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Aqua(2-chloronicotinato)triphenyltin(IV)

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The title complex, $[Sn(C_6H_5)_3(C_6H_3ClNO_2)(H_2O)]$, is five-coordinate with a distorted trigonal–bipyramidal geometry in the solid state. The O atom of the carboxylate group occupies one of the axial sites and the O atom of the water molecule occupies the other. Water H atoms are involved in an intermolecular hydrogen-bonded network with the uncoordinated carboxylate O atom and the pyridine N atom; the interactions lead to two types of rings.

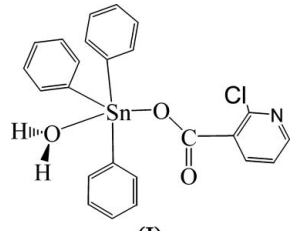
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.031
wR factor = 0.091
Data-to-parameter ratio = 14.5

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

Comment

Organotin esters of carboxylic acids are widely used as biocides, as fungicides and in industry as 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.



(I)

The crystal structure of (I) is shown in Fig. 1. The complex assumes trigonal bipyramidal coordination geometry, formed by three phenyl groups, a monodentate carboxylate group and a coordinated water molecule. The Sn1···O2 distance is 3.201 (3) Å, showing no significant interaction between the two atoms.

In the crystal structure, the water O atoms are linked to adjacent carboxylate O atoms and adjacent N atoms of the pyridine ring *via* O—H···O and O—H···N hydrogen bonds, respectively (Table 2). These interactions form two types of rings (one consists of two coordinated water molecules and two
2-chloronicotinate groups, the other consists of four coordinated water molecules, four 2-chloronicotinate groups and four tin groups) (Fig. 2) and lead to a two-dimensional network.

Experimental

$(C_6H_5)_3SnOH$ (2 mmol) and 2-chloronicotinic acid (2 mmol) were added to dry benzene (30 ml). The mixture was then heated under reflux with stirring for 5 h and the solvent was removed by

evaporation *in vacuo*. The crude adduct was recrystallized from dichloromethane and colourless crystals suitable for X-ray diffraction were obtained (m.p. 403 K). Analysis calculated for $C_{24}H_{20}ClNO_3Sn$: C 54.95, H 3.84, N 2.67%; found: C 54.84, H 3.90, 2.65%.

Crystal data

$[Sn(C_6H_5)_3(C_6H_3ClNO_2)(H_2O)]$	D_x = 1.562 Mg m^{-3}
M_r = 524.55	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 4754 reflections
a = 10.328 (3) Å	θ = 2.3–27.3°
b = 13.861 (3) Å	μ = 1.29 mm^{-1}
c = 15.628 (4) Å	T = 298 (2) K
β = 94.198 (3)°	Block, colourless
V = 2231.2 (10) Å^3	0.53 × 0.41 × 0.37 mm
Z = 4	

Data collection

Siemens SMART CCD area-detector diffractometer	3938 independent reflections
	3128 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.038
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	θ_{max} = 25.0°
	$h = -12 \rightarrow 12$
T_{min} = 0.548, T_{max} = 0.647	$k = -16 \rightarrow 12$
11356 measured reflections	$l = -18 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0479P)^2 + 1.6414P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.031	
$wR(F^2)$ = 0.091	
S = 1.00	$(\Delta/\sigma)_{max} < 0.001$
3938 reflections	$\Delta\rho_{max}$ = 0.77 e Å^{-3}
271 parameters	$\Delta\rho_{min}$ = −0.41 e Å^{-3}
H-atom parameters constraineds treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Sn1—C7	2.122 (4)	Sn1—O1	2.190 (3)
Sn1—C13	2.133 (4)	Sn1—O3	2.370 (3)
Sn1—C19	2.139 (4)		
C7—Sn1—C13	117.42 (16)	C19—Sn1—O1	95.33 (13)
C7—Sn1—C19	131.29 (16)	C7—Sn1—O3	82.45 (13)
C13—Sn1—C19	110.17 (15)	C13—Sn1—O3	87.95 (13)
C7—Sn1—O1	94.27 (13)	C19—Sn1—O3	89.63 (13)
C13—Sn1—O1	90.27 (13)	O1—Sn1—O3	175.03 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H25···O2^{i}	0.82	1.91	2.720 (4)	168
O3—H26···N1^{ii}	0.85	1.99	2.848 (5)	177

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

The water H atoms were refined subject to an O—H distance restraint of 0.85 (2) Å. All other H atoms were placed geometrically and treated as riding on their parent atoms, with C—H distances of 0.93 Å. The U_{iso}(H) values were set at 1.2U_{eq}(C,O).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

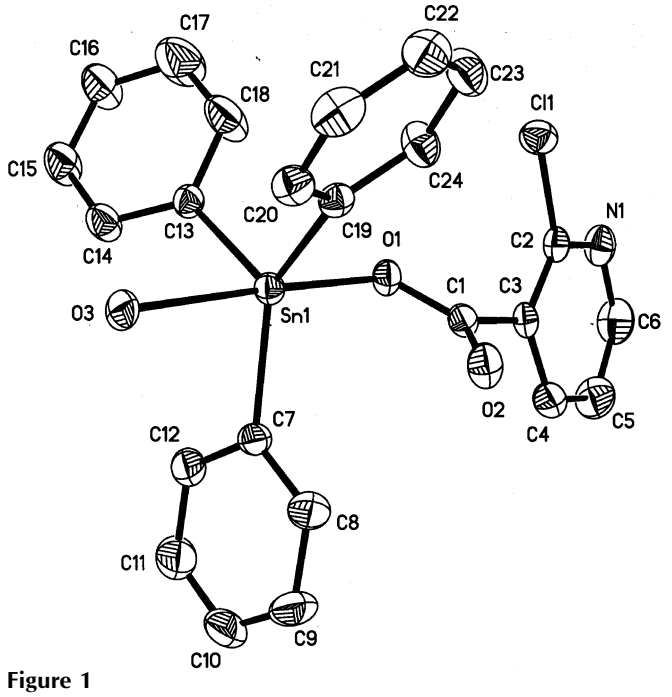


Figure 1
The structure of the title complex (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. H atoms have been omitted for clarity.

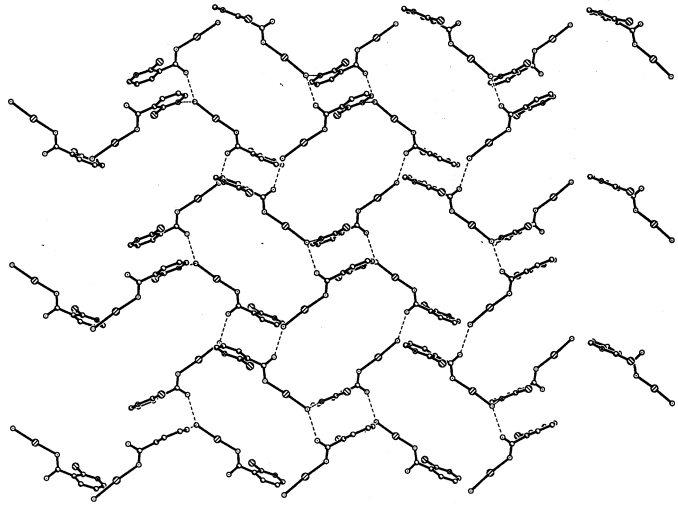


Figure 2
Crystal packing of the title complex. H atoms and phenyl groups have been omitted for clarity. Hydrogen bonds are shown as dashed lines.

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