

## catena-Poly[[tri-*n*-butyltin(IV)]- $\mu$ -pyridine-3-carboxylato- $\kappa^2$ N:O]

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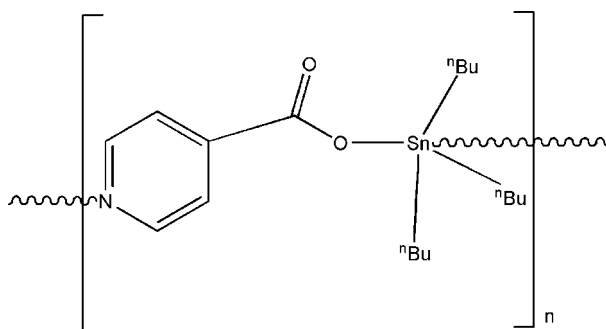
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Key indicators: single-crystal X-ray study;  $T = 298$  K; mean  $\sigma(\text{C}-\text{C}) = 0.020$  Å; disorder in main residue;  $R$  factor = 0.058;  $wR$  factor = 0.163; data-to-parameter ratio = 14.9.

The asymmetric unit of the title compound,  $[\text{Sn}(\text{C}_4\text{H}_9)_3(\text{C}_6\text{H}_4\text{NO}_2)]_n$ , consists of three butyl and one pyridine-3-carboxylate groups bonded to the Sn atom in a distorted trigonal-bipyramidal geometry. In the crystal structure, these units are linked to form an infinite one-dimensional polymeric chain structure. In one *n*-butyl chain three C atoms are disordered over two sites, and in another two C atoms are disordered over two sites.

### Related literature

For bond-length data, see: Allen *et al.* (1987). For general background, see: Gielen *et al.* (1988). For related literature, see: Ma *et al.* (2004).



### Experimental

#### Crystal data

$[\text{Sn}(\text{C}_4\text{H}_9)_3(\text{C}_6\text{H}_4\text{NO}_2)]$   
 $M_r = 412.13$   
 Monoclinic,  $Cc$   
 $a = 9.594$  (4) Å

$b = 24.286$  (11) Å  
 $c = 9.715$  (4) Å  
 $\beta = 114.864$  (5)°  
 $V = 2053.7$  (15) Å<sup>3</sup>

$Z = 4$   
 Mo  $K\alpha$  radiation  
 $\mu = 1.25$  mm<sup>-1</sup>

$T = 298$  (2) K  
 $0.53 \times 0.46 \times 0.41$  mm

#### Data collection

Bruker SMART CCD area-detector diffractometer  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.529$ ,  $T_{\max} = 0.597$

5123 measured reflections  
 3260 independent reflections  
 2741 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.037$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.058$   
 $wR(F^2) = 0.163$   
 $S = 1.00$   
 3260 reflections  
 219 parameters  
 H-atom parameters constrained

$\Delta\rho_{\max} = 1.41$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.73$  e Å<sup>-3</sup>  
 Absolute structure: Flack (1983),  
 1798 Friedel pairs  
 Flack parameter: 0.06 (10)

**Table 1**

Selected geometric parameters (Å, °).

Sn1—C11	2.099 (12)	Sn1—N1 <sup>i</sup>	2.603 (16)
Sn1—C15	2.112 (13)	Sn1—O2	3.186 (9)
Sn1—C7	2.127 (13)		
C11—Sn1—C15	124.9 (5)	O1—Sn1—N1 <sup>i</sup>	179.1 (8)
C11—Sn1—C7	116.3 (6)	C11—Sn1—O2	80.8 (4)
C15—Sn1—C7	116.4 (6)	C15—Sn1—O2	73.3 (4)
C11—Sn1—O1	97.9 (5)	C7—Sn1—O2	135.2 (4)
C15—Sn1—O1	95.9 (6)	O1—Sn1—O2	44.1 (3)
C7—Sn1—O1	91.2 (5)	N1 <sup>i</sup> —Sn1—O2	136.2 (3)
C11—Sn1—N1 <sup>i</sup>	81.4 (5)	C6—O1—Sn1	120.1 (9)
C15—Sn1—N1 <sup>i</sup>	85.0 (6)	C6—O2—Sn1	70.8 (7)
C7—Sn1—N1 <sup>i</sup>	88.5 (5)		

 Symmetry code: (i)  $x, y, z - 1$ .

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); 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: HK2268).

### References

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**supplementary materials**

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## ***catena*-Poly[[tri-*n*-butyltin(IV)]- $\mu$ -pyridine-3-carboxylato- $\kappa^2$ N:O]**

**T.-D. Li and H.-Y. You**

### **Comment**

Self-assembled organotin derivatives of carboxylic acid ligands have been extensively studied due to their biological activities as well as their industrial and agricultural applications (Gielen *et al.*, 1988). pyridine-3-carboxylic acid is a good bridging ligand that can sometimes be used to generate unexpected and interesting coordination polymers, and small changes in experimental conditions can lead to very different architectures.

The asymmetric unit of the title compound, (I), (Fig. 1), consists of three butyl and one (pyridine-3-carboxylate) groups bonded to the tin atom, where the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987).

The tin atom has a distorted trigonal bipyramidal geometry with atoms O1 and N1<sup>i</sup> of the pyridine-3-carboxylic acid [symmetry code: (i)  $x, y, z - 1$ ], in axial and C atoms of the three butyl groups in equatorial positions, as in the similar compound (Ma *et al.*, 2004).

In the crystal structure, (Fig. 2), the molecules are linked to form an infinite one-dimensional polymeric chain structure.

### **Experimental**

For the preparation of the title compound, a mixture of tri-*n*-butyltin oxide (596.1 mg, 2 mmol) and pyridine-3-carboxylic acid (246.2 mg, 2 mmol), in methanol (80 ml) was heated under reflux for 12 h. The resulting clear solution was evaporated under vacuum. The product was crystallized from ethanol (yield; 446.3 mg, 82%, m.p. 398 K).

### **Refinement**

When the crystal structure was solved, the atoms C9, C10, C12, C13 and C14 were found to be disordered. During the refinement process, the occupancies of C9, C12 and C14 were kept fixed as C9 = 1/4, C9' = 3/4, C12 = 1/2, C12' = 1/2, C14 = 0.50 and C14' = 1/2, while the remainings were refined as C10 = 0.39 (3), C10' = 0.61 (3), C13 = 0.39 (3) and C13' = 0.61 (3). H atoms were positioned geometrically, with C—H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H atoms, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C})$ , where  $x = 1.5$  for methyl H, and  $x = 1.2$  for all other H atoms.

## Figures

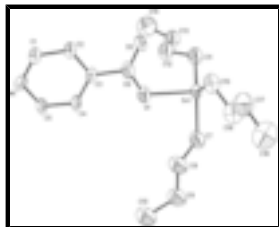


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

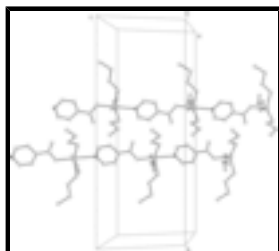


Fig. 2. A packing diagram for (I). H atoms have been omitted for clarity.

## *catena*-Poly[[tri-*n*-butyltin(IV)]- $\mu$ -pyridine-3-carboxylato- $\kappa^2$ N:O]

### Crystal data

[Sn(C<sub>4</sub>H<sub>9</sub>)<sub>3</sub>(C<sub>6</sub>H<sub>4</sub>NO<sub>2</sub>)]

$M_r = 412.13$

Monoclinic, *Cc*

Hall symbol: -C 2yc

$a = 9.594 (4) \text{ \AA}$

$b = 24.286 (11) \text{ \AA}$

$c = 9.715 (4) \text{ \AA}$

$\beta = 114.864 (5)^\circ$

$V = 2053.7 (15) \text{ \AA}^3$

$Z = 4$

$F_{000} = 848$

$D_x = 1.333 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 3313 reflections

$\theta = 2.3\text{--}28.1^\circ$

$\mu = 1.25 \text{ mm}^{-1}$

$T = 298 (2) \text{ K}$

Block, colorless

$0.53 \times 0.46 \times 0.41 \text{ mm}$

### Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 298(2) \text{ K}$

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{\min} = 0.529$ ,  $T_{\max} = 0.597$

5123 measured reflections

3260 independent reflections

2741 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.037$

$\theta_{\max} = 25.0^\circ$

$\theta_{\min} = 2.5^\circ$

$h = -11 \rightarrow 9$

$k = -28 \rightarrow 22$

$l = -11 \rightarrow 11$

Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.058$	$w = 1/[\sigma^2(F_o^2) + (0.1189P)^2 + 1.6655P]$
$wR(F^2) = 0.163$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{\max} = 0.001$
3260 reflections	$\Delta\rho_{\max} = 1.41 \text{ e } \text{\AA}^{-3}$
219 parameters	$\Delta\rho_{\min} = -0.73 \text{ e } \text{\AA}^{-3}$
Primary atom site location: structure-invariant direct methods	Extinction correction: none
Secondary atom site location: difference Fourier map	Absolute structure: Flack (1983), 1798 Friedel pairs
	Flack parameter: 0.06 (10)

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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.5451 (3)	0.87521 (2)	0.0427 (3)	0.0500 (2)	
O1	0.5354 (16)	0.8687 (4)	0.2610 (13)	0.062 (3)	
O2	0.6522 (12)	0.9490 (3)	0.3408 (10)	0.076 (2)	
N1	0.552 (2)	0.8833 (5)	0.779 (2)	0.064 (4)	
C1	0.6275 (15)	0.9254 (5)	0.7557 (12)	0.065 (2)	
H1	0.6718	0.9504	0.8346	0.078*	
C2	0.6459 (14)	0.9350 (5)	0.6238 (12)	0.062 (2)	
H2	0.7027	0.9648	0.6157	0.074*	
C3	0.5757 (14)	0.8981 (5)	0.5027 (12)	0.0552 (18)	
C4	0.4984 (13)	0.8535 (5)	0.5264 (13)	0.061 (2)	
H4	0.4544	0.8273	0.4504	0.073*	
C5	0.4862 (16)	0.8476 (5)	0.6631 (13)	0.0630 (19)	
H5	0.4310	0.8180	0.6754	0.076*	
C6	0.5913 (15)	0.9068 (5)	0.3591 (14)	0.0663 (19)	
C7	0.4511 (18)	0.7949 (5)	-0.0192 (16)	0.083 (2)	
H7A	0.3408	0.7973	-0.0520	0.100*	
H7B	0.4688	0.7830	-0.1058	0.100*	

## supplementary materials

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C8	0.5117 (19)	0.7515 (5)	0.1005 (18)	0.095 (3)	
H8A	0.5009	0.7646	0.1899	0.114*	
H8B	0.6206	0.7471	0.1279	0.114*	
C9	0.4371 (19)	0.6958 (5)	0.0598 (17)	0.098 (3)	0.25
H9A	0.4865	0.6747	0.0081	0.118*	0.25
H9B	0.3298	0.7003	-0.0094	0.118*	0.25
C10	0.448 (6)	0.6638 (16)	0.200 (4)	0.109 (7)	0.39 (3)
H10A	0.3992	0.6286	0.1697	0.163*	0.39 (3)
H10B	0.3973	0.6842	0.2508	0.163*	0.39 (3)
H10C	0.5539	0.6587	0.2683	0.163*	0.39 (3)
C9'	0.4371 (19)	0.6958 (5)	0.0598 (17)	0.098 (3)	0.75
H9'1	0.4335	0.6853	-0.0380	0.118*	0.75
H9'2	0.3318	0.6993	0.0476	0.118*	0.75
C10'	0.512 (4)	0.6492 (11)	0.170 (3)	0.097 (6)	0.61 (3)
H10D	0.4552	0.6158	0.1314	0.145*	0.61 (3)
H10E	0.5113	0.6578	0.2665	0.145*	0.61 (3)
H10F	0.6156	0.6445	0.1825	0.145*	0.61 (3)
C11	0.3914 (15)	0.9411 (6)	-0.0442 (16)	0.081 (2)	
H11A	0.4521	0.9740	-0.0354	0.097*	
H11B	0.3323	0.9344	-0.1517	0.097*	
C12	0.2810 (15)	0.9542 (7)	0.0208 (16)	0.089 (2)	0.50
H12A	0.3310	0.9779	0.1084	0.107*	0.50
H12B	0.2525	0.9204	0.0554	0.107*	0.50
C13	0.133 (3)	0.983 (2)	-0.093 (3)	0.091 (4)	0.39 (3)
H13A	0.1627	1.0105	-0.1486	0.109*	0.39 (3)
H13B	0.0701	0.9560	-0.1654	0.109*	0.39 (3)
C14	0.0394 (19)	1.0105 (8)	-0.025 (2)	0.132 (4)	0.50
H14A	-0.0556	1.0228	-0.1043	0.198*	0.50
H14B	0.0944	1.0415	0.0340	0.198*	0.50
H14C	0.0182	0.9849	0.0391	0.198*	0.50
C12'	0.2810 (15)	0.9542 (7)	0.0208 (16)	0.089 (2)	0.50
H12C	0.3371	0.9558	0.1303	0.107*	0.50
H12D	0.2086	0.9240	-0.0024	0.107*	0.50
C13'	0.188 (3)	1.0082 (10)	-0.032 (4)	0.092 (3)	0.61 (3)
H13C	0.2511	1.0382	0.0284	0.110*	0.61 (3)
H13D	0.1719	1.0150	-0.1366	0.110*	0.61 (3)
C14'	0.0394 (19)	1.0105 (8)	-0.025 (2)	0.132 (4)	0.50
H14D	-0.0082	1.0454	-0.0624	0.198*	0.50
H14E	0.0537	1.0059	0.0782	0.198*	0.50
H14F	-0.0253	0.9815	-0.0862	0.198*	0.50
C15	0.7867 (15)	0.8816 (5)	0.1302 (18)	0.079 (2)	
H15A	0.8117	0.9151	0.0910	0.095*	
H15B	0.8272	0.8854	0.2395	0.095*	
C16	0.8680 (14)	0.8340 (6)	0.0944 (18)	0.094 (3)	
H16A	0.8338	0.8310	-0.0145	0.112*	
H16B	0.8429	0.7999	0.1309	0.112*	
C17	1.0445 (14)	0.8435 (7)	0.1717 (19)	0.100 (3)	
H17A	1.0681	0.8768	0.1306	0.121*	
H17B	1.0756	0.8493	0.2794	0.121*	

C18	1.1349 (18)	0.7980 (8)	0.152 (3)	0.128 (6)
H18A	1.2424	0.8056	0.2075	0.192*
H18B	1.1118	0.7941	0.0459	0.192*
H18C	1.1095	0.7645	0.1884	0.192*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn1	0.0625 (4)	0.0587 (3)	0.0297 (3)	0.0009 (5)	0.0204 (2)	0.0023 (4)
O1	0.068 (6)	0.075 (6)	0.046 (7)	-0.003 (4)	0.027 (5)	-0.001 (4)
O2	0.117 (7)	0.073 (5)	0.060 (5)	-0.028 (5)	0.058 (5)	-0.003 (4)
N1	0.086 (9)	0.067 (7)	0.052 (9)	-0.011 (6)	0.041 (8)	-0.019 (6)
C1	0.088 (4)	0.071 (4)	0.043 (4)	-0.006 (4)	0.035 (3)	-0.004 (3)
C2	0.084 (4)	0.066 (4)	0.042 (4)	-0.007 (4)	0.032 (3)	-0.002 (3)
C3	0.077 (4)	0.058 (4)	0.039 (4)	0.000 (3)	0.034 (3)	-0.005 (3)
C4	0.083 (4)	0.073 (4)	0.040 (4)	-0.012 (3)	0.039 (4)	-0.007 (4)
C5	0.086 (4)	0.075 (4)	0.042 (4)	-0.013 (4)	0.040 (3)	-0.002 (3)
C6	0.082 (4)	0.077 (4)	0.050 (3)	0.002 (3)	0.038 (3)	0.007 (3)
C7	0.096 (5)	0.087 (5)	0.070 (4)	-0.007 (4)	0.038 (4)	0.009 (4)
C8	0.103 (6)	0.085 (5)	0.086 (6)	-0.006 (5)	0.029 (5)	0.016 (5)
C9	0.110 (5)	0.090 (5)	0.085 (5)	-0.005 (4)	0.032 (4)	0.012 (4)
C10	0.115 (11)	0.099 (10)	0.099 (11)	-0.004 (10)	0.032 (10)	0.018 (10)
C9'	0.110 (5)	0.090 (5)	0.085 (5)	-0.005 (4)	0.032 (4)	0.012 (4)
C10'	0.110 (10)	0.101 (10)	0.086 (9)	-0.004 (9)	0.048 (8)	0.013 (9)
C11	0.090 (4)	0.092 (4)	0.068 (4)	0.016 (4)	0.041 (4)	0.014 (4)
C12	0.097 (4)	0.100 (4)	0.076 (4)	0.019 (4)	0.042 (4)	0.009 (4)
C13	0.099 (6)	0.104 (6)	0.077 (6)	0.018 (6)	0.043 (5)	0.010 (5)
C14	0.131 (7)	0.132 (7)	0.107 (7)	0.018 (6)	0.025 (6)	0.012 (6)
C12'	0.097 (4)	0.100 (4)	0.076 (4)	0.019 (4)	0.042 (4)	0.009 (4)
C13'	0.098 (6)	0.104 (6)	0.080 (6)	0.018 (5)	0.043 (5)	0.011 (5)
C14'	0.131 (7)	0.132 (7)	0.107 (7)	0.018 (6)	0.025 (6)	0.012 (6)
C15	0.078 (4)	0.097 (5)	0.069 (5)	0.001 (4)	0.037 (4)	0.007 (4)
C16	0.087 (5)	0.109 (6)	0.086 (6)	0.002 (5)	0.038 (5)	0.005 (5)
C17	0.089 (6)	0.121 (7)	0.092 (7)	-0.002 (6)	0.039 (6)	0.001 (6)
C18	0.097 (9)	0.156 (12)	0.119 (11)	-0.003 (9)	0.033 (9)	-0.021 (10)

Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )

Sn1—C11	2.099 (12)	C10—H10C	0.9600
Sn1—C15	2.112 (13)	C10'—H10D	0.9600
Sn1—C7	2.127 (13)	C10'—H10E	0.9600
Sn1—O1	2.167 (12)	C10'—H10F	0.9600
Sn1—N1 <sup>i</sup>	2.603 (16)	C11—C12	1.477 (13)
Sn1—O2	3.186 (9)	C11—H11A	0.9700
O1—C6	1.274 (13)	C11—H11B	0.9700
O2—C6	1.230 (12)	C12—C13	1.550 (17)
N1—C1	1.322 (19)	C12—H12A	0.9700
N1—C5	1.347 (18)	C12—H12B	0.9700

## supplementary materials

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C1—C2	1.385 (15)	C13—C14	1.480 (18)
C1—H1	0.9300	C13—H13A	0.9700
C2—C3	1.405 (15)	C13—H13B	0.9700
C2—H2	0.9300	C13'—H13C	0.9700
C3—C4	1.386 (16)	C13'—H13D	0.9700
C3—C6	1.479 (15)	C14—H14A	0.9600
C4—C5	1.388 (15)	C14—H14B	0.9600
C4—H4	0.9300	C14—H14C	0.9600
C5—H5	0.9300	C15—C16	1.514 (14)
C7—C8	1.494 (14)	C15—H15A	0.9700
C7—H7A	0.9700	C15—H15B	0.9700
C7—H7B	0.9700	C16—C17	1.554 (14)
C8—C9	1.504 (14)	C16—H16A	0.9700
C8—H8A	0.9700	C16—H16B	0.9700
C8—H8B	0.9700	C17—C18	1.468 (15)
C9—C10	1.535 (18)	C17—H17A	0.9700
C9—H9A	0.9700	C17—H17B	0.9700
C9—H9B	0.9700	C18—H18A	0.9600
C10—H10A	0.9600	C18—H18B	0.9600
C10—H10B	0.9600	C18—H18C	0.9600
C11—Sn1—C15	124.9 (5)	H10A—C10—H10B	109.5
C11—Sn1—C7	116.3 (6)	C9—C10—H10C	109.5
C15—Sn1—C7	116.4 (6)	H10A—C10—H10C	109.5
C11—Sn1—O1	97.9 (5)	H10B—C10—H10C	109.5
C15—Sn1—O1	95.9 (6)	H10D—C10'—H10E	109.5
C7—Sn1—O1	91.2 (5)	H10D—C10'—H10F	109.5
C11—Sn1—N1 <sup>i</sup>	81.4 (5)	H10E—C10'—H10F	109.5
C15—Sn1—N1 <sup>i</sup>	85.0 (6)	C12—C11—Sn1	120.1 (9)
C7—Sn1—N1 <sup>i</sup>	88.5 (5)	C12—C11—H11A	107.3
O1—Sn1—N1 <sup>i</sup>	179.1 (8)	Sn1—C11—H11A	107.3
C11—Sn1—O2	80.8 (4)	C12—C11—H11B	107.3
C15—Sn1—O2	73.3 (4)	Sn1—C11—H11B	107.3
C7—Sn1—O2	135.2 (4)	H11A—C11—H11B	106.9
O1—Sn1—O2	44.1 (3)	C11—C12—C13	113.4 (12)
N1 <sup>i</sup> —Sn1—O2	136.2 (3)	C11—C12—H12A	108.9
C6—O1—Sn1	120.1 (9)	C13—C12—H12A	108.9
C6—O2—Sn1	70.8 (7)	C11—C12—H12B	108.9
C1—N1—C5	117.1 (14)	C13—C12—H12B	108.9
N1—C1—C2	125.2 (12)	H12A—C12—H12B	107.7
N1—C1—H1	117.4	C14—C13—C12	115.6 (17)
C2—C1—H1	117.4	C14—C13—H13A	108.4
C1—C2—C3	117.7 (11)	C12—C13—H13A	108.4
C1—C2—H2	121.2	C14—C13—H13B	108.4
C3—C2—H2	121.2	C12—C13—H13B	108.4
C4—C3—C2	117.4 (10)	H13A—C13—H13B	107.4
C4—C3—C6	122.8 (10)	H13C—C13'—H13D	107.3
C2—C3—C6	119.7 (10)	C13—C14—H14A	109.5
C3—C4—C5	120.4 (11)	C13—C14—H14B	109.5



C3—C4—H4	119.8	H14A—C14—H14B	109.5
C5—C4—H4	119.8	C13—C14—H14C	109.5
N1—C5—C4	122.1 (12)	H14A—C14—H14C	109.5
N1—C5—H5	119.0	H14B—C14—H14C	109.5
C4—C5—H5	119.0	C16—C15—Sn1	115.8 (9)
O2—C6—O1	125.0 (12)	C16—C15—H15A	108.3
O2—C6—C3	119.9 (11)	Sn1—C15—H15A	108.3
O1—C6—C3	115.1 (10)	C16—C15—H15B	108.3
C8—C7—Sn1	116.5 (10)	Sn1—C15—H15B	108.3
C8—C7—H7A	108.2	H15A—C15—H15B	107.4
Sn1—C7—H7A	108.2	C15—C16—C17	109.7 (11)
C8—C7—H7B	108.2	C15—C16—H16A	109.7
Sn1—C7—H7B	108.2	C17—C16—H16A	109.7
H7A—C7—H7B	107.3	C15—C16—H16B	109.7
C7—C8—C9	116.3 (12)	C17—C16—H16B	109.7
C7—C8—H8A	108.2	H16A—C16—H16B	108.2
C9—C8—H8A	108.2	C18—C17—C16	114.1 (13)
C7—C8—H8B	108.2	C18—C17—H17A	108.7
C9—C8—H8B	108.2	C16—C17—H17A	108.7
H8A—C8—H8B	107.4	C18—C17—H17B	108.7
C8—C9—C10	112.0 (16)	C16—C17—H17B	108.7
C8—C9—H9A	109.2	H17A—C17—H17B	107.6
C10—C9—H9A	109.2	C17—C18—H18A	109.5
C8—C9—H9B	109.2	C17—C18—H18B	109.5
C10—C9—H9B	109.2	H18A—C18—H18B	109.5
H9A—C9—H9B	107.9	C17—C18—H18C	109.5
C9—C10—H10A	109.5	H18A—C18—H18C	109.5
C9—C10—H10B	109.5	H18B—C18—H18C	109.5

Symmetry codes: (i)  $x, y, z-1$ .

Fig. 1

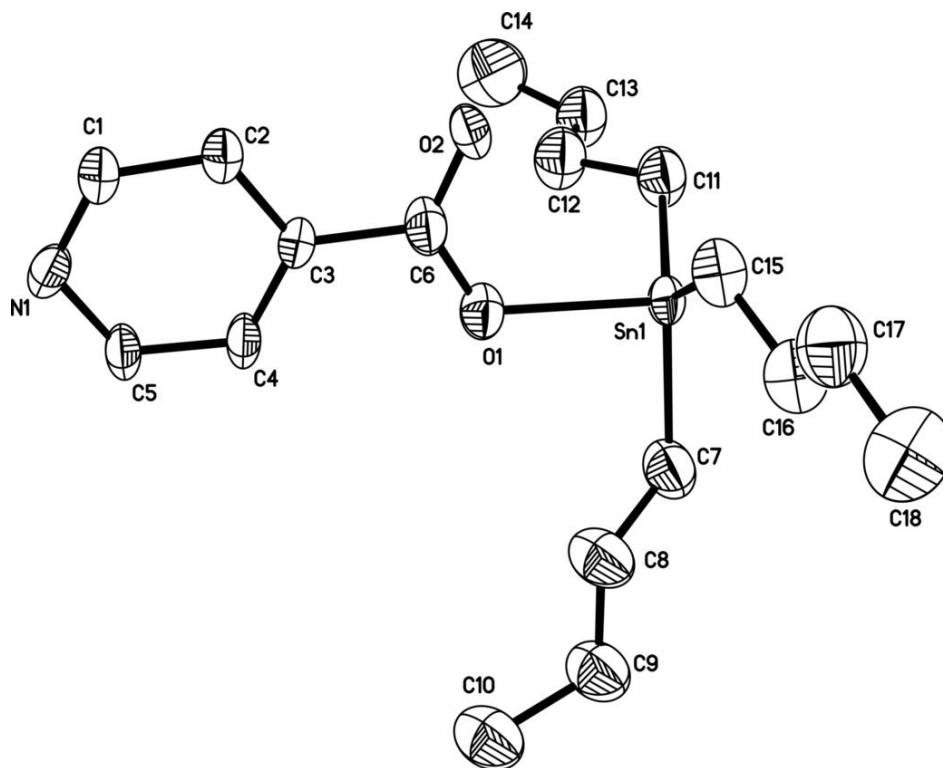


Fig. 2

