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(2-Amino-5-nitrobenzoato)triphenyltin(IV)

Yip Foo Win,[a] Siang-Guan Teoh,[a] Latiffah Zakaria,[b] Shea-Lin Ng[c] and Hoong-Kun Fun[c]*

[a]School of Chemical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, [b]School of Bioogical Sciences, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [c] X-ray Crystallography Unit, School of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia

Correspondence e-mail: hkfun@usm.my

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Key indicators

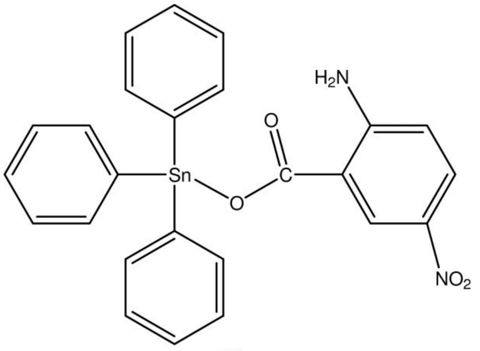
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.033
wR factor = 0.071
Data-to-parameter ratio = 33.4

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

In the title compound, [Sn(C_6H_5)$_3$($C_7H_5N_2O_4$)], the nitro and amino groups are coplanar with the attached benzene ring. The molecules are linked by intermolecular N—H⋯O interactions, forming one-dimensional chains along [010]. In addition, the crystal structure is further stabilized by intermolecular C—H⋯π and π–π interactions.

Comment

Triorganotin(IV) complexes are reported to exhibit antimicrobial and antitumour properties as well as being noted for their significance in industrial applications (Willem *et al.*, 1997; Novelli *et al.*, 1999; Gielen *et al.*, 2000). In general, triphenyltin(IV) carboxylate complexes exist as monomeric structures with four-coordinate distorted tetrahedral or five-coordinate trigonal–bipyramidal geometries (Baul *et al.*, 2001; Yeap & Teoh, 2003; Win, Guan, Ismail *et al.*, 2006). However, (2-chloro-5-aminobenzoato)triphenyltin(IV) was found to exist as a five-coordinate polymeric structure with a linkage of the amino group to an adjacent tin atom and bridging of the carboxylate anion to two neighbouring Sn atoms (Yeap & Teoh, 2003). However, the title compound, (2-amino-5-nitrobenzoato)triphenyltin(IV), (I), is found to exist as a monomeric structure even though the amino group is attached in the *ortho*-position to the benzoate group, as is the case in (2-amino-5-nitrobenzoato)triphenyl(IV).



(I)

Bond lengths and angles in (I) (Fig. 1) have normal values (Allen *et al.*, 1987) and agree well with those found in related structures (Ng *et al.*, 1991; Win, Guan, Ismail *et al.*, 2006; Win, Guan & Yamin, 2006). The nitro group at C4 and amino goup at C1 are coplanar with the attached ring, with torsion angles O3—N2—C4—C3 = 2.0 (2)° and N1—C1—C6—C7 = −0.2 (2)°.

The intramolecular C5—H5*A*⋯O1, N1—H1*B*⋯O2 and C9—H9*A*⋯O2 interactions (Table 2 and Fig. 1) generate

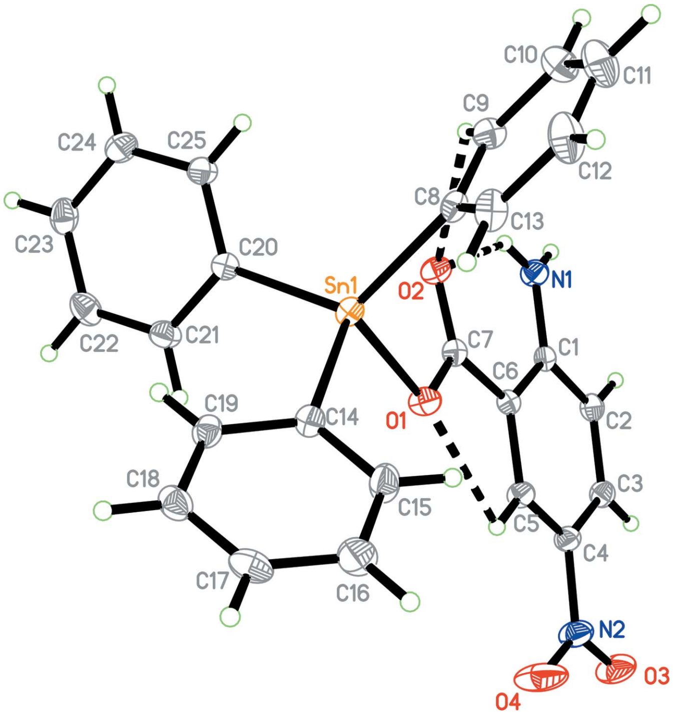


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed lines indicate intramolecular hydrogen bonds.

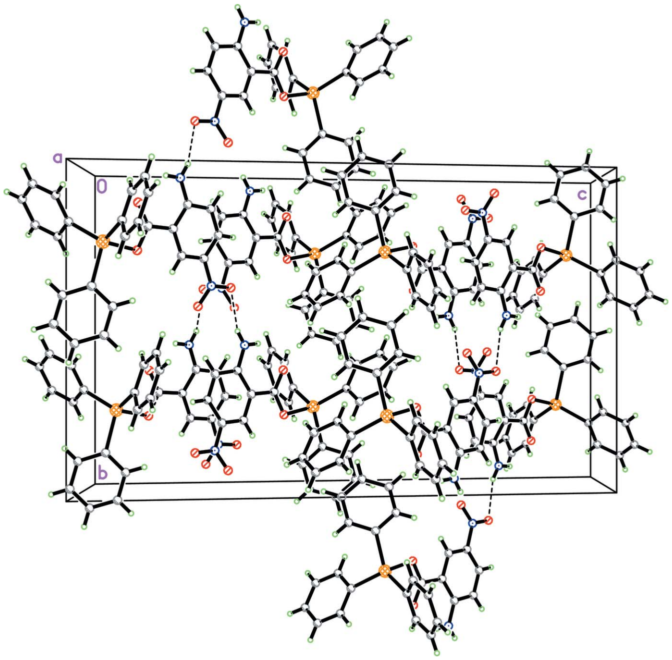


Figure 2
The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

S(5), *S*(6) and *S*(7) ring motifs, respectively (Bernstein *et al.*, 1995). In the crystal structure, the molecules form a one-dimensional chain along the [010] direction by intermolecular N1—H1*A*···O3^{i} interactions (Fig. 2). The crystal packing is stabilized by intermolecular C—H···π interactions involving the C1–C6 (centroid *Cg*1), C8–C13 (centroid *Cg*2), C14–C19 (centroid *Cg*3) and C20–C25 (centroid *Cg*4) benzene rings (Table 2). In addition, the crystal packing is further stabilized by weak intermolecular π–π interactions involving the C1–C6 ring at (x, y, z) and its symmetry equivalent at ($-x$, y, $\frac{1}{2} - z$); the centroid–centroid distance is 3.7260 (9) Å.

Experimental

The complex (2-amino-5-nitrobenzoato)triphenyltin(IV) was obtained by heating under reflux a 1:1 molar mixture of triphenyltin(IV) hydroxide (0.73 g, 2 mmol) and 2-amino-5-nitrobenzoic acid (0.36 g, 2 mmol) in methanol (60 ml) for an hour. A clear yellowish transparent solution was isolated by filtration and kept in a bottle. After 6 days, some yellowish crystals (0.51 g, 96% yield) were obtained (m.p. 481.5–481.9 K. Analysis found for $C_{25}H_{20}N_2O_4Sn_1$: C, 56.41; H, 3.48; N, 5.23; Sn, 22.03%. Calculated for $C_{25}H_{20}N_2O_4Sn_1$: C, 56.53; H, 3.80; N, 5.27; Sn, 22.35%. FTIR from a KBr disc (cm^{-1}): ν(COO)$_{as}$ 1618, ν(COO)$_{s}$ 1310, ν(O—Sn—O) 641, ν(Sn—O) 443. ^{13}C-NMR: δ: phenyl carbons C$_{ipso}$ 142.87 (839.31 Hz), C$_{ortho}$ 136.11 (45.60 Hz), C$_{meta}$ 128.43, C$_{para}$ 129.03 (18.37 Hz); benzene 112.77, 115.75, 127.72, 127.97, 134.89, 155.92; COO 169.52 p.p.m.. ^{119}Sn-NMR: δ: −265.89 p.p.m..

Crystal data

$[Sn(C_6H_5)_3(C_7H_5N_2O_4)]$
$M_r = 531.12$
Monoclinic, $C2/c$
$a = 11.0062\ (4)$ Å
$b = 15.8022\ (4)$ Å
$c = 26.5645\ (8)$ Å
$\beta = 101.415\ (2)°$
$V = 4528.8\ (2)$ Å^3

$Z = 8$
$D_x = 1.558$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.16$ mm^{-1}
$T = 100.0\ (1)$ K
Block, yellow
0.76 × 0.73 × 0.40 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.482$, $T_{max} = 0.657$

47389 measured reflections
9913 independent reflections
9343 reflections with $I > 2\sigma(I)$
$R_{int} = 0.029$
$\theta_{max} = 35.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.071$
$S = 1.24$
9913 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0165P)^2 + 9.0039P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.50$ e Å^{-3}
$\Delta\rho_{min} = -1.18$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.0774 (11)	Sn1—C8	2.1230 (15)
Sn1—C20	2.1224 (15)	Sn1—C14	2.1264 (15)
O1—Sn1—C20	108.88 (5)	O1—Sn1—C14	97.53 (5)
O1—Sn1—C8	106.21 (5)	C20—Sn1—C14	109.30 (6)
C20—Sn1—C8	120.75 (5)		

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1B\cdots O2$	0.84 (2)	2.03 (2)	2.681 (2)	134 (2)
$C5-H5A\cdots O1$	0.93	2.40	2.725 (2)	101
$C9-H9A\cdots O2$	0.93	2.46	3.073 (2)	124
$N1-H1A\cdots O3^{i}$	0.83 (3)	2.25 (3)	3.058 (2)	162 (2)
$C3-H3A\cdots Cg2^{ii}$	0.93	2.77	3.616 (2)	152
$C12-H12A\cdots Cg1^{iii}$	0.93	3.13	3.823 (2)	133
$C13-H13A\cdots Cg4^{iv}$	0.93	3.10	3.661 (2)	120
$C17-H17A\cdots Cg4^{v}$	0.93	3.15	3.804 (2)	129
$C19-H19A\cdots Cg2^{iv}$	0.93	3.00	3.681 (2)	131
$C25-H25A\cdots Cg3^{iv}$	0.93	2.88	3.544 (2)	129

Symmetry codes: (i) $-x-\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, y, -z+\frac{1}{2}$; (iii) $x+1, y, z$; (iv) $-x+\frac{1}{2}, -y+\frac{1}{2}, -z$; (v) $x+\frac{1}{2}, y+\frac{1}{2}, z$. *Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of the C1–C6, C8–C13, C14–C19 and C20–C25 rings, respectively.

The H atoms on N were located in a difference map and refined isotropically, with N—H = 0.84 (3)Å. The remaining H atoms were positional geometrically and refined as riding, with C—H = 0.93Å and $U_{iso}(H) = 1.2U_{eq}(C)$. The deepest hole in the final difference map is 0.61 Å from atom Sn1.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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