18B	1.4672	0.7491	0.4485	0.313*
H18C	1.4919	0.6865	0.3673	0.313*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0755 (5)	0.0549 (4)	0.0733 (6)	0.0017 (3)	0.0260 (3)	0.0032 (3)
O1	0.0755 (5)	0.0549 (4)	0.0733 (6)	0.0017 (3)	0.0260 (3)	0.0032 (3)
O2	0.107 (4)	0.061 (4)	0.094 (5)	−0.002 (3)	0.042 (4)	0.012 (3)
S1	0.123 (3)	0.103 (3)	0.144 (4)	0.007 (2)	0.054 (3)	0.020 (3)
C4′	0.123 (3)	0.103 (3)	0.144 (4)	0.007 (2)	0.054 (3)	0.020 (3)
C1	0.092 (5)	0.060 (4)	0.111 (6)	0.001 (4)	0.037 (5)	0.001 (5)
C2	0.113 (6)	0.062 (5)	0.107 (6)	0.007 (5)	0.046 (5)	0.001 (5)
C3	0.100 (5)	0.086 (5)	0.115 (6)	0.016 (5)	0.050 (5)	−0.003 (5)
C4	0.121 (5)	0.106 (6)	0.145 (5)	0.026 (4)	0.053 (4)	0.010 (5)
S1′	0.121 (5)	0.106 (6)	0.145 (5)	0.026 (4)	0.053 (4)	0.010 (5)
C5	0.121 (7)	0.148 (8)	0.163 (8)	0.017 (7)	0.049 (7)	0.004 (7)
C6	0.132 (7)	0.128 (7)	0.150 (8)	−0.001 (6)	0.067 (6)	0.008 (7)
C7	0.131 (7)	0.089 (6)	0.122 (8)	0.018 (6)	0.047 (6)	0.013 (6)
C8	0.162 (8)	0.135 (8)	0.159 (9)	0.005 (7)	0.033 (8)	0.024 (7)
C9	0.174 (12)	0.158 (11)	0.192 (12)	0.009 (10)	0.034 (11)	0.020 (11)
C10	0.163 (16)	0.229 (19)	0.25 (2)	−0.001 (14)	−0.001 (15)	0.042 (18)
C11	0.113 (6)	0.102 (6)	0.137 (7)	0.010 (5)	0.024 (6)	−0.005 (6)
C12	0.154 (8)	0.141 (8)	0.162 (8)	0.005 (7)	0.007 (7)	0.015 (7)
C13	0.176 (12)	0.204 (12)	0.232 (13)	0.012 (12)	0.013 (12)	0.016 (12)
C14	0.198 (18)	0.31 (2)	0.27 (2)	0.017 (19)	0.083 (17)	−0.01 (2)
C15	0.086 (6)	0.089 (6)	0.121 (7)	−0.008 (5)	0.036 (5)	−0.008 (5)
C16	0.083 (7)	0.128 (9)	0.160 (11)	0.002 (6)	0.009 (7)	−0.027 (8)
C17	0.085 (8)	0.160 (10)	0.194 (12)	0.001 (7)	0.028 (8)	−0.044 (10)
C18	0.124 (13)	0.225 (17)	0.27 (2)	0.019 (13)	0.006 (14)	−0.028 (17)

Geometric parameters (Å, º)

Sn1—C7	2.136 (11)	C9—C10	1.510 (9)
Sn1—C11	2.147 (13)	C9—H9A	0.9700
Sn1—C15	2.159 (10)	C9—H9B	0.9700
Sn1—O1	2.183 (6)	C10—H10A	0.9600
Sn1—O2^{i}	2.482 (7)	C10—H10B	0.9600
O1—C1	1.288 (11)	C10—H10C	0.9600
O2—C1	1.239 (12)	C11—C12	1.531 (9)
O2—Sn1^{ii}	2.482 (7)	C11—H11A	0.9700
S1—C6	1.577 (11)	C11—H11B	0.9700
S1—C3	1.630 (9)	C12—C13	1.497 (10)
C4′—C3	1.432 (9)	C12—H12A	0.9700
C4′—C6	1.432 (9)	C12—H12B	0.9700
C4′—H4′	0.9300	C13—C14	1.539 (10)
C1—C2	1.502 (14)	C13—H13A	0.9700
C2—C3	1.534 (8)	C13—H13B	0.9700
C2—H2A	0.9700	C14—H14A	0.9600
C2—H2B	0.9700	C14—H14B	0.9600
C3—C4	1.443 (9)	C14—H14C	0.9600
C3—S1′	1.601 (13)	C15—C16	1.519 (9)
C4—C5	1.418 (9)	C15—H15A	0.9700
C4—H4	0.9300	C15—H15B	0.9700
S1′—C5	1.585 (14)	C16—C17	1.541 (9)
C5—C6	1.400 (9)	C16—H16A	0.9700
C5—H5	0.9300	C16—H16B	0.9700
C6—H6	0.9300	C17—C18	1.527 (10)
C7—C8	1.526 (9)	C17—H17A	0.9700
C7—H7A	0.9700	C17—H17B	0.9700
C7—H7B	0.9700	C18—H18A	0.9600
C8—C9	1.502 (9)	C18—H18B	0.9600
C8—H8A	0.9700	C18—H18C	0.9600
C8—H8B	0.9700		
C7—Sn1—C11	119.7 (5)	H8A—C8—H8B	107.5
C7—Sn1—C15	116.4 (4)	C8—C9—C10	111.6 (11)
C11—Sn1—C15	122.5 (5)	C8—C9—H9A	109.3
C7—Sn1—O1	89.5 (4)	C10—C9—H9A	109.3
C11—Sn1—O1	97.2 (4)	C8—C9—H9B	109.3
C15—Sn1—O1	94.8 (3)	C10—C9—H9B	109.3
C7—Sn1—O2^{i}	81.9 (4)	H9A—C9—H9B	108.0
C11—Sn1—O2^{i}	85.5 (4)	C9—C10—H10A	109.5
C15—Sn1—O2^{i}	90.6 (3)	C9—C10—H10B	109.5
O1—Sn1—O2^{i}	171.3 (2)	H10A—C10—H10B	109.5
C1—O1—Sn1	124.2 (7)	C9—C10—H10C	109.5
C1—O2—Sn1^{ii}	144.0 (7)	H10A—C10—H10C	109.5
C6—S1—C3	93.6 (5)	H10B—C10—H10C	109.5
C3—C4′—C6	109.4 (8)	C12—C11—Sn1	111.1 (9)

C3—C4′—H4′	125.3	C12—C11—H11A	109.4
C6—C4′—H4′	125.3	Sn1—C11—H11A	109.4
O2—C1—O1	123.6 (10)	C12—C11—H11B	109.4
O2—C1—C2	122.9 (9)	Sn1—C11—H11B	109.4
O1—C1—C2	113.5 (10)	H11A—C11—H11B	108.0
C1—C2—C3	113.4 (9)	C13—C12—C11	114.4 (11)
C1—C2—H2A	108.9	C13—C12—H12A	108.6
C3—C2—H2A	108.9	C11—C12—H12A	108.6
C1—C2—H2B	108.9	C13—C12—H12B	108.6
C3—C2—H2B	108.9	C11—C12—H12B	108.6
H2A—C2—H2B	107.7	H12A—C12—H12B	107.6
C4′—C3—C4	104.3 (7)	C12—C13—C14	109.9 (12)
C4′—C3—C2	129.8 (9)	C12—C13—H13A	109.7
C4—C3—C2	125.8 (9)	C14—C13—H13A	109.7
C4′—C3—S1′	108.2 (13)	C12—C13—H13B	109.7
C4—C3—S1′	20.8 (11)	C14—C13—H13B	109.7
C2—C3—S1′	119.7 (8)	H13A—C13—H13B	108.2
C4′—C3—S1	18 (3)	C13—C14—H14A	109.5
C4—C3—S1	109.4 (7)	C13—C14—H14B	109.5
C2—C3—S1	121.0 (7)	H14A—C14—H14B	109.5
S1′—C3—S1	119.3 (7)	C13—C14—H14C	109.5
C5—C4—C3	108.8 (7)	H14A—C14—H14C	109.5
C5—C4—H4	125.6	H14B—C14—H14C	109.5
C3—C4—H4	125.6	C16—C15—Sn1	114.6 (7)
C5—S1′—C3	93.8 (8)	C16—C15—H15A	108.6
C6—C5—C4	107.6 (7)	Sn1—C15—H15A	108.6
C6—C5—S1′	115.0 (8)	C16—C15—H15B	108.6
C4—C5—S1′	21.0 (11)	Sn1—C15—H15B	108.6
C6—C5—H5	126.2	H15A—C15—H15B	107.6
C4—C5—H5	126.2	C15—C16—C17	111.5 (9)
S1′—C5—H5	115.6	C15—C16—H16A	109.3
C5—C6—C4′	105.8 (9)	C17—C16—H16A	109.3
C5—C6—S1	115.6 (7)	C15—C16—H16B	109.3
C4′—C6—S1	19 (3)	C17—C16—H16B	109.3
C5—C6—H6	122.2	H16A—C16—H16B	108.0
C4′—C6—H6	129.0	C18—C17—C16	110.7 (11)
S1—C6—H6	122.2	C18—C17—H17A	109.5
C8—C7—Sn1	109.3 (8)	C16—C17—H17A	109.5
C8—C7—H7A	109.8	C18—C17—H17B	109.5
Sn1—C7—H7A	109.8	C16—C17—H17B	109.5
C8—C7—H7B	109.8	H17A—C17—H17B	108.1
Sn1—C7—H7B	109.8	C17—C18—H18A	109.5
H7A—C7—H7B	108.3	C17—C18—H18B	109.5
C9—C8—C7	114.8 (10)	H18A—C18—H18B	109.5
C9—C8—H8A	108.6	C17—C18—H18C	109.5
C7—C8—H8A	108.6	H18A—C18—H18C	109.5

C9—C8—H8B	108.6	H18B—C18—H18C	109.5
C7—C8—H8B	108.6		

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