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(3-Amino-4-chlorobenzoato)trimethyltin(IV)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.015
wR factor = 0.038
Data-to-parameter ratio = 17.6

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

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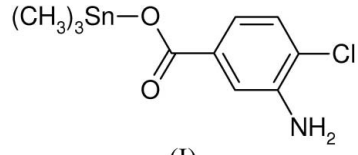
In the title compound, $[Sn(CH_3)_3(C_7H_5ClNO_2)]$, the Sn atom is bonded to three methyl groups and one O atom in a distorted tetrahedral geometry, with Sn—C bond lengths of 2.118 (2)–2.119 (2) Å and an Sn—O bond length of 2.0804 (12) Å.

Comment

In view of our interest in the synthesis, characterization, biological applications and crystal structures of organotin carboxylates (Danish *et al.*, 1995; Parvez *et al.*, 2002; Sadiq-ur-Rehman *et al.*, 2006), we have synthesized a new organotin(IV) carboxylate of 4-chloro-3-aminobenzoic acid, the title compound, (I).



(I)

In compound (I) (Fig. 1), atom Sn1 is bonded to three methyl groups with essentially identical Sn—C distances, comparable with the values reported for the related structure $(C_{16}H_{13}O_3)Sn(CH_3)_3$ (Tahir *et al.*, 1997). The coordination geometry around Sn1 is distorted tetrahedral (Table 1).

The crystal structure of (I) contains centrosymmetric dimers formed *via* intermolecular N—H···O hydrogen bonds (Fig. 2, Table 2).

Experimental

The sodium salt of 4-chloro-3-aminobenzoic acid (0.194 g, 1 mmol) and trimethyltin chloride (0.199 g, 1 mmol) were suspended in dry toluene (150 ml) in a two-necked round-bottomed flask equipped with a water condenser. The mixture was refluxed for 8–10 h, the NaCl formed was filtered off, and the solvent was removed on a rotary evaporator under reduced pressure. The solid product was recrystallized from chloroform to obtain colourless crystals of (I) (yield 70%; m.p. 403–406 K).

Crystal data

$[Sn(CH_3)_3(C_7H_5ClNO_2)]$
M_r = 334.36
Monoclinic, $P2_1/c$
a = 11.9077 (7) Å
b = 9.1237 (5) Å
c = 12.6554 (7) Å
β = 113.086 (1)°
V = 1264.80 (12) Å^3
Z = 4
D_x = 1.756 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 2.21 mm^{-1}
T = 100 (2) K
Block, colourless
0.40 × 0.30 × 0.30 mm

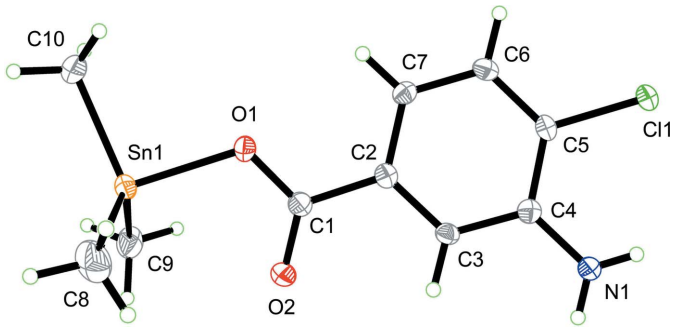


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as spheres of arbitrary radii.

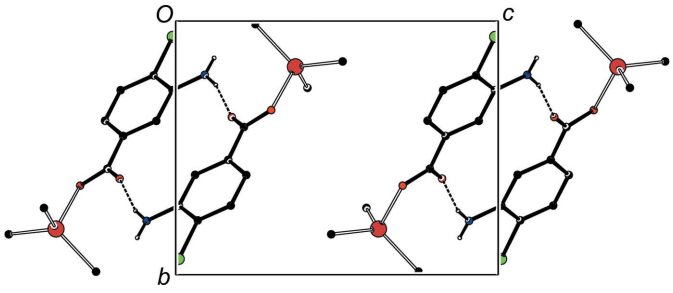


Figure 2
Centrosymmetric dimers formed through intermolecular hydrogen bonding (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity.

Data collection

Bruker SMART APEX CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.435, T_{max} = 0.515
9722 measured reflections
2586 independent reflections
2528 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.038
S = 1.11
2586 reflections
147 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0146P)^2 + 0.9615P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.005
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.0804 (12)	Sn1—C9	2.119 (2)
Sn1—C8	2.118 (2)	Sn1—C10	2.119 (2)
O1—Sn1—C8	102.26 (7)	O1—Sn1—C9	106.60 (6)
O1—Sn1—C10	96.02 (6)	C8—Sn1—C9	118.66 (9)
C8—Sn1—C10	115.55 (9)	C10—Sn1—C9	113.69 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H2N···O2^{i}	0.83 (2)	2.14 (2)	2.947 (2)	166 (2)

Symmetry code: (i) $-x+2, -y+2, -z+1$.

H atoms bound to C atoms were included in calculated positions and allowed to ride during subsequent refinement, with C—H = 0.95 Å and U_{iso}(H) = 1.2U_{eq}(C) for Csp^2, and C—H = 0.98 Å and U_{iso}(H) = 1.5U_{eq}(C) for the methyl groups. The methyl groups were allowed to rotate about their local threefold axes. H atoms bound to N1 were located in a difference Fourier map and refined isotropically, with final N—H distances of 0.80 (2) and 0.83 (2) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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