Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(4-Formyl-2-methoxyphenolato)tris-(2-methyl-2-phenylpropyl)tin(IV)

Yan Dong

Department of Chemistry, Dezhou University, Dezhou 253023, People's Republic of China
Correspondence e-mail: dongyanchem@163.com

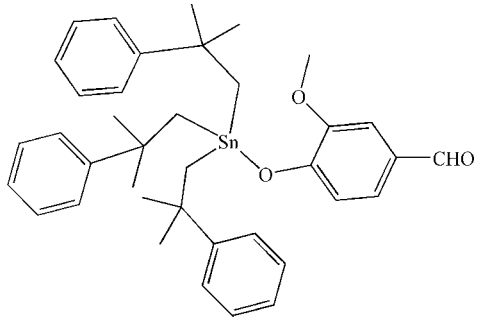
Received 2 October 2007; accepted 31 January 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.007 Å; R factor = 0.048; wR factor = 0.099; data-to-parameter ratio = 17.6.

The Sn atom of the title compound, $[Sn(C_{10}H_{13})_3(C_8H_7O_3)]$, is four-coordinate and possesses a distorted $SnOC_3$ tetrahedral geometry.

Related literature

For related literature, see: Domingos & Sheldrick (1974); Yang *et al.* (2006, 2007); Zhang *et al.* (2002).



Experimental

Crystal data

$[Sn(C_{10}H_{13})_3(C_8H_7O_3)]$
M_r = 669.44
Monoclinic, $P2_1/n$
a = 9.7900 (13) Å
b = 33.761 (4) Å
c = 10.3073 (13) Å
β = 92.873 (2)°
V = 3402.5 (7) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 295 (2) K
0.20 × 0.16 × 0.08 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.859, T_{max} = 0.942
26454 measured reflections
6675 independent reflections
5252 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.099
S = 1.06
6675 reflections
379 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.49 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.038 (3)	Sn1—C11	2.145 (4)
Sn1—C21	2.142 (4)	Sn1—C1	2.148 (4)
O1—Sn1—C21	106.72 (15)	O1—Sn1—C1	93.83 (14)
O1—Sn1—C11	101.37 (13)	C21—Sn1—C1	115.01 (16)
C21—Sn1—C11	118.18 (15)	C11—Sn1—C1	116.65 (16)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The author thanks the Science Foundation of Dezhou University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2240).

References

Bruker (2002). *SADABS*, *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Domingos, A. M. & Sheldrick, G. M. (1974). *Acta Cryst.* B**30**, 519–521.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Yang, G.-M., Tan, G.-X., Ding, Y.-J. & Wu, J. (2006). *Acta Cryst.* E**62**, m1195–m1196.
Yang, H.-J., Tian, L.-J., Mao, W.-T. & Zheng, X.-F. (2007). *Acta Cryst.* E**63**, m1271.
Zhang, Z.-G., Huang, Y.-Q., Zou, Y., Zhang, S.-K. & Xie, Q.-L. (2002). *Chem. J. Chin. Univ.* **23**, 399–402.

  doi:10.1107/S1600536808003437

supporting information

Acta Cryst. (2008). E**64**, m450 [doi:10.1107/S1600536808003437]

(4-Formyl-2-methoxyphenolato)tris(2-methyl-2-phenylpropyl)tin(IV)

Yan Dong

S1. Comment

Little attention has been paid to the condensing reaction of tris(2-methyl-2-phenylpropyl)tin oxide, $\{[C_6H_5C(CH_3)_2CH_2]_3Sn\}_2O$, with phenols in the literature. In reported three structures, tris(2-methyl-2-phenylpropyl)tin pentachlorophenoate, 4-nitrophenolate, and 4-acetylphenolate (Zhang *et al.*, 2002; Yang *et al.*, 2006; Yang *et al.*, 2007), the tin atom is four coordinated.

In the title compound, the Sn atom is also four-coordinate and possess a distorted $SnOC_3$ tetrahedral geometry (Fig. 1). This is different from Me_3SnOMe, in which almost planar trimethyltin groups are linked by two methoxy ligands forming infinite one-dimensional zigzag chains with nearly ideally trigonal-bipyramidal coordinated tin atom (Domingos & Sheldrick,1974), due to the crowding of the four bulky groups at the Sn atom in the title compound. The three Sn—C distances are almost equal [from 2.142 (4) to 2.148 (4) Å] and comparable with those [2.142 (2)–2.158 (2) and 2.144 (2)–2.157 (2) Å, respectively] in tris(2-methyl-2-phenylpropyl)tin 4-nitrophenolate and 4-acetylphenolate (Yang *et al.*, 2006; Yang *et al.*, 2007), but slightly longer than those [2.105 (4)–2.114 (4) Å] in tris(2-methyl-2-phenylpropyl)tin pentachlorophenoate (Zhang *et al.*, 2002). The Sn—O dimension of the title compound is almost same as that [2.045 (2) and 2.041 (2) Å, respectively] of tris(2-methyl-2-phenylpropyl)tin 4-nitrophenolate and 4-acetylphenolate and shorter than that [2.103 (3) Å] found in tris(2-methyl-2-phenylpropyl)tin pentachlorophenoate.

S2. Experimental

The title compound was synthesized by condensing bis[tri(2-phenyl-2-methylpropyl)tin] oxide (1.05 g, 1 mmol) with 4-hydroxy-2-methoxybenzaldehyde (0.30 g, 2 mmol) in toluene (50 ml). Water was removed with a Dean-Stark water separator. The resulting clear solution was evaporated using a rotary evaporator. The white solid obtained was recrystallized from ethanol and crystals of title compound were obtained from chloroform-hexane (V/V, 1:1) by slow evaporation at room temperature (yield 81%, m.p. 388–389 K). Analysis, found: C 68.02, H 6.79%; calculated for $C_{38}H_{46}O_3Sn$: C 68.17, H 6.93%.

S3. Refinement

H atoms were placed at calculated positions and were included in the refinement in the riding-model approximation, with C—H = 0.93 Å and U_{iso}(H) = 1.2Ueq(C) for aromatic and aldehydic H atoms, C—H = 0.96 Å and U_{iso}(H) = 1.5Ueq(C) for methyl H atoms, and C—H = 0.97 Å and U_{iso}(H) = 1.2Ueq(C) for methylene H atoms.

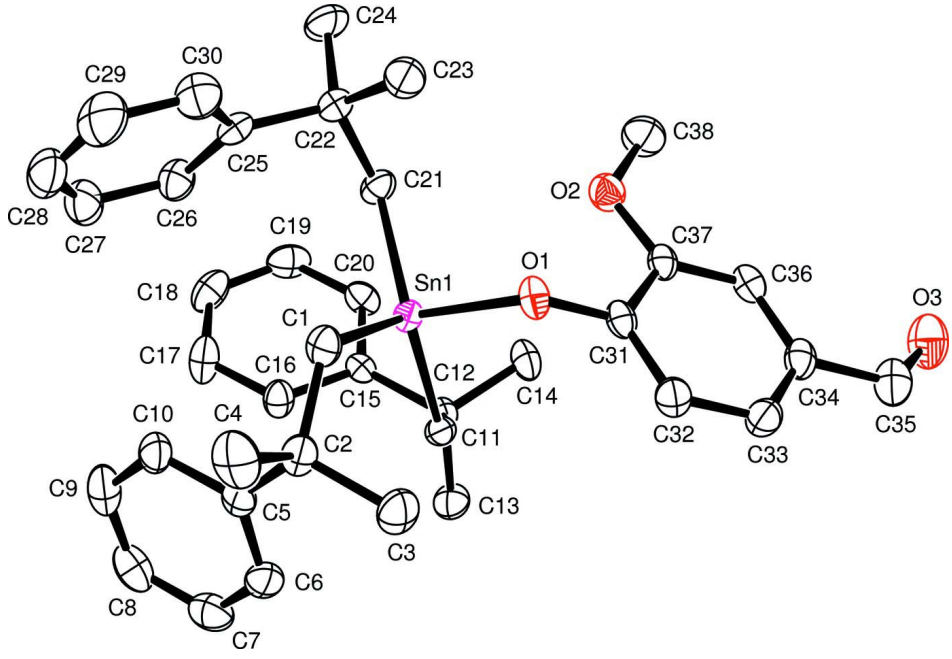


Figure 1

The structure of title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

(4-Formyl-2-methoxyphenolato)tris(2-methyl-2-phenylpropyl)tin(IV)

Crystal data

$[Sn(C_{10}H_{13})_3(C_8H_7O_3)]$
$M_r = 669.44$
Monoclinic, $P2_1/n$
Hall symbol: -p 2yn
$a = 9.7900\ (13)$ Å
$b = 33.761\ (4)$ Å
$c = 10.3073\ (13)$ Å
$\beta = 92.873\ (2)°$
$V = 3402.5\ (7)$ Å^3
$Z = 4$
$F(000) = 1392$
$D_x = 1.307$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4584 reflections
$\theta = 2.2–21.5°$
$\mu = 0.79$ mm^{-1}
$T = 295$ K
Prism, colorless
0.20 × 0.16 × 0.08 mm

Data collection

Bruker SMART APEX area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{min} = 0.859$, $T_{max} = 0.942$
26454 measured reflections
6675 independent reflections
5252 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.2°$
$h = -12\rightarrow12$
$k = -41\rightarrow41$
$l = -12\rightarrow12$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.099$
$S = 1.06$
6675 reflections
379 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.023P)^2 + 3.2918P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.63396 (3)	0.884454 (7)	0.76497 (2)	0.04078 (10)
O1	0.4361 (3)	0.89038 (8)	0.6964 (3)	0.0552 (7)
O2	0.3783 (3)	0.81358 (9)	0.7079 (3)	0.0634 (8)
O3	0.1355 (4)	0.78647 (13)	0.2522 (4)	0.0956 (12)
C1	0.6474 (5)	0.94423 (12)	0.8359 (4)	0.0560 (11)
H1A	0.5552	0.9532	0.8496	0.067*
H1B	0.6958	0.9435	0.9203	0.067*
C2	0.7167 (5)	0.97585 (12)	0.7536 (4)	0.0573 (11)
C3	0.6356 (5)	0.97925 (14)	0.6225 (5)	0.0789 (15)
H3A	0.5417	0.9852	0.6372	0.118*
H3B	0.6406	0.9546	0.5765	0.118*
H3C	0.6737	1.0000	0.5720	0.118*
C4	0.7058 (6)	1.01584 (14)	0.8247 (6)	0.0923 (18)
H4A	0.6112	1.0221	0.8344	0.138*
H4B	0.7473	1.0362	0.7750	0.138*
H4C	0.7521	1.0141	0.9088	0.138*
C5	0.8666 (5)	0.96629 (11)	0.7398 (5)	0.0565 (11)
C6	0.9267 (6)	0.96385 (13)	0.6211 (5)	0.0679 (13)
H6	0.8735	0.9685	0.5454	0.081*
C7	1.0630 (6)	0.95477 (15)	0.6121 (6)	0.0812 (16)
H7	1.0998	0.9530	0.5309	0.097*
C8	1.1438 (6)	0.94842 (16)	0.7202 (7)	0.0866 (17)
H8	1.2359	0.9424	0.7137	0.104*
C9	1.0890 (6)	0.95095 (16)	0.8388 (6)	0.0844 (17)
H9	1.1444	0.9468	0.9135	0.101*

C10	0.9512 (5)	0.95968 (13)	0.8497 (5)	0.0663 (13)
H10	0.9154	0.9611	0.9315	0.080*
C11	0.7350 (4)	0.87195 (11)	0.5896 (4)	0.0445 (9)
H11A	0.6692	0.8760	0.5173	0.053*
H11B	0.8067	0.8915	0.5816	0.053*
C12	0.7994 (4)	0.83075 (11)	0.5732 (4)	0.0436 (9)
C13	0.8845 (5)	0.83177 (14)	0.4515 (4)	0.0664 (13)
H13A	0.8260	0.8381	0.3767	0.100*
H13B	0.9259	0.8063	0.4395	0.100*
H13C	0.9546	0.8516	0.4623	0.100*
C14	0.6860 (5)	0.80029 (14)	0.5503 (5)	0.0675 (13)
H14A	0.6293	0.8078	0.4756	0.101*
H14B	0.6315	0.7991	0.6251	0.101*
H14C	0.7256	0.7748	0.5358	0.101*
C15	0.8936 (4)	0.82085 (11)	0.6905 (4)	0.0396 (9)
C16	0.9885 (4)	0.84824 (13)	0.7388 (4)	0.0575 (11)
H16	0.9940	0.8728	0.6984	0.069*
C17	1.0749 (5)	0.84018 (16)	0.8449 (5)	0.0782 (15)
H17	1.1370	0.8593	0.8753	0.094*
C18	1.0701 (6)	0.80462 (18)	0.9054 (5)	0.0783 (16)
H18	1.1284	0.7993	0.9773	0.094*
C19	0.9787 (5)	0.77666 (16)	0.8598 (5)	0.0741 (15)
H19	0.9750	0.7522	0.9009	0.089*
C20	0.8922 (4)	0.78446 (13)	0.7534 (4)	0.0579 (12)
H20	0.8316	0.7650	0.7230	0.069*
C21	0.6354 (5)	0.83972 (12)	0.9124 (4)	0.0547 (11)
H21A	0.5780	0.8181	0.8803	0.066*
H21B	0.7279	0.8296	0.9235	0.066*
C22	0.5881 (5)	0.85141 (13)	1.0473 (4)	0.0567 (11)
C23	0.4406 (5)	0.8664 (2)	1.0298 (5)	0.0923 (18)
H23A	0.3847	0.8463	0.9879	0.138*
H23B	0.4384	0.8898	0.9772	0.138*
H23C	0.4063	0.8723	1.1132	0.138*
C24	0.5910 (7)	0.81390 (17)	1.1334 (5)	0.102 (2)
H24A	0.5317	0.7942	1.0941	0.153*
H24B	0.5604	0.8205	1.2178	0.153*
H24C	0.6826	0.8038	1.1418	0.153*
C25	0.6838 (4)	0.88179 (13)	1.1135 (4)	0.0511 (10)
C26	0.8219 (5)	0.87993 (15)	1.1027 (5)	0.0671 (13)
H26	0.8587	0.8596	1.0544	0.081*
C27	0.9098 (6)	0.90794 (19)	1.1631 (6)	0.0865 (17)
H27	1.0037	0.9062	1.1545	0.104*
C28	0.8578 (9)	0.93748 (19)	1.2336 (6)	0.098 (2)
H28	0.9155	0.9564	1.2726	0.117*
C29	0.7232 (9)	0.93948 (19)	1.2471 (6)	0.108 (2)
H29	0.6876	0.9597	1.2965	0.130*
C30	0.6361 (6)	0.91187 (16)	1.1888 (5)	0.0819 (16)
H30	0.5427	0.9137	1.2007	0.098*

C31	0.3764 (4)	0.87261 (12)	0.5919 (4)	0.0480 (10)
C32	0.3435 (5)	0.89388 (13)	0.4813 (4)	0.0598 (12)
H32	0.3668	0.9206	0.4781	0.072*
C33	0.2766 (5)	0.87657 (15)	0.3742 (4)	0.0643 (13)
H33	0.2561	0.8914	0.2998	0.077*
C34	0.2407 (4)	0.83744 (15)	0.3786 (4)	0.0579 (12)
C35	0.1688 (5)	0.82004 (18)	0.2631 (5)	0.0753 (15)
H35	0.1480	0.8368	0.1932	0.090*
C36	0.2732 (4)	0.81543 (13)	0.4886 (4)	0.0545 (11)
H36	0.2502	0.7887	0.4904	0.065*
C37	0.3390 (4)	0.83231 (12)	0.5952 (4)	0.0476 (10)
C38	0.3435 (6)	0.77269 (15)	0.7182 (5)	0.0832 (16)
H38A	0.3760	0.7628	0.8015	0.125*
H38B	0.3851	0.7580	0.6509	0.125*
H38C	0.2460	0.7697	0.7093	0.125*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.04377 (16)	0.03930 (15)	0.03881 (15)	0.00142 (13)	−0.00246 (10)	−0.00157 (13)
O1	0.0413 (15)	0.0565 (18)	0.0669 (19)	0.0020 (13)	−0.0061 (14)	−0.0146 (15)
O2	0.062 (2)	0.0576 (19)	0.070 (2)	−0.0053 (15)	−0.0016 (16)	0.0036 (16)
O3	0.092 (3)	0.092 (3)	0.102 (3)	0.005 (2)	−0.014 (2)	−0.037 (2)
C1	0.065 (3)	0.046 (2)	0.057 (3)	0.002 (2)	−0.003 (2)	−0.012 (2)
C2	0.072 (3)	0.037 (2)	0.062 (3)	0.004 (2)	−0.013 (2)	0.002 (2)
C3	0.092 (4)	0.063 (3)	0.078 (4)	0.001 (3)	−0.021 (3)	0.017 (3)
C4	0.103 (4)	0.045 (3)	0.127 (5)	0.003 (3)	−0.010 (4)	−0.013 (3)
C5	0.072 (3)	0.033 (2)	0.063 (3)	−0.011 (2)	−0.009 (2)	0.003 (2)
C6	0.090 (4)	0.051 (3)	0.062 (3)	−0.011 (3)	−0.005 (3)	0.011 (2)
C7	0.092 (4)	0.062 (3)	0.091 (4)	−0.014 (3)	0.017 (4)	0.006 (3)
C8	0.073 (4)	0.063 (3)	0.123 (5)	−0.015 (3)	0.003 (4)	−0.015 (4)
C9	0.076 (4)	0.072 (4)	0.102 (5)	−0.008 (3)	−0.030 (3)	−0.010 (3)
C10	0.075 (3)	0.061 (3)	0.061 (3)	−0.014 (3)	−0.013 (3)	−0.004 (2)
C11	0.041 (2)	0.053 (2)	0.040 (2)	0.0021 (18)	0.0029 (17)	0.0052 (18)
C12	0.038 (2)	0.047 (2)	0.046 (2)	−0.0058 (17)	0.0017 (17)	−0.0083 (18)
C13	0.064 (3)	0.083 (3)	0.053 (3)	0.003 (3)	0.012 (2)	−0.010 (2)
C14	0.055 (3)	0.068 (3)	0.079 (3)	−0.014 (2)	−0.005 (2)	−0.018 (3)
C15	0.034 (2)	0.036 (2)	0.050 (2)	0.0048 (16)	0.0102 (17)	−0.0060 (17)
C16	0.057 (3)	0.049 (3)	0.065 (3)	0.004 (2)	−0.013 (2)	−0.001 (2)
C17	0.075 (3)	0.072 (4)	0.084 (4)	0.008 (3)	−0.031 (3)	−0.018 (3)
C18	0.084 (4)	0.091 (4)	0.058 (3)	0.031 (3)	−0.012 (3)	−0.001 (3)
C19	0.076 (4)	0.069 (3)	0.079 (4)	0.024 (3)	0.013 (3)	0.028 (3)
C20	0.050 (3)	0.045 (2)	0.078 (3)	0.002 (2)	0.006 (2)	0.007 (2)
C21	0.075 (3)	0.045 (2)	0.044 (2)	0.000 (2)	−0.004 (2)	0.0038 (19)
C22	0.062 (3)	0.064 (3)	0.044 (2)	−0.003 (2)	0.000 (2)	0.007 (2)
C23	0.055 (3)	0.155 (6)	0.068 (4)	−0.007 (3)	0.012 (3)	−0.005 (4)
C24	0.149 (6)	0.099 (4)	0.056 (3)	−0.046 (4)	−0.007 (3)	0.029 (3)
C25	0.061 (3)	0.057 (3)	0.035 (2)	0.007 (2)	0.0008 (18)	0.006 (2)

C26	0.063 (3)	0.075 (3)	0.063 (3)	0.007 (3)	−0.005 (2)	−0.004 (3)
C27	0.074 (4)	0.094 (4)	0.089 (4)	−0.011 (3)	−0.020 (3)	0.015 (4)
C28	0.135 (6)	0.080 (4)	0.076 (4)	−0.028 (4)	−0.023 (4)	−0.003 (3)
C29	0.149 (7)	0.088 (5)	0.087 (5)	−0.005 (5)	0.010 (5)	−0.035 (4)
C30	0.084 (4)	0.084 (4)	0.079 (4)	0.010 (3)	0.016 (3)	−0.018 (3)
C31	0.031 (2)	0.052 (2)	0.061 (3)	0.0034 (17)	0.0009 (18)	−0.009 (2)
C32	0.058 (3)	0.056 (3)	0.065 (3)	−0.001 (2)	−0.004 (2)	0.000 (2)
C33	0.060 (3)	0.078 (4)	0.054 (3)	0.004 (2)	−0.002 (2)	0.005 (2)
C34	0.040 (2)	0.076 (3)	0.057 (3)	0.008 (2)	−0.001 (2)	−0.014 (2)
C35	0.062 (3)	0.092 (4)	0.072 (4)	0.012 (3)	0.002 (3)	−0.028 (3)
C36	0.042 (2)	0.052 (3)	0.069 (3)	−0.0024 (19)	0.004 (2)	−0.009 (2)
C37	0.032 (2)	0.055 (3)	0.055 (3)	0.0045 (18)	−0.0007 (18)	−0.004 (2)
C38	0.096 (4)	0.064 (3)	0.090 (4)	−0.008 (3)	0.005 (3)	0.009 (3)

Geometric parameters (Å, º)

Sn1—O1	2.038 (3)	C16—H16	0.9300
Sn1—C21	2.142 (4)	C17—C18	1.355 (7)
Sn1—C11	2.145 (4)	C17—H17	0.9300
Sn1—C1	2.148 (4)	C18—C19	1.368 (7)
O1—C31	1.341 (5)	C18—H18	0.9300
O2—C37	1.361 (5)	C19—C20	1.377 (6)
O2—C38	1.427 (5)	C19—H19	0.9300
O3—C35	1.183 (6)	C20—H20	0.9300
C1—C2	1.541 (6)	C21—C22	1.539 (6)
C1—H1A	0.9700	C21—H21A	0.9700
C1—H1B	0.9700	C21—H21B	0.9700
C2—C5	1.517 (6)	C22—C25	1.527 (6)
C2—C3	1.537 (6)	C22—C23	1.532 (6)
C2—C4	1.542 (6)	C22—C24	1.546 (6)
C3—H3A	0.9600	C23—H23A	0.9600
C3—H3B	0.9600	C23—H23B	0.9600
C3—H3C	0.9600	C23—H23C	0.9600
C4—H4A	0.9600	C24—H24A	0.9600
C4—H4B	0.9600	C24—H24B	0.9600
C4—H4C	0.9600	C24—H24C	0.9600
C5—C6	1.386 (6)	C25—C26	1.364 (6)
C5—C10	1.388 (6)	C25—C30	1.374 (6)
C6—C7	1.377 (7)	C26—C27	1.403 (7)
C6—H6	0.9300	C26—H26	0.9300
C7—C8	1.350 (7)	C27—C28	1.349 (8)
C7—H7	0.9300	C27—H27	0.9300
C8—C9	1.362 (8)	C28—C29	1.334 (8)
C8—H8	0.9300	C28—H28	0.9300
C9—C10	1.390 (7)	C29—C30	1.381 (8)
C9—H9	0.9300	C29—H29	0.9300
C10—H10	0.9300	C30—H30	0.9300
C11—C12	1.540 (5)	C31—C32	1.373 (6)

C11—H11A	0.9700	C31—C37	1.410 (5)
C11—H11B	0.9700	C32—C33	1.384 (6)
C12—C15	1.520 (5)	C32—H32	0.9300
C12—C14	1.523 (5)	C33—C34	1.368 (6)
C12—C13	1.541 (5)	C33—H33	0.9300
C13—H13A	0.9600	C34—C36	1.380 (6)
C13—H13B	0.9600	C34—C35	1.474 (6)
C13—H13C	0.9600	C35—H35	0.9300
C14—H14A	0.9600	C36—C37	1.369 (5)
C14—H14B	0.9600	C36—H36	0.9300
C14—H14C	0.9600	C38—H38A	0.9600
C15—C16	1.386 (5)	C38—H38B	0.9600
C15—C20	1.390 (5)	C38—H38C	0.9600
C16—C17	1.376 (6)		

O1—Sn1—C21	106.72 (15)	C18—C17—H17	119.8
O1—Sn1—C11	101.37 (13)	C16—C17—H17	119.8
C21—Sn1—C11	118.18 (15)	C17—C18—C19	119.3 (5)
O1—Sn1—C1	93.83 (14)	C17—C18—H18	120.3
C21—Sn1—C1	115.01 (16)	C19—C18—H18	120.3
C11—Sn1—C1	116.65 (16)	C18—C19—C20	120.5 (5)
C31—O1—Sn1	127.1 (2)	C18—C19—H19	119.7
C37—O2—C38	117.1 (4)	C20—C19—H19	119.7
C2—C1—Sn1	119.0 (3)	C19—C20—C15	121.4 (4)
C2—C1—H1A	107.6	C19—C20—H20	119.3
Sn1—C1—H1A	107.6	C15—C20—H20	119.3
C2—C1—H1B	107.6	C22—C21—Sn1	118.0 (3)
Sn1—C1—H1B	107.6	C22—C21—H21A	107.8
H1A—C1—H1B	107.0	Sn1—C21—H21A	107.8
C5—C2—C3	113.1 (4)	C22—C21—H21B	107.8
C5—C2—C1	111.0 (3)	Sn1—C21—H21B	107.8
C3—C2—C1	108.2 (4)	H21A—C21—H21B	107.2
C5—C2—C4	108.8 (4)	C25—C22—C23	112.7 (4)
C3—C2—C4	107.9 (4)	C25—C22—C21	111.7 (4)
C1—C2—C4	107.6 (4)	C23—C22—C21	107.6 (4)
C2—C3—H3A	109.5	C25—C22—C24	107.5 (4)
C2—C3—H3B	109.5	C23—C22—C24	109.1 (4)
H3A—C3—H3B	109.5	C21—C22—C24	108.1 (4)
C2—C3—H3C	109.5	C22—C23—H23A	109.5
H3A—C3—H3C	109.5	C22—C23—H23B	109.5
H3B—C3—H3C	109.5	H23A—C23—H23B	109.5
C2—C4—H4A	109.5	C22—C23—H23C	109.5
C2—C4—H4B	109.5	H23A—C23—H23C	109.5
H4A—C4—H4B	109.5	H23B—C23—H23C	109.5
C2—C4—H4C	109.5	C22—C24—H24A	109.5
H4A—C4—H4C	109.5	C22—C24—H24B	109.5
H4B—C4—H4C	109.5	H24A—C24—H24B	109.5
C6—C5—C10	116.7 (5)	C22—C24—H24C	109.5

C6—C5—C2	123.5 (4)	H24A—C24—H24C	109.5
C10—C5—C2	119.9 (4)	H24B—C24—H24C	109.5
C7—C6—C5	121.9 (5)	C26—C25—C30	116.5 (5)
C7—C6—H6	119.1	C26—C25—C22	121.4 (4)
C5—C6—H6	119.1	C30—C25—C22	122.0 (4)
C8—C7—C6	120.6 (6)	C25—C26—C27	121.4 (5)
C8—C7—H7	119.7	C25—C26—H26	119.3
C6—C7—H7	119.7	C27—C26—H26	119.3
C7—C8—C9	119.3 (6)	C28—C27—C26	119.9 (6)
C7—C8—H8	120.3	C28—C27—H27	120.1
C9—C8—H8	120.3	C26—C27—H27	120.1
C8—C9—C10	120.9 (5)	C29—C28—C27	119.7 (6)
C8—C9—H9	119.6	C29—C28—H28	120.2
C10—C9—H9	119.6	C27—C28—H28	120.2
C5—C10—C9	120.6 (5)	C28—C29—C30	120.8 (6)
C5—C10—H10	119.7	C28—C29—H29	119.6
C9—C10—H10	119.7	C30—C29—H29	119.6
C12—C11—Sn1	118.6 (3)	C25—C30—C29	121.6 (6)
C12—C11—H11A	107.7	C25—C30—H30	119.2
Sn1—C11—H11A	107.7	C29—C30—H30	119.2
C12—C11—H11B	107.7	O1—C31—C32	120.5 (4)
Sn1—C11—H11B	107.7	O1—C31—C37	121.1 (4)
H11A—C11—H11B	107.1	C32—C31—C37	118.3 (4)
C15—C12—C14	112.5 (3)	C31—C32—C33	121.6 (4)
C15—C12—C11	110.3 (3)	C31—C32—H32	119.2
C14—C12—C11	109.1 (3)	C33—C32—H32	119.2
C15—C12—C13	108.7 (3)	C34—C33—C32	119.6 (4)
C14—C12—C13	108.0 (3)	C34—C33—H33	120.2
C11—C12—C13	108.1 (3)	C32—C33—H33	120.2
C12—C13—H13A	109.5	C33—C34—C36	119.8 (4)
C12—C13—H13B	109.5	C33—C34—C35	118.1 (5)
H13A—C13—H13B	109.5	C36—C34—C35	122.0 (5)
C12—C13—H13C	109.5	O3—C35—C34	125.2 (6)
H13A—C13—H13C	109.5	O3—C35—H35	117.4
H13B—C13—H13C	109.5	C34—C35—H35	117.4
C12—C14—H14A	109.5	C37—C36—C34	121.0 (4)
C12—C14—H14B	109.5	C37—C36—H36	119.5
H14A—C14—H14B	109.5	C34—C36—H36	119.5
C12—C14—H14C	109.5	O2—C37—C36	126.4 (4)
H14A—C14—H14C	109.5	O2—C37—C31	114.0 (4)
H14B—C14—H14C	109.5	C36—C37—C31	119.7 (4)
C16—C15—C20	116.4 (4)	O2—C38—H38A	109.5
C16—C15—C12	120.5 (3)	O2—C38—H38B	109.5
C20—C15—C12	123.1 (4)	H38A—C38—H38B	109.5
C17—C16—C15	121.9 (4)	O2—C38—H38C	109.5
C17—C16—H16	119.1	H38A—C38—H38C	109.5
C15—C16—H16	119.1	H38B—C38—H38C	109.5
C18—C17—C16	120.5 (5)		

C21—Sn1—O1—C31	−95.1 (3)	C16—C15—C20—C19	1.4 (6)
C11—Sn1—O1—C31	29.2 (4)	C12—C15—C20—C19	−179.7 (4)
C1—Sn1—O1—C31	147.4 (3)	O1—Sn1—C21—C22	−78.4 (3)
O1—Sn1—C1—C2	−99.6 (3)	C11—Sn1—C21—C22	168.4 (3)
C21—Sn1—C1—C2	149.9 (3)	C1—Sn1—C21—C22	24.2 (4)
C11—Sn1—C1—C2	5.2 (4)	Sn1—C21—C22—C25	−64.9 (4)
Sn1—C1—C2—C5	−63.6 (4)	Sn1—C21—C22—C23	59.2 (5)
Sn1—C1—C2—C3	61.1 (4)	Sn1—C21—C22—C24	177.0 (3)
Sn1—C1—C2—C4	177.5 (3)	C23—C22—C25—C26	−159.5 (4)
C3—C2—C5—C6	4.7 (6)	C21—C22—C25—C26	−38.2 (5)
C1—C2—C5—C6	126.6 (4)	C24—C22—C25—C26	80.2 (5)
C4—C2—C5—C6	−115.2 (5)	C23—C22—C25—C30	21.8 (6)
C3—C2—C5—C10	−175.7 (4)	C21—C22—C25—C30	143.1 (4)
C1—C2—C5—C10	−53.8 (5)	C24—C22—C25—C30	−98.5 (5)
C4—C2—C5—C10	64.4 (5)	C30—C25—C26—C27	−1.5 (7)
C10—C5—C6—C7	0.9 (6)	C22—C25—C26—C27	179.7 (4)
C2—C5—C6—C7	−179.5 (4)	C25—C26—C27—C28	0.1 (8)
C5—C6—C7—C8	−0.9 (8)	C26—C27—C28—C29	1.0 (9)
C6—C7—C8—C9	0.2 (8)	C27—C28—C29—C30	−0.6 (10)
C7—C8—C9—C10	0.4 (8)	C26—C25—C30—C29	1.9 (8)
C6—C5—C10—C9	−0.2 (6)	C22—C25—C30—C29	−179.3 (5)
C2—C5—C10—C9	−179.9 (4)	C28—C29—C30—C25	−0.9 (10)
C8—C9—C10—C5	−0.4 (8)	Sn1—O1—C31—C32	−108.0 (4)
O1—Sn1—C11—C12	−113.5 (3)	Sn1—O1—C31—C37	75.5 (4)
C21—Sn1—C11—C12	2.6 (4)	O1—C31—C32—C33	−177.2 (4)
C1—Sn1—C11—C12	146.3 (3)	C37—C31—C32—C33	−0.6 (6)
Sn1—C11—C12—C15	−52.1 (4)	C31—C32—C33—C34	0.7 (7)
Sn1—C11—C12—C14	72.0 (4)	C32—C33—C34—C36	−1.0 (7)
Sn1—C11—C12—C13	−170.8 (3)	C32—C33—C34—C35	179.7 (4)
C14—C12—C15—C16	−169.4 (4)	C33—C34—C35—O3	177.7 (5)
C11—C12—C15—C16	−47.3 (5)	C36—C34—C35—O3	−1.7 (8)
C13—C12—C15—C16	71.0 (5)	C33—C34—C36—C37	1.2 (6)
C14—C12—C15—C20	11.7 (5)	C35—C34—C36—C37	−179.4 (4)
C11—C12—C15—C20	133.8 (4)	C38—O2—C37—C36	−2.4 (6)
C13—C12—C15—C20	−107.8 (4)	C38—O2—C37—C31	179.8 (4)
C20—C15—C16—C17	−1.2 (6)	C34—C36—C37—O2	−178.8 (4)
C12—C15—C16—C17	179.8 (4)	C34—C36—C37—C31	−1.2 (6)
C15—C16—C17—C18	0.5 (8)	O1—C31—C37—O2	−4.7 (5)
C16—C17—C18—C19	0.2 (8)	C32—C31—C37—O2	178.8 (4)
C17—C18—C19—C20	0.0 (8)	O1—C31—C37—C36	177.4 (4)
C18—C19—C20—C15	−0.9 (7)	C32—C31—C37—C36	0.9 (6)