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(4-Acetylphenolato)tris(2-methyl-2-phenylpropyl)tin(IV)

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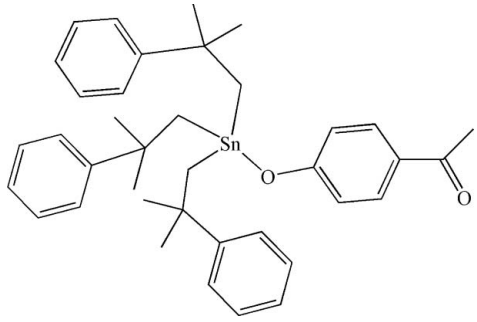
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.004 Å; R factor = 0.026; wR factor = 0.067; data-to-parameter ratio = 17.6.

The Sn^{IV} atom of the title compound, $[Sn(C_{10}H_{13})_3(C_8H_7O_2)]$, displays a distorted $SnOC_3$ tetrahedral geometry, with Sn—C = 2.144 (2)–2.157 (2)Å and Sn—O = 2.041 (2) Å.

Related literature

For related complexes containing the tris(2-methyl-2-phenylpropyl)tin fragment and a distorted tetrahedral $SnOC_3$ grouping, see Domingos & Sheldrick (1974), Zhang *et al.* (2002) and Yang *et al.* (2006).



Experimental

Crystal data

$[Sn(C_{10}H_{13})_3(C_8H_7O_2)]$
M_r = 653.44
Triclinic, $P\overline{1}$
a = 9.5062 (7) Å
b = 9.7309 (7) Å
c = 19.0769 (15) Å
α = 78.704 (2)°
β = 87.906 (1)°
γ = 76.874 (1)°
V = 1685.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.79 mm^{-1}
T = 295 (2) K
0.41 × 0.30 × 0.22 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
T_{min} = 0.738, T_{max} = 0.846
13220 measured reflections
6532 independent reflections
6022 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.067
S = 1.02
6532 reflections
371 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.041 (2)	Sn1—C21	2.154 (2)
Sn1—C11	2.144 (2)	Sn1—C1	2.157 (2)
O1—Sn1—C11	93.55 (7)	O1—Sn1—C1	109.00 (7)
O1—Sn1—C21	99.90 (7)	C11—Sn1—C1	115.07 (8)
C11—Sn1—C21	119.21 (8)	C21—Sn1—C1	115.49 (8)

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2357).

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supplementary materials

Acta Cryst. (2007). E**63**, m1271 [**doi:10.1107/S1600536807015449**]

(4-Acetylphenolato)tris(2-methyl-2-phenylpropyl)tin(IV)

H.-J. Yang, L.-J. Tian, W.-T. Mao and X.-F. Zheng

Comment

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

In the title compound, (I), the Sn atom is also four-coordinate and possess a distorted $SnOC_3$ tetrahedral geometry (Fig. 1 & Table 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 (I). The Sn—C distances lie in the narrow range of 2.144 (2)–2.157 (2) Å, in agreement with those [2.142 (2)–2.158 (2) Å] in tris(2-methyl-2-phenylpropyl)tin 4-nitrophenolate (Yang *et al.*, 2006), 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 separation in (I) of 2.045 (2) Å is almost same as that of tris(2-methyl-2-phenylpropyl)tin 4-nitrophenolate and shorter than that [2.103 (3) Å] found in tris(2-methyl-2-phenylpropyl)tin pentachlorophenoate.

Experimental

Bis[tris(2-phenyl-2-methylpropyl)tin] oxide (1.05 g, 1 mmol) was condensed with 4-hydroxyphenylethanone (0.27 g, 2 mmol) in toluene (50 ml). Water was removed with a Dean–Stark water separator. The resulting clear solution was evaporated to dryness using a rotary evaporator. The white solid obtained was recrystallized from ethanol and crystals of (I) were obtained from cyclohexane by slow evaporation at 298 K (yield 78%; m.p. 358–359 K).

Refinement

The H atoms were placed at calculated positions (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

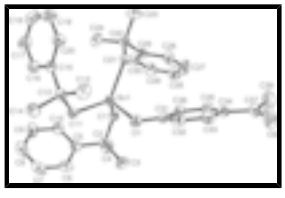


Fig. 1. The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level. H atoms have been omitted for clarity.

(4-Acetylphenolato)tris(2-methyl-2-phenylpropyl)tin(IV)

Crystal data

$[Sn(C_{10}H_{13})_3(C_8H_7O_2)]$	$Z = 2$
$M_r = 653.44$	$F_{000} = 680$
Triclinic, $P\overline{1}$	$D_x = 1.288$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.5062$ (7) Å	Cell parameters from 7970 reflections
$b = 9.7309$ (7) Å	$\theta = 2.2$–26.4º
$c = 19.0769$ (15) Å	$\mu = 0.79$ mm^{-1}
$\alpha = 78.704$ (2)º	$T = 295$ (2) K
$\beta = 87.906$ (1)º	Block, colorless
$\gamma = 76.874$ (1)º	0.41 × 0.30 × 0.22 mm
$V = 1685.2$ (2) Å^3	

Data collection

Bruker SMART APEX CCD diffractometer	6532 independent reflections
Radiation source: fine-focus sealed tube	6022 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 295$(2) K	$\theta_{max} = 26.0$º
ω scans	$\theta_{min} = 2.2$º
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$h = -11 \rightarrow 11$
$T_{min} = 0.738$, $T_{max} = 0.846$	$k = -11 \rightarrow 11$
13220 measured reflections	$l = -23 \rightarrow 23$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.0822P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.026$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.067$	$\Delta\rho_{max} = 0.43$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.29$ e Å^{-3}
6532 reflections	Extinction correction: none
371 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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.

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 $F^2 > 2\text{sigma}(F^2)$ 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.317898 (13)	0.629091 (14)	0.227412 (7)	0.03998 (6)
O1	0.52017 (16)	0.51431 (17)	0.21076 (8)	0.0568 (4)
O2	0.9387 (3)	−0.0669 (3)	0.35029 (17)	0.1349 (11)
C1	0.3299 (2)	0.7556 (2)	0.30715 (11)	0.0472 (5)
H1A	0.2319	0.7952	0.3205	0.057*
H1B	0.3767	0.6905	0.3492	0.057*
C2	0.4082 (2)	0.8807 (2)	0.28908 (12)	0.0507 (5)
C3	0.5696 (3)	0.8193 (3)	0.28176 (17)	0.0736 (7)
H3A	0.6058	0.7540	0.3251	0.110*
H3B	0.6196	0.8962	0.2729	0.110*
H3C	0.5850	0.7689	0.2426	0.110*
C4	0.3876 (3)	0.9623 (3)	0.35178 (15)	0.0777 (8)
H4A	0.2866	1.0026	0.3570	0.117*
H4B	0.4391	1.0381	0.3422	0.117*
H4C	0.4241	0.8970	0.3951	0.117*
C5	0.3417 (2)	0.9854 (2)	0.22192 (12)	0.0498 (5)
C6	0.4219 (3)	1.0272 (3)	0.16242 (16)	0.0725 (7)
H6	0.5218	0.9949	0.1637	0.087*
C7	0.3552 (4)	1.1164 (3)	0.10115 (17)	0.0879 (9)
H7	0.4113	1.1424	0.0620	0.106*
C8	0.2095 (4)	1.1667 (3)	0.09735 (16)	0.0827 (9)
H8	0.1654	1.2243	0.0557	0.099*
C9	0.1297 (3)	1.1309 (3)	0.15570 (15)	0.0738 (7)
H9	0.0304	1.1674	0.1545	0.089*
C10	0.1941 (3)	1.0405 (3)	0.21730 (13)	0.0596 (6)
H10	0.1367	1.0165	0.2563	0.072*
C11	0.2938 (2)	0.7468 (2)	0.11949 (11)	0.0474 (5)
H11A	0.2351	0.8420	0.1204	0.057*
H11B	0.3886	0.7587	0.1027	0.057*
C12	0.2271 (2)	0.6850 (2)	0.06371 (10)	0.0482 (5)
C13	0.3191 (3)	0.5349 (3)	0.06031 (14)	0.0693 (7)
H13A	0.4170	0.5412	0.0493	0.104*
H13B	0.2813	0.4976	0.0238	0.104*

H13C	0.3164	0.4720	0.1056	0.104*
C14	0.2323 (3)	0.7832 (3)	−0.00954 (12)	0.0731 (8)
H14A	0.3309	0.7852	−0.0215	0.110*
H14B	0.1788	0.8788	−0.0077	0.110*
H14C	0.1905	0.7470	−0.0452	0.110*
C15	0.0697 (2)	0.6840 (2)	0.08094 (10)	0.0464 (5)
C16	−0.0250 (3)	0.8086 (3)	0.09183 (13)	0.0612 (6)
H16	0.0094	0.8916	0.0894	0.073*
C17	−0.1686 (3)	0.8130 (4)	0.10622 (16)	0.0825 (9)
H17	−0.2296	0.8982	0.1136	0.099*
C18	−0.2220 (3)	0.6928 (5)	0.10974 (15)	0.0886 (10)
H18	−0.3192	0.6957	0.1193	0.106*
C19	−0.1318 (4)	0.5696 (4)	0.09911 (14)	0.0828 (9)
H19	−0.1676	0.4874	0.1019	0.099*
C20	0.0132 (3)	0.5637 (3)	0.08411 (12)	0.0622 (6)
H20	0.0729	0.4783	0.0761	0.075*
C21	0.2088 (2)	0.4559 (2)	0.25972 (10)	0.0442 (5)
H21A	0.1647	0.4415	0.2175	0.053*
H21B	0.2814	0.3690	0.2769	0.053*
C22	0.0910 (2)	0.4712 (2)	0.31761 (11)	0.0438 (4)
C23	0.0239 (3)	0.3390 (3)	0.32729 (14)	0.0693 (7)
H23A	−0.0185	0.3358	0.2829	0.104*
H23B	−0.0492	0.3454	0.3633	0.104*
H23C	0.0977	0.2533	0.3417	0.104*
C24	−0.0271 (3)	0.6045 (3)	0.29186 (13)	0.0670 (7)
H24A	−0.0663	0.5975	0.2474	0.100*
H24B	0.0129	0.6883	0.2851	0.100*
H24C	−0.1022	0.6119	0.3268	0.100*
C25	0.1581 (2)	0.4748 (2)	0.38874 (10)	0.0426 (4)
C26	0.2682 (3)	0.3640 (3)	0.41985 (13)	0.0645 (6)
H26	0.3015	0.2863	0.3973	0.077*
C27	0.3310 (3)	0.3660 (4)	0.48461 (16)	0.0872 (9)
H27	0.4052	0.2899	0.5049	0.105*
C28	0.2841 (4)	0.4785 (4)	0.51789 (14)	0.0861 (9)
H28	0.3263	0.4803	0.5608	0.103*
C29	0.1750 (4)	0.5889 (3)	0.48842 (14)	0.0747 (8)
H29	0.1423	0.6660	0.5114	0.090*
C30	0.1130 (3)	0.5872 (3)	0.42491 (12)	0.0555 (6)
H30	0.0384	0.6637	0.4056	0.067*
C31	0.5915 (2)	0.3940 (2)	0.25247 (12)	0.0483 (5)
C32	0.6787 (3)	0.2864 (3)	0.22104 (14)	0.0604 (6)
H32	0.6834	0.2983	0.1715	0.073*
C33	0.7573 (3)	0.1634 (3)	0.26260 (16)	0.0665 (7)
H33	0.8155	0.0939	0.2405	0.080*
C34	0.7522 (2)	0.1401 (2)	0.33631 (15)	0.0591 (6)
C35	0.6640 (3)	0.2438 (3)	0.36739 (14)	0.0592 (6)
H35	0.6567	0.2292	0.4169	0.071*
C36	0.5859 (2)	0.3697 (3)	0.32638 (13)	0.0560 (6)
H36	0.5287	0.4390	0.3489	0.067*

C37	0.8452 (3)	0.0082 (3)	0.3789 (2)	0.0812 (9)
C38	0.8200 (5)	−0.0289 (4)	0.4578 (2)	0.1201 (14)
H38A	0.8626	−0.1287	0.4751	0.180*
H38B	0.7181	−0.0108	0.4667	0.180*
H38C	0.8633	0.0291	0.4820	0.180*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03956 (9)	0.04239 (9)	0.03860 (9)	−0.01044 (6)	−0.00066 (6)	−0.00760 (6)
O1	0.0426 (8)	0.0607 (10)	0.0603 (10)	−0.0036 (7)	0.0056 (7)	−0.0058 (8)
O2	0.123 (2)	0.0682 (14)	0.170 (3)	0.0354 (14)	0.0357 (19)	0.0092 (15)
C1	0.0523 (12)	0.0480 (12)	0.0415 (11)	−0.0092 (9)	−0.0026 (9)	−0.0108 (9)
C2	0.0508 (12)	0.0488 (12)	0.0563 (13)	−0.0123 (10)	−0.0049 (10)	−0.0168 (10)
C3	0.0521 (14)	0.0729 (17)	0.101 (2)	−0.0172 (13)	−0.0109 (14)	−0.0222 (15)
C4	0.099 (2)	0.0668 (17)	0.0731 (18)	−0.0108 (15)	−0.0217 (15)	−0.0320 (14)
C5	0.0573 (13)	0.0402 (11)	0.0569 (13)	−0.0161 (10)	0.0010 (10)	−0.0155 (9)
C6	0.0704 (17)	0.0702 (17)	0.0834 (19)	−0.0322 (14)	0.0112 (14)	−0.0129 (15)
C7	0.123 (3)	0.0736 (19)	0.0697 (19)	−0.043 (2)	0.0186 (18)	0.0026 (15)
C8	0.125 (3)	0.0522 (16)	0.0641 (18)	−0.0138 (17)	−0.0079 (18)	−0.0007 (13)
C9	0.0839 (19)	0.0561 (15)	0.0718 (18)	0.0042 (14)	−0.0120 (15)	−0.0105 (13)
C10	0.0654 (15)	0.0547 (14)	0.0554 (14)	−0.0044 (11)	0.0005 (11)	−0.0132 (11)
C11	0.0488 (12)	0.0508 (12)	0.0437 (11)	−0.0172 (10)	0.0016 (9)	−0.0046 (9)
C12	0.0524 (12)	0.0566 (13)	0.0354 (10)	−0.0117 (10)	0.0016 (9)	−0.0095 (9)
C13	0.0700 (16)	0.0784 (18)	0.0613 (15)	−0.0032 (13)	0.0036 (12)	−0.0339 (13)
C14	0.0761 (18)	0.102 (2)	0.0401 (12)	−0.0310 (16)	0.0055 (12)	0.0008 (13)
C15	0.0551 (12)	0.0535 (12)	0.0311 (9)	−0.0154 (10)	−0.0044 (9)	−0.0051 (9)
C16	0.0558 (14)	0.0591 (14)	0.0654 (15)	−0.0112 (11)	0.0032 (11)	−0.0067 (12)
C17	0.0554 (16)	0.103 (2)	0.0771 (19)	−0.0049 (16)	0.0058 (14)	−0.0050 (17)
C18	0.0577 (17)	0.157 (3)	0.0544 (16)	−0.042 (2)	−0.0022 (13)	−0.0060 (19)
C19	0.098 (2)	0.117 (3)	0.0534 (15)	−0.069 (2)	−0.0098 (15)	−0.0082 (16)
C20	0.0793 (17)	0.0670 (15)	0.0489 (13)	−0.0319 (13)	−0.0067 (12)	−0.0120 (11)
C21	0.0504 (12)	0.0470 (11)	0.0388 (10)	−0.0155 (9)	0.0020 (9)	−0.0119 (9)
C22	0.0437 (11)	0.0493 (11)	0.0413 (10)	−0.0137 (9)	0.0005 (8)	−0.0115 (9)
C23	0.0752 (17)	0.0871 (19)	0.0650 (15)	−0.0503 (15)	0.0161 (13)	−0.0266 (14)
C24	0.0499 (13)	0.0900 (19)	0.0539 (14)	0.0001 (13)	−0.0072 (11)	−0.0137 (13)
C25	0.0462 (11)	0.0457 (11)	0.0367 (10)	−0.0155 (9)	0.0014 (8)	−0.0043 (8)
C26	0.0748 (17)	0.0596 (15)	0.0525 (13)	−0.0027 (12)	−0.0076 (12)	−0.0080 (11)
C27	0.085 (2)	0.097 (2)	0.0633 (17)	−0.0034 (18)	−0.0250 (15)	0.0086 (16)
C28	0.109 (3)	0.114 (3)	0.0461 (14)	−0.043 (2)	−0.0140 (15)	−0.0181 (16)
C29	0.105 (2)	0.0792 (19)	0.0503 (14)	−0.0315 (17)	0.0058 (15)	−0.0245 (14)
C30	0.0676 (15)	0.0556 (13)	0.0439 (12)	−0.0137 (11)	0.0042 (10)	−0.0117 (10)
C31	0.0347 (10)	0.0504 (12)	0.0621 (13)	−0.0120 (9)	0.0020 (9)	−0.0138 (10)
C32	0.0571 (14)	0.0621 (15)	0.0674 (15)	−0.0162 (12)	0.0167 (12)	−0.0246 (12)
C33	0.0606 (15)	0.0452 (13)	0.096 (2)	−0.0101 (11)	0.0197 (14)	−0.0254 (13)
C34	0.0461 (12)	0.0433 (12)	0.0891 (19)	−0.0129 (10)	0.0008 (12)	−0.0122 (12)
C35	0.0544 (13)	0.0588 (14)	0.0634 (14)	−0.0060 (11)	−0.0084 (11)	−0.0155 (11)
C36	0.0503 (13)	0.0540 (13)	0.0620 (14)	0.0009 (10)	−0.0050 (11)	−0.0205 (11)

C37	0.0652 (17)	0.0453 (14)	0.125 (3)	−0.0074 (13)	0.0036 (17)	−0.0026 (15)
C38	0.120 (3)	0.087 (2)	0.122 (3)	0.011 (2)	−0.017 (3)	0.019 (2)

Geometric parameters (Å, °)

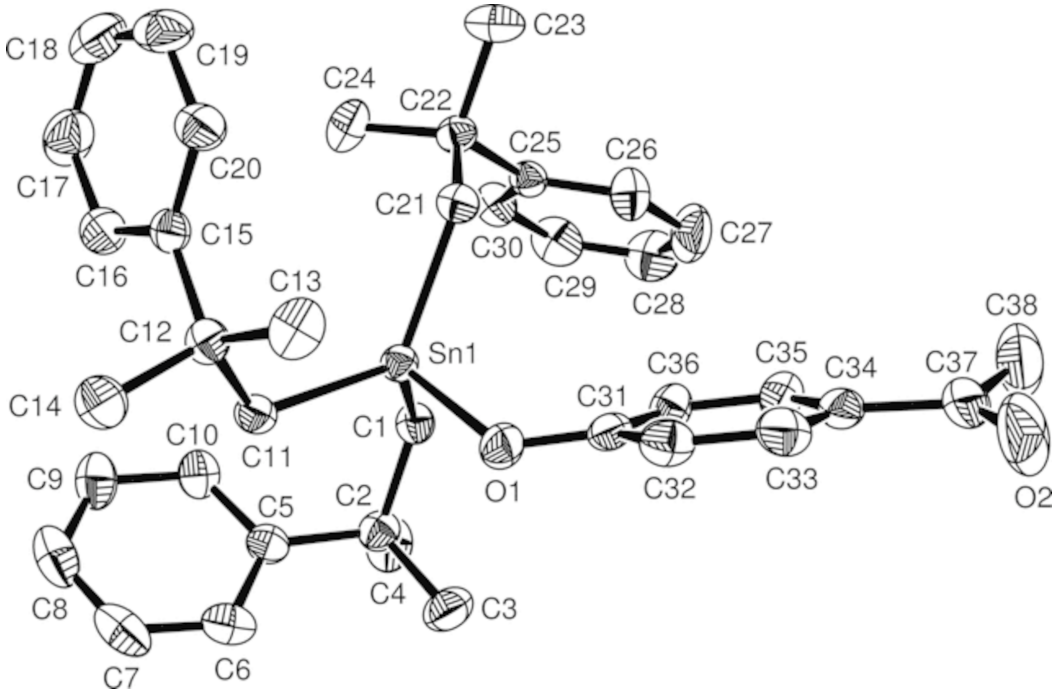
Sn1—O1	2.041 (2)	C17—C18	1.367 (5)
Sn1—C11	2.144 (2)	C17—H17	0.9300
Sn1—C21	2.154 (2)	C18—C19	1.353 (5)
Sn1—C1	2.157 (2)	C18—H18	0.9300
O1—C31	1.333 (3)	C19—C20	1.388 (4)
O2—C37	1.203 (4)	C19—H19	0.9300
C1—C2	1.544 (3)	C20—H20	0.9300
C1—H1A	0.9700	C21—C22	1.547 (3)
C1—H1B	0.9700	C21—H21A	0.9700
C2—C3	1.527 (3)	C21—H21B	0.9700
C2—C5	1.528 (3)	C22—C24	1.521 (3)
C2—C4	1.544 (3)	C22—C25	1.530 (3)
C3—H3A	0.9600	C22—C23	1.538 (3)
C3—H3B	0.9600	C23—H23A	0.9600
C3—H3C	0.9600	C23—H23B	0.9600
C4—H4A	0.9600	C23—H23C	0.9600
C4—H4B	0.9600	C24—H24A	0.9600
C4—H4C	0.9600	C24—H24B	0.9600
C5—C10	1.383 (3)	C24—H24C	0.9600
C5—C6	1.390 (3)	C25—C26	1.376 (3)
C6—C7	1.389 (4)	C25—C30	1.385 (3)
C6—H6	0.9300	C26—C27	1.397 (4)
C7—C8	1.360 (5)	C26—H26	0.9300
C7—H7	0.9300	C27—C28	1.354 (4)
C8—C9	1.357 (4)	C27—H27	0.9300
C8—H8	0.9300	C28—C29	1.358 (4)
C9—C10	1.390 (3)	C28—H28	0.9300
C9—H9	0.9300	C29—C30	1.372 (3)
C10—H10	0.9300	C29—H29	0.9300
C11—C12	1.539 (3)	C30—H30	0.9300
C11—H11A	0.9700	C31—C36	1.384 (3)
C11—H11B	0.9700	C31—C32	1.399 (3)
C12—C15	1.522 (3)	C32—C33	1.373 (3)
C12—C13	1.535 (3)	C32—H32	0.9300
C12—C14	1.537 (3)	C33—C34	1.381 (4)
C13—H13A	0.9600	C33—H33	0.9300
C13—H13B	0.9600	C34—C35	1.374 (3)
C13—H13C	0.9600	C34—C37	1.490 (4)
C14—H14A	0.9600	C35—C36	1.385 (3)
C14—H14B	0.9600	C35—H35	0.9300
C14—H14C	0.9600	C36—H36	0.9300
C15—C16	1.382 (3)	C37—C38	1.500 (5)
C15—C20	1.385 (3)	C38—H38A	0.9600
C16—C17	1.376 (4)	C38—H38B	0.9600

C16—H16	0.9300	C38—H38C	0.9600
O1—Sn1—C11	93.55 (7)	C18—C17—H17	119.9
O1—Sn1—C21	99.90 (7)	C16—C17—H17	119.9
C11—Sn1—C21	119.21 (8)	C19—C18—C17	119.1 (3)
O1—Sn1—C1	109.00 (7)	C19—C18—H18	120.4
C11—Sn1—C1	115.07 (8)	C17—C18—H18	120.4
C21—Sn1—C1	115.49 (8)	C18—C19—C20	121.2 (3)
C31—O1—Sn1	126.62 (13)	C18—C19—H19	119.4
C2—C1—Sn1	119.10 (14)	C20—C19—H19	119.4
C2—C1—H1A	107.5	C15—C20—C19	120.5 (3)
Sn1—C1—H1A	107.5	C15—C20—H20	119.8
C2—C1—H1B	107.5	C19—C20—H20	119.8
Sn1—C1—H1B	107.5	C22—C21—Sn1	118.13 (13)
H1A—C1—H1B	107.0	C22—C21—H21A	107.8
C3—C2—C5	112.8 (2)	Sn1—C21—H21A	107.8
C3—C2—C4	108.1 (2)	C22—C21—H21B	107.8
C5—C2—C4	108.25 (19)	Sn1—C21—H21B	107.8
C3—C2—C1	109.03 (19)	H21A—C21—H21B	107.1
C5—C2—C1	110.00 (17)	C24—C22—C25	112.32 (18)
C4—C2—C1	108.5 (2)	C24—C22—C23	108.2 (2)
C2—C3—H3A	109.5	C25—C22—C23	108.86 (18)
C2—C3—H3B	109.5	C24—C22—C21	109.37 (18)
H3A—C3—H3B	109.5	C25—C22—C21	110.23 (16)
C2—C3—H3C	109.5	C23—C22—C21	107.75 (17)
H3A—C3—H3C	109.5	C22—C23—H23A	109.5
H3B—C3—H3C	109.5	C22—C23—H23B	109.5
C2—C4—H4A	109.5	H23A—C23—H23B	109.5
C2—C4—H4B	109.5	C22—C23—H23C	109.5
H4A—C4—H4B	109.5	H23A—C23—H23C	109.5
C2—C4—H4C	109.5	H23B—C23—H23C	109.5
H4A—C4—H4C	109.5	C22—C24—H24A	109.5
H4B—C4—H4C	109.5	C22—C24—H24B	109.5
C10—C5—C6	116.5 (2)	H24A—C24—H24B	109.5
C10—C5—C2	120.1 (2)	C22—C24—H24C	109.5
C6—C5—C2	123.3 (2)	H24A—C24—H24C	109.5
C7—C6—C5	121.1 (3)	H24B—C24—H24C	109.5
C7—C6—H6	119.5	C26—C25—C30	116.7 (2)
C5—C6—H6	119.5	C26—C25—C22	120.58 (19)
C8—C7—C6	121.3 (3)	C30—C25—C22	122.73 (19)
C8—C7—H7	119.4	C25—C26—C27	121.3 (3)
C6—C7—H7	119.4	C25—C26—H26	119.4
C9—C8—C7	118.5 (3)	C27—C26—H26	119.4
C9—C8—H8	120.7	C28—C27—C26	120.0 (3)
C7—C8—H8	120.7	C28—C27—H27	120.0
C8—C9—C10	121.1 (3)	C26—C27—H27	120.0
C8—C9—H9	119.5	C27—C28—C29	119.8 (3)
C10—C9—H9	119.5	C27—C28—H28	120.1
C5—C10—C9	121.4 (2)	C29—C28—H28	120.1
C5—C10—H10	119.3	C28—C29—C30	120.3 (3)

C9—C10—H10	119.3	C28—C29—H29	119.9
C12—C11—Sn1	118.51 (14)	C30—C29—H29	119.9
C12—C11—H11A	107.7	C29—C30—C25	121.9 (2)
Sn1—C11—H11A	107.7	C29—C30—H30	119.0
C12—C11—H11B	107.7	C25—C30—H30	119.0
Sn1—C11—H11B	107.7	O1—C31—C36	123.31 (19)
H11A—C11—H11B	107.1	O1—C31—C32	119.3 (2)
C15—C12—C13	112.7 (2)	C36—C31—C32	117.4 (2)
C15—C12—C14	108.08 (18)	C33—C32—C31	120.7 (2)
C13—C12—C14	108.4 (2)	C33—C32—H32	119.7
C15—C12—C11	110.59 (17)	C31—C32—H32	119.7
C13—C12—C11	108.87 (18)	C32—C33—C34	121.7 (2)
C14—C12—C11	108.05 (19)	C32—C33—H33	119.1
C12—C13—H13A	109.5	C34—C33—H33	119.1
C12—C13—H13B	109.5	C35—C34—C33	117.8 (2)
H13A—C13—H13B	109.5	C35—C34—C37	122.6 (3)
C12—C13—H13C	109.5	C33—C34—C37	119.6 (2)
H13A—C13—H13C	109.5	C34—C35—C36	121.2 (2)
H13B—C13—H13C	109.5	C34—C35—H35	119.4
C12—C14—H14A	109.5	C36—C35—H35	119.4
C12—C14—H14B	109.5	C31—C36—C35	121.1 (2)
H14A—C14—H14B	109.5	C31—C36—H36	119.4
C12—C14—H14C	109.5	C35—C36—H36	119.4
H14A—C14—H14C	109.5	O2—C37—C34	120.2 (3)
H14B—C14—H14C	109.5	O2—C37—C38	120.9 (3)
C16—C15—C20	117.1 (2)	C34—C37—C38	118.9 (3)
C16—C15—C12	119.9 (2)	C37—C38—H38A	109.5
C20—C15—C12	123.0 (2)	C37—C38—H38B	109.5
C17—C16—C15	121.8 (3)	H38A—C38—H38B	109.5
C17—C16—H16	119.1	C37—C38—H38C	109.5
C15—C16—H16	119.1	H38A—C38—H38C	109.5
C18—C17—C16	120.3 (3)	H38B—C38—H38C	109.5
C11—Sn1—O1—C31	−163.81 (17)	C16—C15—C20—C19	−1.3 (3)
C21—Sn1—O1—C31	−43.34 (18)	C12—C15—C20—C19	−179.1 (2)
C1—Sn1—O1—C31	78.13 (18)	C18—C19—C20—C15	1.2 (4)
O1—Sn1—C1—C2	67.67 (17)	O1—Sn1—C21—C22	144.23 (15)
C11—Sn1—C1—C2	−35.82 (19)	C11—Sn1—C21—C22	−116.01 (15)
C21—Sn1—C1—C2	179.11 (15)	C1—Sn1—C21—C22	27.53 (18)
Sn1—C1—C2—C3	−68.2 (2)	Sn1—C21—C22—C24	59.0 (2)
Sn1—C1—C2—C5	56.0 (2)	Sn1—C21—C22—C25	−64.9 (2)
Sn1—C1—C2—C4	174.23 (16)	Sn1—C21—C22—C23	176.41 (15)
C3—C2—C5—C10	174.1 (2)	C24—C22—C25—C26	−179.1 (2)
C4—C2—C5—C10	−66.3 (3)	C23—C22—C25—C26	61.1 (3)
C1—C2—C5—C10	52.1 (3)	C21—C22—C25—C26	−56.9 (3)
C3—C2—C5—C6	−4.1 (3)	C24—C22—C25—C30	0.9 (3)
C4—C2—C5—C6	115.6 (3)	C23—C22—C25—C30	−118.9 (2)
C1—C2—C5—C6	−126.1 (2)	C21—C22—C25—C30	123.1 (2)
C10—C5—C6—C7	−1.8 (4)	C30—C25—C26—C27	−0.2 (4)
C2—C5—C6—C7	176.4 (2)	C22—C25—C26—C27	179.7 (2)

C5—C6—C7—C8	0.4 (5)	C25—C26—C27—C28	−0.2 (5)
C6—C7—C8—C9	1.7 (5)	C26—C27—C28—C29	0.5 (5)
C7—C8—C9—C10	−2.4 (4)	C27—C28—C29—C30	−0.4 (5)
C6—C5—C10—C9	1.1 (3)	C28—C29—C30—C25	−0.1 (4)
C2—C5—C10—C9	−177.1 (2)	C26—C25—C30—C29	0.4 (4)
C8—C9—C10—C5	1.0 (4)	C22—C25—C30—C29	−179.6 (2)
O1—Sn1—C11—C12	90.31 (16)	Sn1—O1—C31—C36	−37.9 (3)
C21—Sn1—C11—C12	−13.1 (2)	Sn1—O1—C31—C32	143.00 (17)
C1—Sn1—C11—C12	−156.78 (15)	O1—C31—C32—C33	177.8 (2)
Sn1—C11—C12—C15	66.0 (2)	C36—C31—C32—C33	−1.4 (3)
Sn1—C11—C12—C13	−58.4 (2)	C31—C32—C33—C34	0.9 (4)
Sn1—C11—C12—C14	−175.93 (16)	C32—C33—C34—C35	0.8 (4)
C13—C12—C15—C16	174.6 (2)	C32—C33—C34—C37	−177.0 (2)
C14—C12—C15—C16	−65.6 (3)	C33—C34—C35—C36	−1.9 (4)
C11—C12—C15—C16	52.5 (3)	C37—C34—C35—C36	175.8 (2)
C13—C12—C15—C20	−7.6 (3)	O1—C31—C36—C35	−178.9 (2)
C14—C12—C15—C20	112.2 (2)	C32—C31—C36—C35	0.3 (3)
C11—C12—C15—C20	−129.7 (2)	C34—C35—C36—C31	1.4 (4)
C20—C15—C16—C17	0.9 (3)	C35—C34—C37—O2	−167.0 (3)
C12—C15—C16—C17	178.8 (2)	C33—C34—C37—O2	10.7 (4)
C15—C16—C17—C18	−0.4 (4)	C35—C34—C37—C38	13.0 (4)
C16—C17—C18—C19	0.2 (4)	C33—C34—C37—C38	−169.3 (3)
C17—C18—C19—C20	−0.6 (4)		

Fig. 1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