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catena-Poly[[triphenyltin(IV)]-μ-6-oxo-1,6-dihydropyridine-3-carboxylato]

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The title compound, $[Sn(C_6H_5)_3(C_6H_4NO_3)]$, possesses an infinite chain structure. The SnO_2C_3 centre has distorted trigonal–bipyramidal geometry with the O atoms in the apical positions. A strong intermolecular N—H···O hydrogen bond results in the formation of double chains.

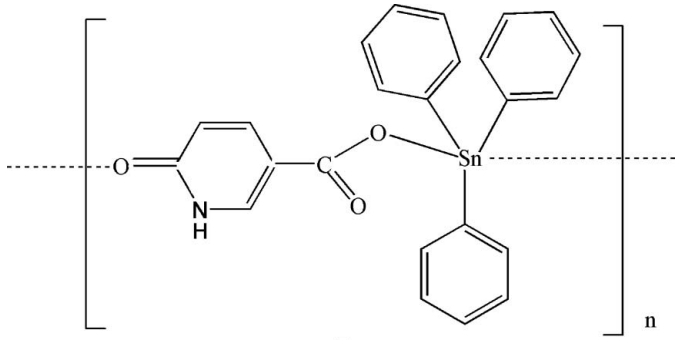
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.027
wR factor = 0.071
Data-to-parameter ratio = 14.3

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

The title compound, (I) (Fig. 1), possesses an infinite one-dimensional chain structure arising from Sn—O bridges to the 6-hydroxy-3-pyridinecarboxylate ligand, one of which is substantially longer than the other (Table 1).



(I)

The Sn atom has distorted trigonal–bipyramidal geometry, with atoms O1 and O3^{i} [symmetry code: (i) $x, y-1, z$] in axial positions [O1—Sn1—O3^{i} = 175.31 (9)°] and the C atoms of the three phenyl groups in equatorial positions. The sum of the equatorial C—Sn—C angles is 359.2°, indicating approximate coplanarity for these atoms. The SnO_2C_3 geometry in (I) is similar to those seen previously in related compounds (Xie *et al.*, 1991).

A strong intermolecular N—H···O hydrogen bond (Table 2) between the NH group of the pyridine ring and the non-coordinated O2 atom of a nearby carboxylate group results in the formation of a double chain parallel to *b* (Fig. 2).

Experimental

A mixture of triphenyltin oxide (1.4322 g, 2.0 mmol) and 6-hydroxynicotinic acid (0.5564 g, 4.0 mmol) in methanol (80 ml) was heated under reflux for 8 h. The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/ethanol (1:1) to yield blocks of (I). Yield 1.3862 g, 71%, m.p. 483 K. Analysis calculated for $C_{24}H_{19}NO_3Sn$: C 59.05, H 3.92, N 2.87%; found: C 59.02, H 3.96, N 2.91%.

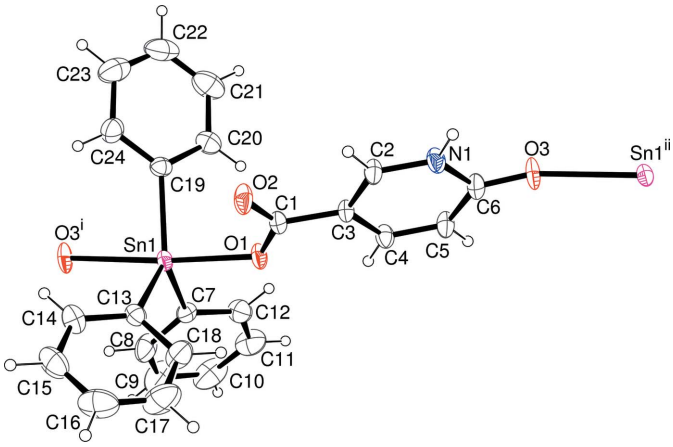


Figure 1
The molecular structure of (I), with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry codes: (i) $x, y-1, z$; (ii) $x, y+1, z$.]

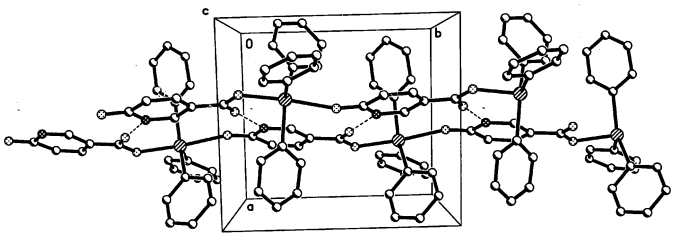


Figure 2
Part of a double chain in (I), with the N···O hydrogen-bond contacts shown by dashed lines. H atoms have been omitted for clarity.

Crystal data

$[Sn(C_6H_5)_3(C_6H_4NO_3)]$
$M_r = 488.09$
Monoclinic, $P2_1/c$
$a = 9.5629$ (17) Å
$b = 10.6579$ (19) Å
$c = 21.353$ (4) Å
$\beta = 101.155$ (3)°
$V = 2135.2$ (7) Å^3
$Z = 4$
$D_x = 1.518$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5143 reflections
$\theta = 2.2$–$27.8°$
$\mu = 1.22$ mm^{-1}
$T = 298$ (2) K
Block, colourless
0.49 × 0.46 × 0.41 mm

Data collection

Bruker SMART CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
$T_{min} = 0.586$, $T_{max} = 0.635$
10839 measured reflections
3755 independent reflections
3053 reflections with $I > 2\sigma(I)$
$R_{int} = 0.041$
$\theta_{max} = 25.0°$
$h = -9 \rightarrow 11$
$k = -12 \rightarrow 12$
$l = -24 \rightarrow 25$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.071$
$S = 1.00$
3755 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.034P)^2 + 0.6145P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.52$ e Å^{-3}
$\Delta\rho_{min} = -0.47$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C19	2.133 (3)	Sn1—O3^{i}	2.356 (2)
Sn1—C13	2.134 (3)	C1—O1	1.292 (4)
Sn1—C7	2.137 (3)	C1—O2	1.233 (4)
Sn1—O1	2.150 (2)		
C19—Sn1—C13	130.80 (12)	C7—Sn1—O1	90.01 (10)
C19—Sn1—C7	115.76 (12)	C19—Sn1—O3^{i}	83.52 (11)
C13—Sn1—C7	112.63 (12)	C13—Sn1—O3^{i}	87.84 (11)
C19—Sn1—O1	92.09 (10)	C7—Sn1—O3^{i}	90.42 (10)
C13—Sn1—O1	96.30 (11)	O1—Sn1—O3^{i}	175.31 (9)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{ii}	0.86	1.95	2.785 (4)	165

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

H atoms were positioned geometrically [N—H = 0.86 Å and C—H = 0.93 Å] and refined as riding with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

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: *SHELXTL*.

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