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Methanoltriphenyl(quinoline-2-carboxylato)tin(IV)

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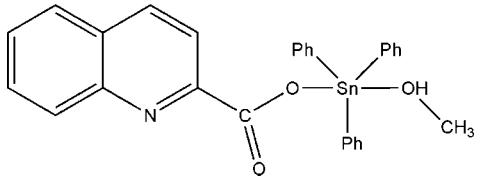
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.029; wR factor = 0.098; data-to-parameter ratio = 14.8.

The Sn atom in the title compound, $[Sn(C_6H_5)_3(C_{10}H_6NO_2)(CH_4O)]$, adopts a distorted SnO_2C_3 trigonal–bipyramidal geometry. The O atom of the carboxylate group occupies one of the axial sites and the O atom of the methanol molecule occupies the other. In the crystal structure, a bifurcated O—H···(O,N) hydrogen bond links adjacent molecules.

Related literature

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



Experimental

Crystal data

$[Sn(C_6H_5)_3(C_{10}H_6NO_2)(CH_4O)]$
M_r = 554.19
Monoclinic, $P2_1/n$
a = 11.1774 (11) Å
b = 14.3964 (12) Å
c = 16.098 (2) Å
β = 93.572 (2)°
V = 2585.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.02 mm^{-1}
T = 298 (2) K
0.54 × 0.46 × 0.45 mm

Data collection

Siemens SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.610, T_{max} = 0.657
12574 measured reflections
4551 independent reflections
3424 reflections with $I > 2\sigma(I)$
R_{int} = 0.040

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.099
S = 1.00
4551 reflections
307 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.90 e Å^{-3}
$\Delta\rho_{min}$ = −0.47 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C17	2.135 (4)	Sn1—C23	2.145 (4)
Sn1—C11	2.138 (4)	Sn1—O3	2.437 (2)
Sn1—O1	2.145 (3)		
O1—Sn1—O3	173.17 (9)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2^{i}	0.82	2.44	3.000 (4)	127
O3—H3···N1^{i}	0.82	2.08	2.827 (4)	151

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

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: HB2644).

References

Ma, C., Li, J., Zhang, R. & Wang, D. (2006). *J. Organomet. Chem.* **691**, 1713–1721.
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  doi:10.1107/S1600536807056851

supplementary materials

Acta Cryst. (2007). E**63**, m2994 [**doi:10.1107/S1600536807056851**]

Methanoltriphenyl(quinoline-2-carboxylato)tin(IV)

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Comment

Organotin esters of carboxylic acids are widely used as biocides, fungicides and homogeneous catalysts. Studies on organotin complexes containing carboxylate ligands with an additional donor atom (*e.g.* N, O or S) that is available for coordinating to the Sn atom have revealed that new structural types may lead to different activities. We have therefore synthesized the title compound, (I), and present its crystal structure here (Fig. 1).

The Sn in (I) atom assumes a trigonal-bipyramidal coordination geometry, formed by three phenyl groups, a monodentate carboxylate group and a coordinated methanol molecule (Table 1). The Sn—O distances in (I) are are close to those in related structures (Ma *et al.*, 2006).

In the crystal of (I), the methanol O—H group makes a bifurcated O—H···(O,*N*) hydrogen bond (Table 2) to the carboxylate O atom and quinoline N atom in an adjacent molecule (Fig. 2).

Experimental

The reaction was carried out under nitrogen atmosphere. Quinaldic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to a solution of methanol (30 ml) in a Schlenk flask and stirred for 0.5 h. Triphenyltin 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) to yield colourless blocks of (I) (yield 83%; m.p. 446 K). Analysis calculated (%) for $C_{29}H_{25}NO_3Sn$: C 62.85; H 4.55; N 2.53. Found: C 62.79; H 4.63; N 2.62%.

Refinement

The H atoms were positioned geometrically (C—H = 0.93–0.96 Å, O—H = 0.82 Å) and refined as riding with U_{iso}(H) = 1.2xU_{eq}(C,*O*) or 1.5U_{eq}(methyl C).

Figures

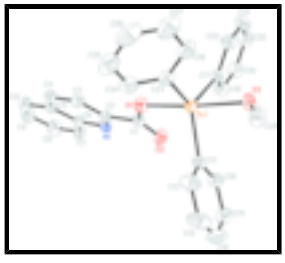

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids. H atoms have been omitted for clarity.

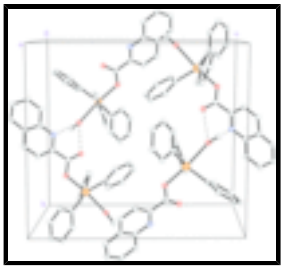

Fig. 2. The unit cell of (I). H atoms have been omitted for clarity. Hydrogen bonds are shown as dashed lines joining the donor and acceptor atoms.

Methanoltriphenyl(quinoline-2-carboxylato)tin(IV)

Crystal data

$[Sn(C_6H_5)_3(C_{10}H_6NO_2)(CH_4O)]$	F_{000} = 1120
M_r = 554.19	D_x = 1.424 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 5687 reflections
a = 11.1774 (11) Å	θ = 2.3–26.9º
b = 14.3964 (12) Å	μ = 1.02 mm^{-1}
c = 16.098 (2) Å	T = 298 (2) K
β = 93.572 (2)º	Block, colourless
V = 2585.3 (5) Å^3	0.54 × 0.46 × 0.45 mm
Z = 4	

Data collection

Siemens SMART CCD diffractometer	4551 independent reflections
Radiation source: fine-focus sealed tube	3424 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.040
T = 298(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 1.9º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −10→13
T_{min} = 0.610, T_{max} = 0.657	k = −17→14
12574 measured reflections	l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.029	H-atom parameters constrained
$wR(F^2)$ = 0.099	$w = 1/[\sigma^2(F_o^2) + (0.0547P)^2 + 0.777P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.00	$(\Delta/\sigma)_{max}$ = 0.002
4551 reflections	$\Delta\rho_{max}$ = 0.90 e Å^{-3}

307 parameters	$\Delta\rho_{min} = -0.47$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.62676 (2)	0.142033 (17)	0.775590 (15)	0.03955 (11)
N1	0.7000 (3)	0.4632 (2)	0.94373 (18)	0.0415 (7)
O1	0.6090 (2)	0.24000 (17)	0.87443 (16)	0.0510 (7)
O2	0.6980 (3)	0.35405 (18)	0.80596 (17)	0.0559 (8)
O3	0.6358 (2)	0.01729 (19)	0.67387 (16)	0.0503 (7)
H3	0.6984	−0.0016	0.6559	0.075*
C1	0.6512 (3)	0.3235 (3)	0.8669 (2)	0.0431 (9)
C2	0.6403 (3)	0.3839 (3)	0.9437 (2)	0.0403 (8)
C3	0.5728 (4)	0.3546 (3)	1.0098 (2)	0.0493 (10)
H3A	0.5318	0.2984	1.0070	0.059*
C4	0.5685 (4)	0.4104 (3)	1.0787 (2)	0.0546 (11)
H4	0.5237	0.3925	1.1227	0.066*
C5	0.6322 (4)	0.4953 (3)	1.0825 (2)	0.0504 (10)
C6	0.6972 (3)	0.5194 (3)	1.0128 (2)	0.0425 (9)
C7	0.7603 (4)	0.6051 (3)	1.0128 (3)	0.0577 (11)
H7	0.8037	0.6215	0.9676	0.069*
C8	0.7567 (5)	0.6632 (4)	1.0797 (3)	0.0735 (14)
H8	0.7976	0.7194	1.0795	0.088*
C9	0.6926 (5)	0.6395 (4)	1.1484 (3)	0.0734 (14)
H9	0.6911	0.6804	1.1931	0.088*
C10	0.6328 (4)	0.5583 (3)	1.1510 (3)	0.0657 (13)
H10	0.5917	0.5432	1.1976	0.079*
C11	0.5416 (3)	0.2169 (3)	0.6736 (2)	0.0453 (9)
C12	0.4221 (4)	0.2014 (3)	0.6513 (3)	0.0710 (13)
H12	0.3772	0.1629	0.6838	0.085*
C13	0.3681 (5)	0.2434 (4)	0.5801 (4)	0.098 (2)
H13	0.2873	0.2331	0.5659	0.118*
C14	0.4336 (6)	0.2999 (4)	0.5309 (3)	0.0874 (17)
H14	0.3980	0.3261	0.4826	0.105*
C15	0.5488 (5)	0.3167 (4)	0.5531 (3)	0.0766 (15)
H15	0.5926	0.3559	0.5206	0.092*
C16	0.6043 (4)	0.2762 (3)	0.6241 (3)	0.0585 (11)
H16	0.6844	0.2892	0.6385	0.070*
C17	0.8172 (3)	0.1293 (3)	0.7900 (2)	0.0421 (9)
C18	0.8935 (3)	0.2035 (3)	0.7736 (2)	0.0506 (10)
H18	0.8609	0.2591	0.7533	0.061*
C19	1.0165 (4)	0.1954 (4)	0.7871 (3)	0.0637 (12)
H19	1.0654	0.2451	0.7747	0.076*
C20	1.0673 (4)	0.1157 (4)	0.8184 (3)	0.0686 (13)
H20	1.1500	0.1117	0.8282	0.082*
C21	0.9949 (4)	0.0407 (4)	0.8356 (3)	0.0689 (13)

H21	1.0291	−0.0139	0.8567	0.083*
C22	0.8711 (4)	0.0474 (3)	0.8210 (3)	0.0572 (11)
H22	0.8233	−0.0034	0.8321	0.069*
C23	0.5185 (4)	0.0463 (3)	0.8402 (2)	0.0472 (10)
C24	0.4280 (4)	0.0796 (4)	0.8874 (3)	0.0631 (12)
H24	0.4131	0.1431	0.8895	0.076*
C25	0.3593 (4)	0.0181 (5)	0.9317 (3)	0.0863 (17)
H25	0.2980	0.0405	0.9627	0.104*
C26	0.3825 (6)	−0.0759 (5)	0.9295 (4)	0.097 (2)
H26	0.3369	−0.1169	0.9590	0.117*
C27	0.4729 (7)	−0.1092 (4)	0.8837 (4)	0.099 (2)
H27	0.4890	−0.1725	0.8830	0.119*
C28	0.5397 (5)	−0.0493 (3)	0.8388 (3)	0.0719 (14)
H28	0.5997	−0.0727	0.8072	0.086*
C29	0.5361 (4)	−0.0265 (3)	0.6299 (3)	0.0616 (12)
H29A	0.4684	−0.0262	0.6638	0.092*
H29B	0.5566	−0.0895	0.6171	0.092*
H29C	0.5163	0.0066	0.5791	0.092*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.04301 (18)	0.03095 (17)	0.04461 (17)	−0.00319 (11)	0.00217 (11)	0.00156 (11)
N1	0.0432 (18)	0.0352 (18)	0.0464 (17)	−0.0011 (14)	0.0049 (14)	−0.0061 (14)
O1	0.0639 (18)	0.0323 (15)	0.0577 (16)	−0.0089 (13)	0.0118 (13)	−0.0063 (12)
O2	0.077 (2)	0.0455 (18)	0.0469 (16)	−0.0086 (14)	0.0153 (15)	−0.0054 (13)
O3	0.0460 (16)	0.0493 (17)	0.0560 (16)	−0.0015 (12)	0.0073 (12)	−0.0165 (13)
C1	0.044 (2)	0.036 (2)	0.049 (2)	0.0019 (17)	0.0013 (18)	−0.0047 (18)
C2	0.046 (2)	0.031 (2)	0.044 (2)	0.0039 (16)	0.0027 (17)	0.0016 (16)
C3	0.060 (3)	0.037 (2)	0.052 (2)	−0.0028 (18)	0.0107 (19)	0.0076 (19)
C4	0.065 (3)	0.054 (3)	0.047 (2)	0.004 (2)	0.016 (2)	0.007 (2)
C5	0.061 (3)	0.048 (3)	0.043 (2)	0.011 (2)	0.0046 (19)	−0.0029 (19)
C6	0.044 (2)	0.039 (2)	0.045 (2)	0.0043 (17)	0.0054 (17)	−0.0040 (17)
C7	0.065 (3)	0.047 (3)	0.062 (3)	−0.010 (2)	0.013 (2)	−0.018 (2)
C8	0.075 (3)	0.063 (3)	0.082 (4)	−0.010 (3)	0.003 (3)	−0.023 (3)
C9	0.092 (4)	0.068 (4)	0.061 (3)	0.004 (3)	0.002 (3)	−0.027 (3)
C10	0.083 (3)	0.070 (3)	0.046 (2)	0.009 (3)	0.013 (2)	−0.010 (2)
C11	0.049 (2)	0.036 (2)	0.051 (2)	0.0026 (17)	−0.0009 (18)	−0.0014 (18)
C12	0.054 (3)	0.065 (3)	0.091 (4)	−0.002 (2)	−0.009 (2)	0.011 (3)
C13	0.067 (4)	0.096 (5)	0.126 (5)	0.007 (3)	−0.044 (4)	0.000 (4)
C14	0.112 (5)	0.077 (4)	0.069 (3)	0.018 (4)	−0.031 (3)	0.004 (3)
C15	0.099 (4)	0.076 (4)	0.055 (3)	0.014 (3)	0.007 (3)	0.012 (3)
C16	0.061 (3)	0.055 (3)	0.059 (3)	0.001 (2)	0.002 (2)	0.010 (2)
C17	0.044 (2)	0.044 (2)	0.0381 (19)	0.0039 (17)	0.0000 (16)	−0.0055 (17)
C18	0.047 (2)	0.047 (3)	0.057 (2)	−0.0047 (19)	−0.0012 (18)	−0.005 (2)
C19	0.051 (3)	0.069 (3)	0.070 (3)	−0.009 (2)	0.000 (2)	−0.007 (3)
C20	0.045 (3)	0.090 (4)	0.069 (3)	0.009 (3)	−0.006 (2)	−0.012 (3)
C21	0.067 (3)	0.067 (3)	0.071 (3)	0.024 (3)	−0.008 (2)	−0.001 (3)

C22	0.063 (3)	0.045 (3)	0.063 (3)	0.002 (2)	−0.003 (2)	0.000 (2)
C23	0.056 (2)	0.043 (2)	0.042 (2)	−0.0148 (18)	−0.0002 (18)	0.0018 (17)
C24	0.052 (3)	0.069 (3)	0.068 (3)	−0.008 (2)	0.003 (2)	0.010 (2)
C25	0.056 (3)	0.126 (5)	0.078 (3)	−0.019 (3)	0.013 (3)	0.021 (4)
C26	0.124 (5)	0.089 (5)	0.079 (4)	−0.058 (4)	0.010 (4)	0.022 (4)
C27	0.168 (7)	0.058 (3)	0.072 (4)	−0.042 (4)	0.022 (4)	0.006 (3)
C28	0.122 (4)	0.041 (3)	0.055 (3)	−0.016 (3)	0.021 (3)	0.003 (2)
C29	0.055 (3)	0.070 (3)	0.059 (3)	−0.011 (2)	0.000 (2)	−0.020 (2)

Geometric parameters (Å, °)

Sn1—C17	2.135 (4)	C13—H13	0.9300
Sn1—C11	2.138 (4)	C14—C15	1.337 (7)
Sn1—O1	2.145 (3)	C14—H14	0.9300
Sn1—C23	2.145 (4)	C15—C16	1.394 (6)
Sn1—O3	2.437 (2)	C15—H15	0.9300
N1—C2	1.323 (5)	C16—H16	0.9300
N1—C6	1.376 (4)	C17—C22	1.402 (5)
O1—C1	1.299 (4)	C17—C18	1.402 (5)
O2—C1	1.222 (4)	C18—C19	1.384 (6)
O3—C29	1.430 (4)	C18—H18	0.9300
O3—H3	0.8200	C19—C20	1.362 (7)
C1—C2	1.522 (5)	C19—H19	0.9300
C2—C3	1.407 (5)	C20—C21	1.387 (7)
C3—C4	1.372 (6)	C20—H20	0.9300
C3—H3A	0.9300	C21—C22	1.393 (6)
C4—C5	1.414 (6)	C21—H21	0.9300
C4—H4	0.9300	C22—H22	0.9300
C5—C6	1.417 (5)	C23—C24	1.387 (6)
C5—C10	1.427 (6)	C23—C28	1.398 (6)
C6—C7	1.421 (5)	C24—C25	1.397 (7)
C7—C8	1.366 (6)	C24—H24	0.9300
C7—H7	0.9300	C25—C26	1.379 (8)
C8—C9	1.397 (7)	C25—H25	0.9300
C8—H8	0.9300	C26—C27	1.373 (9)
C9—C10	1.349 (7)	C26—H26	0.9300
C9—H9	0.9300	C27—C28	1.374 (7)
C10—H10	0.9300	C27—H27	0.9300
C11—C12	1.379 (6)	C28—H28	0.9300
C11—C16	1.388 (6)	C29—H29A	0.9600
C12—C13	1.399 (7)	C29—H29B	0.9600
C12—H12	0.9300	C29—H29C	0.9600
C13—C14	1.378 (8)		
C17—Sn1—C11	121.34 (15)	C12—C13—H13	119.7
C17—Sn1—O1	96.50 (12)	C15—C14—C13	119.3 (5)
C11—Sn1—O1	100.43 (13)	C15—C14—H14	120.3
C17—Sn1—C23	118.77 (15)	C13—C14—H14	120.3
C11—Sn1—C23	117.28 (15)	C14—C15—C16	121.1 (5)
O1—Sn1—C23	88.95 (13)	C14—C15—H15	119.4

C17—Sn1—O3	85.81 (11)	C16—C15—H15	119.4
C11—Sn1—O3	83.72 (12)	C11—C16—C15	120.8 (4)
O1—Sn1—O3	173.17 (9)	C11—C16—H16	119.6
C23—Sn1—O3	84.31 (12)	C15—C16—H16	119.6
C2—N1—C6	118.1 (3)	C22—C17—C18	117.1 (4)
C1—O1—Sn1	119.2 (2)	C22—C17—Sn1	121.0 (3)
C29—O3—Sn1	126.5 (2)	C18—C17—Sn1	121.9 (3)
C29—O3—H3	109.5	C19—C18—C17	121.0 (4)
Sn1—O3—H3	123.7	C19—C18—H18	119.5
O2—C1—O1	125.7 (4)	C17—C18—H18	119.5
O2—C1—C2	120.4 (3)	C20—C19—C18	121.1 (4)
O1—C1—C2	113.9 (3)	C20—C19—H19	119.4
N1—C2—C3	123.5 (3)	C18—C19—H19	119.4
N1—C2—C1	115.3 (3)	C19—C20—C21	119.6 (4)
C3—C2—C1	121.2 (3)	C19—C20—H20	120.2
C4—C3—C2	118.9 (4)	C21—C20—H20	120.2
C4—C3—H3A	120.6	C20—C21—C22	119.9 (4)
C2—C3—H3A	120.6	C20—C21—H21	120.1
C3—C4—C5	119.9 (4)	C22—C21—H21	120.1
C3—C4—H4	120.1	C21—C22—C17	121.3 (4)
C5—C4—H4	120.1	C21—C22—H22	119.4
C4—C5—C6	117.3 (3)	C17—C22—H22	119.4
C4—C5—C10	124.1 (4)	C24—C23—C28	118.6 (4)
C6—C5—C10	118.6 (4)	C24—C23—Sn1	119.8 (3)
N1—C6—C5	122.3 (3)	C28—C23—Sn1	121.6 (3)
N1—C6—C7	118.3 (3)	C23—C24—C25	120.3 (5)
C5—C6—C7	119.4 (4)	C23—C24—H24	119.9
C8—C7—C6	119.5 (4)	C25—C24—H24	119.9
C8—C7—H7	120.2	C26—C25—C24	119.9 (5)
C6—C7—H7	120.2	C26—C25—H25	120.1
C7—C8—C9	121.1 (5)	C24—C25—H25	120.1
C7—C8—H8	119.5	C27—C26—C25	120.2 (5)
C9—C8—H8	119.5	C27—C26—H26	119.9
C10—C9—C8	121.0 (4)	C25—C26—H26	119.9
C10—C9—H9	119.5	C26—C27—C28	120.3 (6)
C8—C9—H9	119.5	C26—C27—H27	119.8
C9—C10—C5	120.4 (4)	C28—C27—H27	119.8
C9—C10—H10	119.8	C27—C28—C23	120.8 (5)
C5—C10—H10	119.8	C27—C28—H28	119.6
C12—C11—C16	117.8 (4)	C23—C28—H28	119.6
C12—C11—Sn1	119.7 (3)	O3—C29—H29A	109.5
C16—C11—Sn1	122.3 (3)	O3—C29—H29B	109.5
C11—C12—C13	120.3 (5)	H29A—C29—H29B	109.5
C11—C12—H12	119.9	O3—C29—H29C	109.5
C13—C12—H12	119.9	H29A—C29—H29C	109.5
C14—C13—C12	120.6 (5)	H29B—C29—H29C	109.5
C14—C13—H13	119.7		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2^{i}	0.82	2.44	3.000 (4)	127
O3—H3···N1^{i}	0.82	2.08	2.827 (4)	151

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

Fig. 1

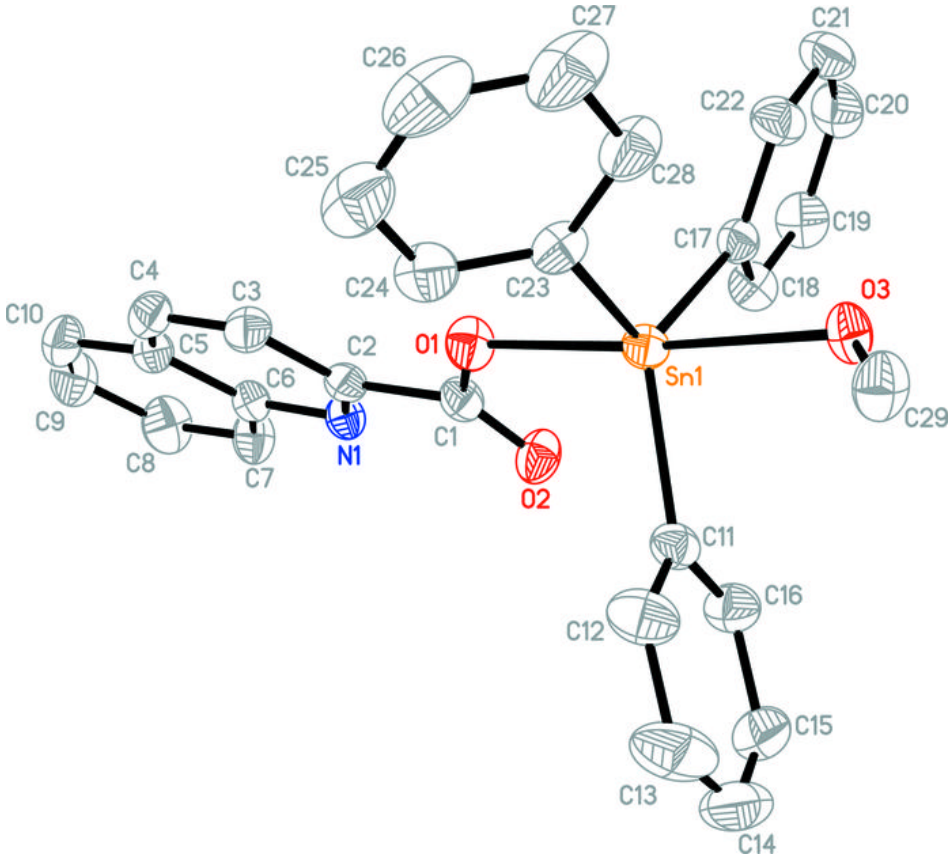
C27
C21
C26
C22
C20
C25
C28
C19
C17
C4
C24
C23
C18
O3
C10
C3
O1
C2
C5
Sn1
C6
C29
C9
C1
N1
C8
C7
O2
C11
C16
C12
C15
C13
C14

Fig. 2