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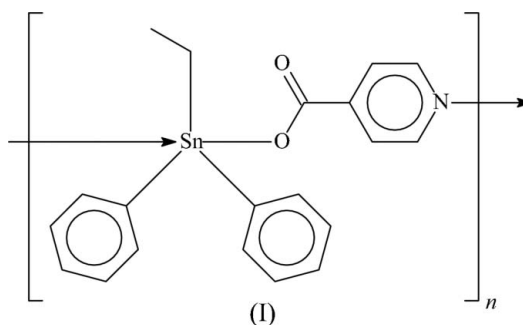
Key indicators

Single-crystal X-ray study
 $T = 173\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
Disorder in main residue
 R factor = 0.028
 wR factor = 0.089
Data-to-parameter ratio = 18.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[ethylidiphenyltin(IV)]- μ -isonicotinato- $\kappa^2\text{O:N}$]**In the title compound, $[\text{Sn}(\text{C}_2\text{H}_5)(\text{C}_6\text{H}_5)_2(\text{C}_6\text{H}_4\text{NO}_2)]_n$, the isonicotinate group functions in an N,O-bridging mode to link adjacent triorganotin groups into an infinite chain. The metal centre shows SnC_3NO trigonal-bipyramidal coordination, with the N and O atoms in axial positions.

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Comment

This study continues our work on carboxylic acid derivatives of ethyldiphenyltin(IV). The previous study (Amini *et al.*, 2006) described the chloroacetate derivative, which exists as a carboxylate-bridged chain compound. The carboxylic acid used in the present study is isonicotinic acid. This acid was also used in the synthesis of the triphenyltin derivative, reported by Ng & Kumar Das (1992); its crystal structure features bridging through the carboxylate O and pyridyl N atoms, to give rise to a zig-zag chain structure. The dative $\text{Sn}-\text{N}$ bond is, however, relatively long [2.582 (3) Å], so that the geometry about Sn is severely distorted.In the title compound, (I), replacing the phenyl group by an ethyl group leads to no significant difference in the SnC_3NO trigonal-bipyramidal coordination environment (Table 1; Fig. 1). The compound adopts a linear bridged motif, and the $\text{Sn}-\text{N}$ bond is similarly weak [2.546 (2) Å]. The very different carboxylate $\text{C}15-\text{O}1$ and $\text{C}15-\text{O}2$ bond lengths in (I) imply charge localisation for this group.

Experimental

Ethyldiphenyltin iodide was prepared by the method of Davison & Rakita (1970). This reagent (0.86 g, 2 mmol) was then treated with sodium isopropoxide (0.16 g, 2 mmol) in propan-2-ol (20 ml) to give ethyldiphenyltin isopropoxide and sodium iodide. The sodium iodide precipitate was removed by filtration. Isonicotinic acid (0.24 g, 2 mmol) was added to the filtrate and evaporation of the solvent gave a white solid, which was purified by recrystallization from a dichloromethane-methanol (1:1 v/v) mixture at 278 K to furnish colourless crystals of (I) (m.p. >573 K).

Crystal data

[Sn(C ₂ H ₅)(C ₆ H ₅) ₂ (C ₆ H ₄ NO ₂)]	$V = 912.97 (2) \text{ \AA}^3$
$M_r = 424.05$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.543 \text{ Mg m}^{-3}$
$a = 9.7562 (1) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.9711 (1) \text{ \AA}$	$\mu = 1.41 \text{ mm}^{-1}$
$c = 10.2908 (1) \text{ \AA}$	$T = 173 (2) \text{ K}$
$\alpha = 78.990 (1)^\circ$	Plate, colourless
$\beta = 77.066 (1)^\circ$	$0.38 \times 0.20 \times 0.10 \text{ mm}$
$\gamma = 70.622 (1)^\circ$	

Data collection

Bruker APEXII CCD area-detector diffractometer	13345 measured reflections
φ and ω scans	4146 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	3983 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.616$, $T_{\max} = 0.872$	$R_{\text{int}} = 0.029$
	$\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.061P)^2 + 0.7851P]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.089$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.12$	$\Delta\rho_{\text{max}} = 2.36 \text{ e \AA}^{-3}$
4146 reflections	$\Delta\rho_{\text{min}} = -1.10 \text{ e \AA}^{-3}$
227 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Sn1—C1	2.155 (3)	Sn1—O1	2.212 (2)
Sn1—C7	2.186 (3)	C15—O1	1.313 (3)
Sn1—C13	2.168 (3)	C15—O2	1.243 (3)
Sn1—N1 ⁱ	2.546 (2)		
C1—Sn1—C7	107.9 (1)	C7—Sn1—O1	95.5 (1)
C1—Sn1—C13	120.8 (1)	C7—Sn1—N1 ⁱ	89.1 (1)
C1—Sn1—O1	89.3 (1)	C13—Sn1—O1	93.6 (1)
C1—Sn1—N1 ⁱ	88.2 (1)	C13—Sn1—N1 ⁱ	84.2 (1)
C7—Sn1—C13	130.5 (1)	N1 ⁱ —Sn1—O1	175.3 (1)

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

The terminal C atom of the ethyl group is disordered over two sites, C14 and C14', in a 0.54 (1):0.46 (1) population ratio. The C13—C14 and C13—C14' distances were restrained to be within 0.01 \AA of each other. H atoms were placed in calculated positions, with C—H = 0.93–0.97 \AA , and were refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. The largest difference peak and deepest difference hole are within 1 \AA of Sn1.

Data collection: SMART (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve

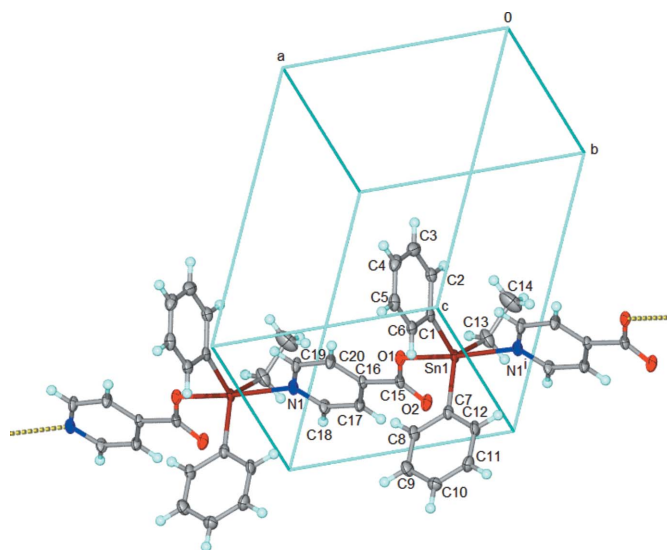


Figure 1

A view of part of the polymeric chain in (I) that runs along [100]. Displacement ellipsoids are drawn at the 70% probability level and H atoms are shown as spheres of arbitrary radii. The minor disorder component is not shown. [Symmetry code: (i) $x - 1, y, z$.]

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: SHELXL97.

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