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(2-Hydroxybenzoato-κO)triphenyl(triphenylphosphine oxide-κO)tin(IV)

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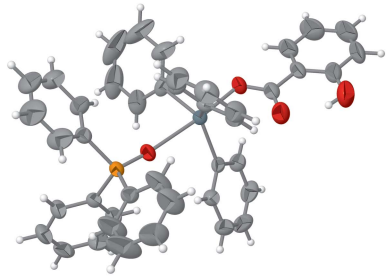
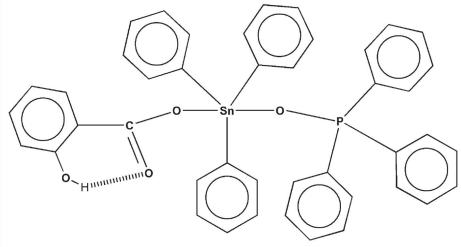
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $[Sn\{C_6H_4(OH)COO\}(C_6H_5)_3\{OP(C_6H_5)_3\}]$, is comprised of discrete molecules with the Sn^{IV} atom in a trigonal–bipyramidal coordination environment. The carboxylate O atom of the salicylate anion and the O atom of the triphenylphosphine oxide moiety are in the axial positions and the three *ipso* C atoms occupy the equatorial positions. An intramolecular O—H···O hydrogen bond is present in the anion between the hydroxy group and the carbonyl atom O of the carboxylate group.

3D view



Chemical scheme



Structure description

The applications of organotin compounds in various fields (Omae, 1989) might explain the effort to synthesize and structurally determine new representatives of this family of compounds. In this context, the crystal structure of the derivative $C_6H_4(OH)CO_2SnPh_3$ has been determined by Vollano *et al.* (1984), followed by a redetermination by Rauf *et al.* (2008). The structure consists of discrete molecules, with a tetrahedral coordination of the Sn^{IV} atom by the carboxylate $-CO_2$ moiety and three phenyl groups. Related structures, *viz.* $[Sn(C_6H_5COC_6H_4COO)(C_6H_5)_3\{(C_6H_5)_3OP\}]$ and $[Sn(OOCC_6HF_4)(C_6H_5)_3\{(C_6H_5)_3OP\}]$ were reported by Diop *et al.* (2006) and Ma *et al.* (2006), respectively. In these structures, the $OPPh_3$ moiety coordinates in a monodentate manner through the O atom to an $SnPh_3$ residue. The scarcity of data on $OPPh_3$ moieties coordinating to an $SnPh_3$ residue that is additionally linked to a carboxylate group has prompted us to study the interactions between $C_6H_4(OH)CO_2SnPh_3$ and $OPPh_3$, which has yielded the mononuclear title compound.

The molecular structure consists of a salicylate anion and a $OPPh_3$ molecule, each coordinating to the Sn^{IV} atom of the $SnPh_3$ group in a monodentate mode. The Sn^{IV} atom has a distorted trigonal–bipyramidal coordination environment, with the three phenyl

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O5	0.82	1.82	2.546 (4)	147
C8—H8···O5	0.93	2.43	3.071 (4)	126

groups in the equatorial positions (Fig. 1). The Sn—O1 bond involving the anion [2.124 (2) Å] and the Sn—O4 bond involving the $OPPh_3$ group [2.451 (2) Å] are markedly different. The O1—Sn—O4 angle [171.65 (9)°] deviates from linearity. The sum of the C(*ipso*)—Sn—C(*ipso*) angles amounts to 357.36°. Comparable C(*ipso*)—Sn—C(*ipso*) angular sums of 359.07 and 357.63° were observed for the related structures reported by Diop *et al.* (2006) and Ma *et al.* (2006), respectively. The corresponding O—Sn—O angles in these structures are 175.46 (11) and 178.03 (11)°. The P—O4 bond length [1.489 (2) Å] in (I) is very similar to that in the structure reported by Ma *et al.* (1.486 Å), but different to the one reported by Diop *et al.* [1.511 (3) Å]. In the free $OPPh_3$ ligand, the P—O bond length is 1.460 (1) Å (Bandoli *et al.*, 1970). An intramolecular hydrogen bond is present between the hydroxy group and the C=O group of the carboxylate moiety (Table 1). In addition, a weak intramolecular C—H···O interaction between one of the phenyl H atoms and the carbonyl O atom is observed. The packing of molecules in the crystal has no special features and is depicted in Fig. 2.

A search of the Cambridge Structural Database (Version 5.37 plus two updates; Groom *et al.*, 2016) for structures containing salicylate moieties revealed 2105 hits while the $Sn(Ph_3)(OPPh_3)$ fragment is present in 12 structures.

Synthesis and crystallization

$C_6H_4(OH)CO_2SnPh_3$, (I), was obtained from the condensation of salicylic acid (0.5 g, 4 mmol) with triphenyltin(IV) hydroxide (1.328 g, 4 mmol) in ethanol (50 ml). The title

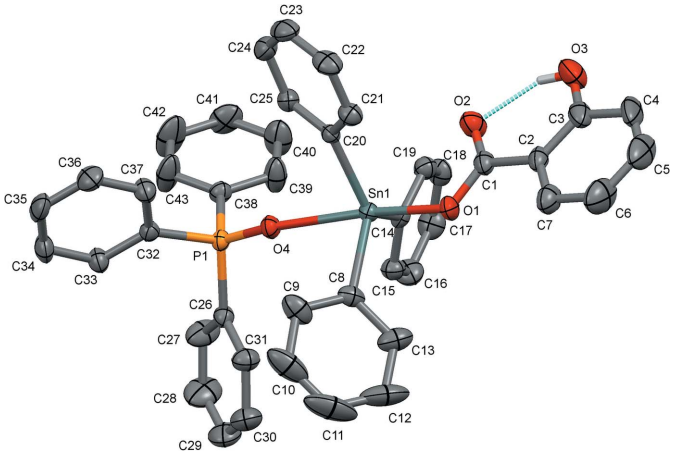


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 50% probability level. C-bound H atoms have been omitted for clarity. The intramolecular O—H···O hydrogen bond is shown with a dashed line.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Sn(C_6H_5)_3(C_7H_5O_3)(C_{18}H_{15}OP)]$
M_r	765.37
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	293
a, b, c (Å)	9.3620 (3), 17.7187 (7), 22.1796 (9)
V (Å^3)	3679.2 (2)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.78
Crystal size (mm)	0.10 × 0.05 × 0.02
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.69, 0.75
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11302, 11302, 8849
R_{int}	0.067
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.037, 0.063, 1.05
No. of reflections	11302
No. of parameters	443
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.24
Absolute structure	Flack x determined using 3310 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.026 (5)

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2006) and *publCIF* (Westrip, 2010).

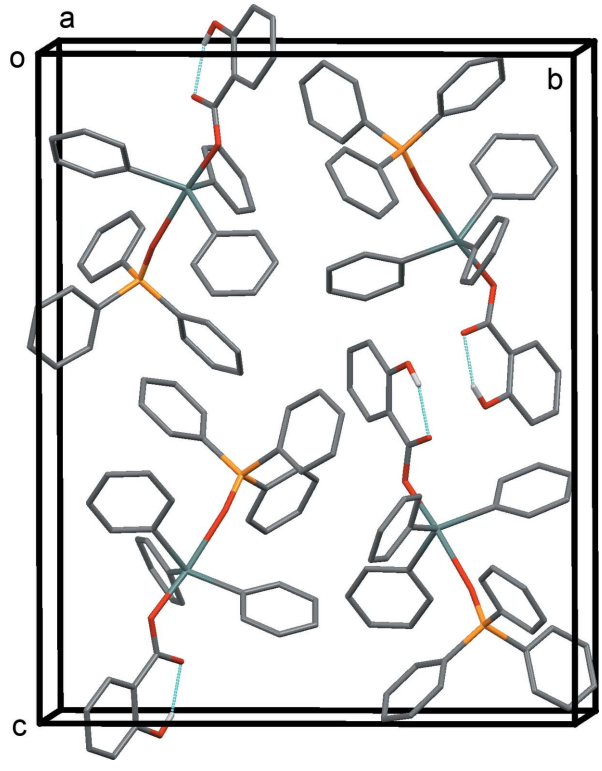


Figure 2
The crystal packing of the title compound viewed along the *a* axis. The intramolecular O—H···O hydrogen bond is shown as a dashed line, and C-bound H atoms have been omitted for clarity.

compound was obtained by reacting an ethanolic solution of (I) (0.487 g, 1 mmol) with $OPPh_3$ (0.278 g, 1 mmol). The mixture was stirred for several hours. Slow solvent evaporation yielded colourless single crystals suitable for X-ray analysis.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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full crystallographic data

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(2-Hydroxybenzoato-κO)triphenyl(triphenylphosphine oxide-κO)tin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_7H_5O_3)(C_{18}H_{15}OP)]$
M_r = 765.37
Orthorhombic, $P2_12_12_1$
a = 9.3620 (3) Å
b = 17.7187 (7) Å
c = 22.1796 (9) Å
V = 3679.2 (2) Å^3
Z = 4
F(000) = 1560
D_x = 1.382 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 162157 reflections
θ = 2.3–30.6°
μ = 0.78 mm^{-1}
T = 293 K
Platelet, colorless
0.10 × 0.05 × 0.02 mm

Data collection

Bruker D8 Venture diffractometer
Radiation source: fine-focus sealed-tube
Detector resolution: 8.33 pixels mm^{-1}
combinatoin of /w– and /f–scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.69, T_{max} = 0.75
11302 measured reflections
11302 independent reflections
8849 reflections with $I > 2\sigma(I)$
R_{int} = 0.067
θ_{max} = 30.6°, θ_{min} = 2.3°
h = −13→13
k = 0→25
l = 0→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.063
S = 1.05
11302 reflections
443 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
$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.2485P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Absolute structure: Flack x determined using 3310 quotients $[(I^+) - (I^-)]/[(I^+) + (I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.026 (5)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.92470 (2)	0.23909 (2)	0.79019 (2)	0.03537 (6)
P1	1.10239 (8)	0.33513 (4)	0.65040 (3)	0.03534 (18)
O1	0.8198 (3)	0.17642 (14)	0.85879 (10)	0.0509 (6)
O2	0.9484 (5)	0.1873 (2)	1.03685 (13)	0.0999 (11)
H2	0.9810	0.2090	1.0072	0.150*
O4	1.0151 (2)	0.30745 (12)	0.70199 (9)	0.0432 (5)
O5	0.9652 (3)	0.22689 (17)	0.92674 (11)	0.0664 (7)
C1	0.7881 (4)	0.1037 (2)	0.7273 (2)	0.0715 (12)
H1	0.8369	0.0772	0.7571	0.086*
C2	0.6626 (5)	0.1038 (2)	0.9478 (2)	0.0709 (12)
H2A	0.6300	0.1020	0.9082	0.085*
C3	1.3704 (4)	0.1963 (2)	0.84320 (18)	0.0570 (10)
H3	1.4309	0.2108	0.8744	0.068*
C4	1.3334 (5)	0.1325 (2)	0.7513 (2)	0.0666 (11)
H4	1.3682	0.1026	0.7202	0.080*
C5	1.2605 (4)	0.2594 (3)	0.5616 (2)	0.0773 (12)
H5	1.3313	0.2955	0.5673	0.093*
C6	0.8541 (5)	0.5160 (2)	0.61409 (18)	0.0655 (11)
H6	0.7915	0.5465	0.6357	0.079*
C7	1.3407 (5)	0.3410 (3)	0.7212 (2)	0.0781 (14)
H7	1.2989	0.3002	0.7408	0.094*
C8	1.2282 (3)	0.21838 (18)	0.84431 (15)	0.0470 (8)
H8	1.1934	0.2465	0.8765	0.056*
C9	1.4699 (5)	0.3668 (3)	0.7407 (2)	0.0880 (16)
H9	1.5149	0.3429	0.7728	0.106*
C10	1.5328 (4)	0.4259 (2)	0.7145 (2)	0.0807 (13)
H10	1.6193	0.4443	0.7290	0.097*
C11	0.7223 (4)	0.2195 (3)	0.68116 (17)	0.0694 (12)
H11	0.7264	0.2719	0.6793	0.083*
C12	1.3371 (5)	0.4329 (3)	0.6466 (2)	0.0926 (18)
H12	1.2927	0.4567	0.6143	0.111*
C13	0.9754 (5)	0.4869 (2)	0.52329 (17)	0.0633 (11)
H13	0.9944	0.4975	0.4830	0.076*
C14	1.0123 (3)	0.40946 (17)	0.61023 (13)	0.0379 (7)
C15	1.0377 (4)	0.2061 (2)	0.58802 (17)	0.0569 (9)
H15	0.9556	0.2059	0.6116	0.068*
C16	1.0562 (5)	0.1502 (2)	0.54498 (19)	0.0739 (12)
H16	0.9870	0.1132	0.5396	0.089*
C17	1.2782 (7)	0.2043 (3)	0.5187 (2)	0.1018 (18)
H17	1.3601	0.2039	0.4950	0.122*
C19	1.1918 (4)	0.15498 (19)	0.75101 (15)	0.0478 (8)
H19	1.1326	0.1406	0.7193	0.057*
C20	0.9343 (4)	0.41208 (17)	0.81022 (14)	0.0462 (7)
H20	1.0159	0.4098	0.7864	0.055*
C21	0.8898 (5)	0.4812 (2)	0.83324 (17)	0.0612 (11)

H21	0.9422	0.5246	0.8251	0.073*
C22	0.7383 (4)	0.3524 (2)	0.85800 (15)	0.0486 (8)
H22	0.6865	0.3091	0.8671	0.058*
C23	0.6935 (4)	0.4217 (2)	0.88043 (17)	0.0638 (11)
H23	0.6118	0.4247	0.9041	0.077*
C24	0.8303 (6)	0.1478 (2)	1.02070 (18)	0.0712 (12)
C25	0.6367 (7)	0.1028 (6)	0.6416 (3)	0.136 (4)
H25	0.5850	0.0761	0.6128	0.163*
C26	0.7584 (8)	0.1079 (3)	1.0650 (2)	0.104 (2)
H26	0.7906	0.1092	1.1047	0.124*
C27	0.6406 (5)	0.1796 (5)	0.6392 (2)	0.110 (2)
H27	0.5893	0.2053	0.6097	0.132*
C28	0.7072 (7)	0.0648 (4)	0.6854 (3)	0.116 (2)
H28	0.7013	0.0125	0.6873	0.139*
C29	1.4689 (6)	0.4584 (3)	0.6666 (3)	0.113 (2)
H29	1.5135	0.4982	0.6468	0.136*
C30	0.8634 (4)	0.1858 (2)	0.91366 (16)	0.0493 (9)
C31	0.7700 (5)	0.4853 (2)	0.86754 (19)	0.0686 (12)
H31	0.7397	0.5317	0.8824	0.082*
C32	0.6431 (9)	0.0675 (3)	1.0507 (3)	0.119 (3)
H32	0.5969	0.0403	1.0808	0.143*
C35	0.7822 (4)	0.14517 (19)	0.96130 (15)	0.0533 (9)
C36	0.5897 (7)	0.0646 (3)	0.9921 (3)	0.109 (2)
H36	0.5077	0.0373	0.9831	0.131*
C37	0.9180 (4)	0.45468 (19)	0.64161 (15)	0.0544 (8)
H37	0.8972	0.4438	0.6817	0.065*
C38	1.0404 (4)	0.4262 (2)	0.55051 (14)	0.0494 (9)
H38	1.1036	0.3963	0.5287	0.059*
C39	0.8835 (5)	0.5316 (2)	0.55470 (19)	0.0655 (11)
H39	0.8407	0.5728	0.5360	0.079*
C40	1.1376 (3)	0.26135 (19)	0.59650 (13)	0.0419 (7)
C41	1.2718 (3)	0.37294 (19)	0.67417 (14)	0.0432 (8)
C42	1.1766 (6)	0.1501 (3)	0.5107 (2)	0.0888 (16)
H42	1.1896	0.1130	0.4816	0.107*
C43	0.7969 (3)	0.1814 (2)	0.72536 (14)	0.0445 (8)
C44	1.4224 (4)	0.1539 (2)	0.79708 (19)	0.0653 (10)
H44	1.5179	0.1395	0.7967	0.078*
C45	1.1377 (3)	0.19839 (15)	0.79707 (14)	0.0380 (7)
C46	0.8592 (3)	0.34689 (17)	0.82223 (13)	0.0370 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03818 (10)	0.03418 (9)	0.03376 (9)	0.00002 (9)	0.00066 (9)	−0.00042 (8)
P1	0.0374 (4)	0.0353 (4)	0.0333 (4)	−0.0011 (3)	0.0024 (3)	0.0046 (3)
O1	0.0659 (16)	0.0497 (14)	0.0371 (13)	−0.0038 (12)	0.0077 (12)	0.0078 (11)
O2	0.145 (3)	0.107 (3)	0.0478 (17)	0.009 (3)	−0.009 (2)	0.0028 (17)
O4	0.0484 (12)	0.0442 (12)	0.0371 (12)	−0.0013 (9)	0.0060 (10)	0.0081 (10)

O5	0.0704 (17)	0.0788 (19)	0.0501 (14)	−0.0145 (16)	0.0038 (12)	0.0017 (14)
C1	0.062 (2)	0.061 (2)	0.091 (3)	−0.011 (2)	0.013 (2)	−0.029 (2)
C2	0.086 (3)	0.062 (3)	0.065 (3)	−0.002 (2)	0.023 (2)	0.009 (2)
C3	0.045 (2)	0.063 (2)	0.063 (2)	−0.0003 (17)	−0.0127 (18)	0.006 (2)
C4	0.066 (3)	0.064 (3)	0.070 (3)	0.020 (2)	0.009 (2)	−0.011 (2)
C5	0.068 (2)	0.067 (3)	0.097 (3)	−0.003 (2)	0.034 (2)	−0.018 (3)
C6	0.073 (3)	0.050 (2)	0.073 (3)	0.019 (2)	0.000 (2)	−0.004 (2)
C7	0.060 (2)	0.080 (3)	0.094 (4)	−0.023 (2)	−0.026 (2)	0.043 (3)
C8	0.0473 (19)	0.0444 (19)	0.0494 (18)	−0.0006 (15)	−0.0019 (15)	−0.0003 (15)
C9	0.064 (3)	0.099 (4)	0.101 (4)	−0.021 (3)	−0.035 (3)	0.033 (3)
C10	0.054 (2)	0.073 (3)	0.116 (4)	−0.015 (2)	−0.030 (3)	−0.001 (3)
C11	0.045 (2)	0.109 (4)	0.055 (2)	−0.010 (2)	−0.0049 (17)	0.001 (2)
C12	0.080 (3)	0.079 (3)	0.119 (4)	−0.036 (3)	−0.046 (3)	0.047 (3)
C13	0.080 (3)	0.062 (2)	0.047 (2)	0.003 (2)	−0.0060 (19)	0.0218 (19)
C14	0.0409 (17)	0.0352 (16)	0.0376 (17)	−0.0023 (13)	−0.0018 (13)	0.0033 (13)
C15	0.057 (2)	0.056 (2)	0.058 (2)	−0.0040 (18)	0.0066 (17)	−0.0107 (18)
C16	0.088 (3)	0.056 (2)	0.077 (3)	−0.005 (2)	−0.003 (3)	−0.018 (2)
C17	0.112 (4)	0.091 (4)	0.103 (4)	0.009 (3)	0.057 (3)	−0.026 (3)
C19	0.051 (2)	0.0448 (19)	0.0473 (19)	0.0029 (16)	0.0005 (16)	−0.0046 (15)
C20	0.054 (2)	0.0420 (17)	0.0421 (16)	0.0007 (18)	−0.0024 (16)	0.0023 (12)
C21	0.080 (3)	0.0413 (19)	0.063 (2)	0.0031 (19)	−0.012 (2)	0.0004 (17)
C22	0.046 (2)	0.054 (2)	0.0459 (19)	0.0026 (16)	0.0040 (16)	−0.0044 (16)
C23	0.060 (2)	0.077 (3)	0.055 (2)	0.021 (2)	0.0067 (19)	−0.016 (2)
C24	0.109 (4)	0.060 (3)	0.045 (2)	0.021 (3)	0.015 (2)	0.002 (2)
C25	0.076 (4)	0.227 (10)	0.105 (5)	−0.058 (5)	0.010 (4)	−0.095 (6)
C26	0.196 (7)	0.072 (3)	0.043 (2)	0.021 (4)	0.037 (3)	0.014 (2)
C27	0.061 (3)	0.209 (8)	0.060 (3)	−0.021 (4)	−0.010 (2)	−0.019 (4)
C28	0.093 (4)	0.111 (5)	0.143 (6)	−0.037 (4)	0.025 (4)	−0.084 (4)
C29	0.085 (4)	0.084 (4)	0.170 (6)	−0.048 (3)	−0.047 (4)	0.051 (4)
C30	0.062 (2)	0.044 (2)	0.0421 (19)	0.0105 (17)	0.0093 (17)	0.0049 (15)
C31	0.087 (3)	0.051 (2)	0.068 (3)	0.022 (2)	−0.013 (2)	−0.019 (2)
C32	0.192 (7)	0.081 (4)	0.085 (4)	−0.008 (4)	0.079 (5)	0.015 (3)
C35	0.075 (3)	0.0419 (19)	0.0428 (19)	0.0124 (19)	0.0186 (18)	0.0094 (15)
C36	0.133 (5)	0.089 (4)	0.105 (4)	−0.027 (4)	0.053 (4)	0.009 (3)
C37	0.066 (2)	0.054 (2)	0.0434 (17)	0.012 (2)	0.0039 (19)	0.0048 (15)
C38	0.056 (2)	0.053 (2)	0.0393 (17)	0.0060 (16)	0.0022 (15)	0.0072 (15)
C39	0.081 (3)	0.041 (2)	0.074 (3)	0.0030 (19)	−0.020 (2)	0.0190 (19)
C40	0.0465 (16)	0.0382 (16)	0.0410 (15)	0.0045 (15)	0.0043 (13)	0.0035 (15)
C41	0.0411 (18)	0.0420 (18)	0.0466 (18)	−0.0036 (15)	−0.0024 (15)	0.0013 (15)
C42	0.125 (5)	0.062 (3)	0.079 (3)	0.019 (3)	0.013 (3)	−0.025 (2)
C43	0.0335 (16)	0.060 (2)	0.0397 (18)	−0.0100 (16)	0.0085 (13)	−0.0109 (15)
C44	0.0451 (19)	0.068 (2)	0.083 (3)	0.011 (2)	0.005 (2)	0.008 (2)
C45	0.0412 (16)	0.0288 (14)	0.0440 (17)	0.0015 (12)	0.0001 (15)	0.0049 (14)
C46	0.0428 (17)	0.0383 (17)	0.0298 (15)	0.0074 (14)	−0.0031 (13)	−0.0006 (12)

Geometric parameters (Å, º)

Sn1—C45	2.126 (3)	C12—H12	0.9300
Sn1—O1	2.124 (2)	C13—C39	1.362 (6)
Sn1—C46	2.128 (3)	C13—C38	1.376 (5)
Sn1—C43	2.132 (3)	C13—H13	0.9300
Sn1—O4	2.451 (2)	C14—C37	1.380 (5)
P1—O4	1.489 (2)	C14—C38	1.383 (4)
P1—C14	1.800 (3)	C15—C40	1.368 (5)
P1—C41	1.800 (3)	C15—C16	1.386 (5)
P1—C40	1.802 (3)	C15—H15	0.9300
O1—C30	1.294 (4)	C16—C42	1.360 (6)
O2—C24	1.357 (6)	C16—H16	0.9300
O2—H2	0.8200	C17—C42	1.363 (7)
O5—C30	1.234 (4)	C17—H17	0.9300
C1—C28	1.382 (7)	C19—C45	1.375 (4)
C1—C43	1.381 (5)	C19—H19	0.9300
C1—H1	0.9300	C20—C46	1.378 (5)
C2—C35	1.372 (6)	C20—C21	1.391 (5)
C2—C36	1.382 (6)	C20—H20	0.9300
C2—H2A	0.9300	C21—C31	1.358 (6)
C3—C44	1.360 (5)	C21—H21	0.9300
C3—C8	1.387 (5)	C22—C46	1.385 (4)
C3—H3	0.9300	C22—C23	1.390 (5)
C4—C44	1.366 (6)	C22—H22	0.9300
C4—C19	1.385 (5)	C23—C31	1.365 (6)
C4—H4	0.9300	C23—H23	0.9300
C5—C17	1.373 (6)	C24—C26	1.385 (6)
C5—C40	1.387 (5)	C24—C35	1.393 (6)
C5—H5	0.9300	C25—C28	1.353 (11)
C6—C39	1.374 (5)	C25—C27	1.363 (10)
C6—C37	1.382 (5)	C25—H25	0.9300
C6—H6	0.9300	C26—C32	1.334 (9)
C7—C41	1.350 (5)	C26—H26	0.9300
C7—C9	1.364 (6)	C27—H27	0.9300
C7—H7	0.9300	C28—H28	0.9300
C8—C45	1.393 (4)	C29—H29	0.9300
C8—H8	0.9300	C30—C35	1.487 (5)
C9—C10	1.335 (6)	C31—H31	0.9300
C9—H9	0.9300	C32—C36	1.393 (8)
C10—C29	1.348 (7)	C32—H32	0.9300
C10—H10	0.9300	C36—H36	0.9300
C11—C43	1.380 (5)	C37—H37	0.9300
C11—C27	1.397 (7)	C38—H38	0.9300
C11—H11	0.9300	C39—H39	0.9300
C12—C41	1.369 (5)	C42—H42	0.9300
C12—C29	1.387 (6)	C44—H44	0.9300

C45—Sn1—O1	101.83 (11)	C46—C20—H20	119.5
C45—Sn1—C46	123.43 (12)	C21—C20—H20	119.5
O1—Sn1—C46	95.55 (11)	C31—C21—C20	120.0 (4)
C45—Sn1—C43	114.36 (12)	C31—C21—H21	120.0
O1—Sn1—C43	88.45 (11)	C20—C21—H21	120.0
C46—Sn1—C43	119.57 (13)	C46—C22—C23	120.9 (4)
C45—Sn1—O4	84.32 (9)	C46—C22—H22	119.6
O1—Sn1—O4	171.65 (9)	C23—C22—H22	119.6
C46—Sn1—O4	85.56 (10)	C31—C23—C22	119.8 (4)
C43—Sn1—O4	83.82 (11)	C31—C23—H23	120.1
O4—P1—C14	111.35 (14)	C22—C23—H23	120.1
O4—P1—C41	112.40 (14)	O2—C24—C26	118.2 (5)
C14—P1—C41	106.59 (15)	O2—C24—C35	122.0 (4)
O4—P1—C40	111.79 (13)	C26—C24—C35	119.8 (5)
C14—P1—C40	106.75 (14)	C28—C25—C27	120.8 (6)
C41—P1—C40	107.63 (15)	C28—C25—H25	119.6
C30—O1—Sn1	117.4 (2)	C27—C25—H25	119.6
C24—O2—H2	109.5	C32—C26—C24	119.9 (5)
P1—O4—Sn1	164.85 (13)	C32—C26—H26	120.1
C28—C1—C43	120.6 (5)	C24—C26—H26	120.1
C28—C1—H1	119.7	C25—C27—C11	119.6 (6)
C43—C1—H1	119.7	C25—C27—H27	120.2
C35—C2—C36	121.0 (5)	C11—C27—H27	120.2
C35—C2—H2A	119.5	C25—C28—C1	120.1 (6)
C36—C2—H2A	119.5	C25—C28—H28	119.9
C44—C3—C8	120.8 (4)	C1—C28—H28	119.9
C44—C3—H3	119.6	C10—C29—C12	120.5 (4)
C8—C3—H3	119.6	C10—C29—H29	119.7
C44—C4—C19	120.5 (4)	C12—C29—H29	119.7
C44—C4—H4	119.7	O5—C30—O1	122.7 (3)
C19—C4—H4	119.7	O5—C30—C35	120.9 (3)
C17—C5—C40	120.3 (4)	O1—C30—C35	116.4 (3)
C17—C5—H5	119.8	C21—C31—C23	120.5 (4)
C40—C5—H5	119.8	C21—C31—H31	119.8
C39—C6—C37	119.7 (4)	C23—C31—H31	119.8
C39—C6—H6	120.1	C26—C32—C36	122.1 (5)
C37—C6—H6	120.1	C26—C32—H32	118.9
C41—C7—C9	121.9 (4)	C36—C32—H32	118.9
C41—C7—H7	119.0	C2—C35—C24	119.2 (4)
C9—C7—H7	119.0	C2—C35—C30	121.4 (4)
C3—C8—C45	119.9 (3)	C24—C35—C30	119.4 (4)
C3—C8—H8	120.0	C2—C36—C32	117.9 (6)
C45—C8—H8	120.0	C2—C36—H36	121.0
C10—C9—C7	121.0 (4)	C32—C36—H36	121.0
C10—C9—H9	119.5	C14—C37—C6	120.7 (3)
C7—C9—H9	119.5	C14—C37—H37	119.7
C9—C10—C29	118.8 (4)	C6—C37—H37	119.7
C9—C10—H10	120.6	C13—C38—C14	120.2 (3)

C29—C10—H10	120.6	C13—C38—H38	119.9
C43—C11—C27	120.2 (5)	C14—C38—H38	119.9
C43—C11—H11	119.9	C13—C39—C6	119.9 (3)
C27—C11—H11	119.9	C13—C39—H39	120.0
C41—C12—C29	120.5 (4)	C6—C39—H39	120.0
C41—C12—H12	119.8	C15—C40—C5	118.2 (3)
C29—C12—H12	119.8	C15—C40—P1	119.1 (2)
C39—C13—C38	120.7 (4)	C5—C40—P1	122.7 (3)
C39—C13—H13	119.6	C7—C41—C12	117.1 (4)
C38—C13—H13	119.6	C7—C41—P1	119.4 (3)
C37—C14—C38	118.7 (3)	C12—C41—P1	123.5 (3)
C37—C14—P1	118.3 (2)	C16—C42—C17	120.3 (4)
C38—C14—P1	122.8 (3)	C16—C42—H42	119.8
C40—C15—C16	121.4 (4)	C17—C42—H42	119.8
C40—C15—H15	119.3	C11—C43—C1	118.7 (4)
C16—C15—H15	119.3	C11—C43—Sn1	121.9 (3)
C42—C16—C15	119.3 (4)	C1—C43—Sn1	119.4 (3)
C42—C16—H16	120.3	C3—C44—C4	119.6 (4)
C15—C16—H16	120.3	C3—C44—H44	120.2
C42—C17—C5	120.5 (5)	C4—C44—H44	120.2
C42—C17—H17	119.8	C19—C45—C8	118.5 (3)
C5—C17—H17	119.8	C19—C45—Sn1	118.8 (2)
C45—C19—C4	120.6 (3)	C8—C45—Sn1	122.6 (2)
C45—C19—H19	119.7	C20—C46—C22	118.0 (3)
C4—C19—H19	119.7	C20—C46—Sn1	122.7 (2)
C46—C20—C21	121.0 (4)	C22—C46—Sn1	119.3 (2)

C14—P1—O4—Sn1	178.5 (5)	P1—C14—C37—C6	175.1 (3)
C41—P1—O4—Sn1	−61.9 (6)	C39—C6—C37—C14	0.7 (6)
C40—P1—O4—Sn1	59.2 (5)	C39—C13—C38—C14	0.5 (6)
C44—C3—C8—C45	−1.4 (5)	C37—C14—C38—C13	0.1 (5)
C41—C7—C9—C10	1.0 (9)	P1—C14—C38—C13	−175.5 (3)
C7—C9—C10—C29	−2.3 (9)	C38—C13—C39—C6	−0.5 (6)
O4—P1—C14—C37	28.6 (3)	C37—C6—C39—C13	−0.1 (7)
C41—P1—C14—C37	−94.4 (3)	C16—C15—C40—C5	−1.4 (6)
C40—P1—C14—C37	150.8 (3)	C16—C15—C40—P1	176.7 (3)
O4—P1—C14—C38	−155.8 (3)	C17—C5—C40—C15	1.8 (6)
C41—P1—C14—C38	81.3 (3)	C17—C5—C40—P1	−176.2 (4)
C40—P1—C14—C38	−33.5 (3)	O4—P1—C40—C15	32.3 (3)
C40—C15—C16—C42	0.3 (7)	C14—P1—C40—C15	−89.7 (3)
C40—C5—C17—C42	−1.2 (8)	C41—P1—C40—C15	156.2 (3)
C44—C4—C19—C45	−0.9 (6)	O4—P1—C40—C5	−149.8 (3)
C46—C20—C21—C31	−0.7 (5)	C14—P1—C40—C5	88.3 (3)
C46—C22—C23—C31	−0.5 (6)	C41—P1—C40—C5	−25.9 (4)
O2—C24—C26—C32	−179.1 (5)	C9—C7—C41—C12	0.0 (7)
C35—C24—C26—C32	−0.4 (8)	C9—C7—C41—P1	179.3 (4)
C28—C25—C27—C11	2.2 (10)	C29—C12—C41—C7	0.5 (8)
C43—C11—C27—C25	−0.9 (7)	C29—C12—C41—P1	−178.9 (5)

C27—C25—C28—C1	−2.0 (10)	O4—P1—C41—C7	35.5 (4)
C43—C1—C28—C25	0.6 (8)	C14—P1—C41—C7	157.7 (3)
C9—C10—C29—C12	2.7 (10)	C40—P1—C41—C7	−88.0 (4)
C41—C12—C29—C10	−1.8 (10)	O4—P1—C41—C12	−145.2 (4)
Sn1—O1—C30—O5	−2.7 (4)	C14—P1—C41—C12	−22.9 (4)
Sn1—O1—C30—C35	176.1 (2)	C40—P1—C41—C12	91.3 (4)
C20—C21—C31—C23	1.0 (6)	C15—C16—C42—C17	0.3 (8)
C22—C23—C31—C21	−0.4 (6)	C5—C17—C42—C16	0.2 (9)
C24—C26—C32—C36	−1.0 (9)	C27—C11—C43—C1	−0.5 (6)
C36—C2—C35—C24	−0.2 (6)	C27—C11—C43—Sn1	179.4 (3)
C36—C2—C35—C30	178.3 (4)	C28—C1—C43—C11	0.6 (6)
O2—C24—C35—C2	179.6 (4)	C28—C1—C43—Sn1	−179.3 (3)
C26—C24—C35—C2	0.9 (6)	C8—C3—C44—C4	−0.2 (6)
O2—C24—C35—C30	1.0 (6)	C19—C4—C44—C3	1.3 (6)
C26—C24—C35—C30	−177.6 (4)	C4—C19—C45—C8	−0.8 (5)
O5—C30—C35—C2	175.1 (3)	C4—C19—C45—Sn1	174.7 (3)
O1—C30—C35—C2	−3.7 (5)	C3—C8—C45—C19	1.9 (5)
O5—C30—C35—C24	−6.3 (5)	C3—C8—C45—Sn1	−173.4 (3)
O1—C30—C35—C24	174.8 (3)	C21—C20—C46—C22	−0.1 (5)
C35—C2—C36—C32	−1.1 (8)	C21—C20—C46—Sn1	−178.4 (3)
C26—C32—C36—C2	1.8 (10)	C23—C22—C46—C20	0.7 (5)
C38—C14—C37—C6	−0.7 (6)	C23—C22—C46—Sn1	179.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O5	0.82	1.82	2.546 (4)	147
C8—H8···O5	0.93	2.43	3.071 (4)	126