Dichlorobis(pyridine-κN)bis(3,3,3-trifluoropropyl-κC^1)tin(IV)

Hassan Allouchi,[a] Michel Cotrait,[b] Bernard Jousseaume,[b]* Marie-Claude Rascle[b] and Thierry Toupance[b]

[a]Laboratoire de Chimie Physique, PIMIR EA 2098, Faculté de Pharmacie, Université de Tours, 31, Avenue Monge, 37200 Tours, France, and [b]Laboratoire de Chimie Organique et Organométallique, UMR 5802, Université Bordeaux I, 351, Cours de la Libération, 33405 Talence, France

Correspondence e-mail: b.jousseaume@lcoo.u-bordeaux.fr

In the title compound, $[Sn(C_3H_4F_3)_2Cl_2(C_5H_5N)_2]$, the Sn atom lies on an inversion centre and is octahedrally coordinated by two Cl atoms, two trifluoropropyl groups and two N atoms in an all-*trans* configuration. The electronegative trifluoropropyl groups increase the electrophilic properties of the Sn atom, and the Sn—Cl and Sn—N bonds are shortened in comparison with those reported for analogous compounds.

Comment

Organotin compounds, which show a great variety of applications in organic (Jousseaume & Pereyre, 1998) and industrial (Evans, 1998) chemistry, have mainly been developed with simple organic residues such as methyl, butyl, octyl or phenyl groups, the corresponding raw materials being cheap and easily available. It is therefore of interest to study the influence of other organic groups on the chemical and physicochemical properties of the corresponding organotin compounds, in order to change or improve these properties and to establish structure–reactivity relationships.

The introduction of electronegative elements, such as oxygen or halogens, on to an Sn-linked alkyl group lowers the stability of the corresponding organotin compounds (Davies, 1997; Jousseaume et al., 1992), which can be expressed by a lengthening of the corresponding Sn—C bond (White & Giordano, 2001), and this should increase the electrophilic properties of the metal. We have thus been interested in (3,3,3-trifluoropropyl)tin compounds (Franc et al., 2000), where an electronegative trifluoromethyl group is situated in a β position relative to the Sn atom. However, dichlorobis(3,3,3-trifluoropropyl)tin, unlike most dichlorodiorganotin compounds, is liquid at room temperature. The title compound, (I), with the addition of pyridine ligands, has thus been prepared and its crystal structure is presented here.

In this compound, which is a discrete 1:2 adduct of dichlorobis(3,3,3-trifluoropropyl)tin with pyridine, no intermolecular Sn—Cl or Sn—N contacts shorter than 4 Å are present in the unit cell. The Sn atom, which is at a centre of symmetry, is six-coordinate and shows an octahedral geometry. The ligands are in an all-*trans* configuration.

(I)
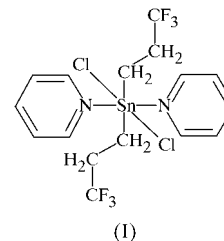
A comparison of the Sn—C bonds with those of analogous compounds with methyl (Aslanov et al., 1978) or ethyl groups (Casas et al., 2000), i.e. dichlorodimethylbis(pyridine-N)tin and dichlorodiethylbis(pyridine-N)tin, shows a lengthening of 0.01 Å, while the Sn—N and Sn—Cl bonds are shortened by 0.03 and 0.05 Å, and 0.04 and 0.06 Å, respectively. These findings can be interpreted as an increase of the electrophilic properties of the Sn atom due to the presence of three F atoms at the end of the carbon chain.
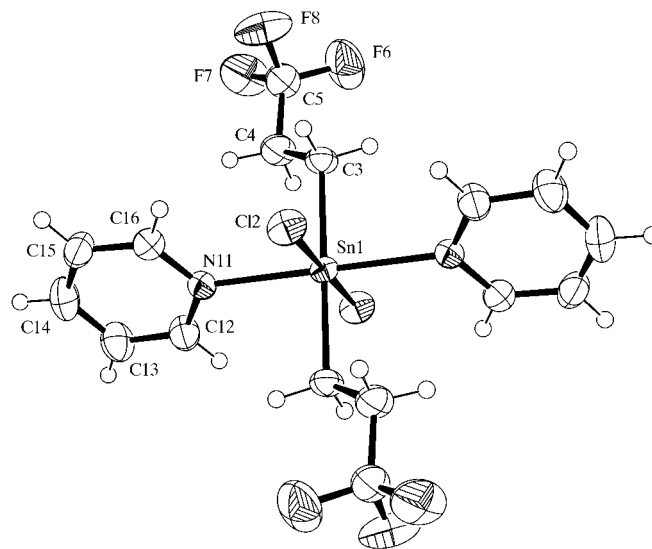

Figure 1
A view of the molecule of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.

The dihedral angle between the C—C bond and the Sn—Cl bond is the same (127°) as in the corresponding diethyl derivative. The pyridine ring is more tilted with respect to the N—Sn—Cl plane, by 31° instead of 22°, which decreases possible $H(C16)\cdots Cl$ interactions, as the interatomic distance increases from 1.86 to 2.90 Å.

Crystal cohesion is assumed to occur through very weak van der Waals interactions. In addition, there is no superposition of the pyridine molecules.

Experimental

The title complex was prepared by the addition of a solution of pyridine in chloroform to a solution of dichlorobis(3,3,3-trifluoro-propyl)tin in the same solvent. After 10 d, crystals of (I) suitable for X-ray analysis were obtained.

Crystal data

$[Sn(C_3H_4F_3)_2Cl_2(C_5H_5N)_2]$	$D_x = 1.773$ Mg m^{-3}
$M_r = 541.92$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4606
$a = 10.4684$ (4) Å	reflections
$b = 10.3551$ (3) Å	$\theta = 3.4$–27.5°
$c = 9.4337$ (3) Å	$\mu = 1.58$ mm^{-1}
$\beta = 96.939$ (2)°	$T = 293$ (2) K
$V = 1015.14$ (6) Å^3	Needle, colourless
$Z = 2$	$0.33 \times 0.09 \times 0.08$ mm

Data collection

Nonius KappaCCD area-detector diffractometer	$R_{int} = 0.045$
	$\theta_{max} = 27.5°$
ω scans	$h = -13 \rightarrow 13$
4606 measured reflections	$k = -13 \rightarrow 13$
2314 independent reflections	$l = -12 \rightarrow 12$
1648 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.039$	$w = 1/[\sigma^2(F_o^2) + (0.0441P)^2]$
$wR(F^2) = 0.085$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.99$	$(\Delta/\sigma)_{max} < 0.001$
2246 reflections	$\Delta\rho_{max} = 0.70$ e Å^{-3}
124 parameters	$\Delta\rho_{min} = -0.67$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C3	2.160 (3)	C5—F8	1.336 (4)
Sn1—N11	2.365 (3)	N11—C12	1.331 (5)
Sn1—Cl2	2.5357 (7)	N11—C16	1.340 (4)
C3—C4	1.502 (4)	C12—C13	1.379 (5)
C4—C5	1.479 (5)	C13—C14	1.377 (6)
C5—F6	1.322 (4)	C14—C15	1.359 (5)
C5—F7	1.328 (4)	C15—C16	1.375 (5)
C3—Sn1—N11	91.39 (11)	C16—N11—Sn1	121.2 (2)
C3—Sn1—Cl2	90.32 (9)	N11—C12—C13	123.1 (3)
N11—Sn1—Cl2	90.07 (7)	C14—C13—C12	118.2 (4)
C4—C3—Sn1	115.6 (2)	C15—C14—C13	119.3 (3)
C5—C4—C3	114.4 (3)	C14—C15—C16	119.4 (3)
C12—N11—C16	117.7 (3)	N11—C16—C15	122.3 (3)
C12—N11—Sn1	121.1 (2)		

Table 2
Comparison of bond lengths in R_2SnCl_2(pyridine)$_2$ complexes (Å).

R	Sn—C	Sn—Cl	Sn—N	Reference
Methyl	2.15 (2)	2.570 (1)	2.39 (2)	i
Ethyl	2.151 (4)	2.591 (1)	2.410 (3)	ii
3,3,3-Trifluoropropyl	2.160 (3)	2.5357 (7)	2.365 (3)	iii

References: (i) Aslanov *et al.* (1978); (ii) Casas *et al.* (2000); (iii) this work.

All H atoms were located in difference Fourier syntheses but were included in the refinement using a riding-model approximation, with isotropic displacement parameters fixed at $1.2U_{eq}$ of the parent atom, and with C—H distances of 0.97 Å for CH$_2$ and 0.93 Å for C$_6$H$_5$.

Data collection: *KappaCCD Reference Manual* (Nonius, 1998); data reduction: *DENZO-SMN* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: DN1011). Services for accessing these data are described at the back of the journal.

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