metal-organic papers

Aquatriphenyl(trifluoroacetato)tin–2,2':6',2''-terpyridine (1/1)

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Key indicators

Single-crystal X-ray study
T = 158 K
Mean σ(C–C) = 0.004 Å
R factor = 0.027
wR factor = 0.062
Data-to-parameter ratio = 15.3

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

The coordinated water molecule in the 1:1 adduct of triphenyltin trifluoroacetate with 2,2':6',2''-terpyridine, [Sn(C$_2$F$_3$O$_2$)(C$_6$H$_5$)$_3$(H$_2$O)]·C$_{15}$H$_{11}$N$_3$, interacts with the N atoms of the two outer pyridyl rings of the terpyridine heterocycle [O···N = 2.771 (3) and 2.797 (3) Å]; these outer rings are twisted by 25.6 (1) and 32.7 (1)° with respect to the central ring. The Sn atom is five-coordinate in a *trans*–C$_3$SnO$_2$ trigonal-bipyramidal environment [Sn—O = 2.221 (2) Å and Sn← O = 2.274 (2) Å].

Comment

In our previously reported structure of the 1:1 complex of aquatrifluoroacetatotriphenyltin and 2,4,6-tris(2-pyridyl)-1,3,5-triazine (Chee *et al.*, 2002), the water molecule [Sn← O = 2.311 (3) Å] forms hydrogen bonds to two of the N atoms of the 2-pyridyl and 6-pyridyl rings of the N-heterocycle [O···N = 2.841 (4) and 2.826 (4) Å]; the N atom in the 1-position of the triazine ring is not involved in any interaction. The heterocyclic ligand is relatively flat, the 2-pyridyl and 4-pyridyl rings being twisted by only 7.7 (2) and 13.4 (2)° with respect to the triazine ring. Without the 4-pyridyl group, the resulting N-heterocycle, *viz*. terpyridine, also furnishes a similar outer-sphere coordination complex. However, the terpyridine ligand in the title complex, (I) (Fig. 1), is severely twisted, the dihedral angles of the two outer rings with respect to the central pyridyl ring being 25.6 (1) and 32.7 (1)°. This twist contrasts with the virtually flat conformation of terpyridine itself, the corresponding dihedral angles being only only 5.1 and 7.2°. As the ligand exists in the *trans,trans*-conformation in the solid state (and also in solution) (Bessel *et al.*, 1992), it would have to reorganize itself in order to function as a terdentate chelate. Interestingly, the two terpyridine ligands in 2-methyl-3-trimethylsilyl-2,3-dicarba-1-stanna-*closo*-heptaborane(6) bis-(terpyridine) both exist in the *cis,cis*-conformation, although only one of them chelates to the Sn^{II} atom (Siriwardane & Hosmane, 1988).

(I)
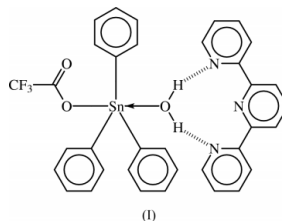
The ligand also forms outer-sphere coordination complexes with triphenyltin chloride [Sn—O$_{water}$ = 2.317 (2) Å; Prasad *et al.*, 1982] and triphenyltin isothiocyanate [Sn—O$_{water}$ = 2.252 (2) Å; Prasad & Smith, 1982]; the ligand is also severely

twisted [14.3 (3) and 32.0 (2)° in the chloride, and 19.6 (3) and 29.5 (3)° in the isothiocyanate]. The Sn—O$_{water}$ bond length in the trifluoroacetate is similar to the distances found in the two complexes, but is much shorter than that [Sn—O$_{water}$ = 2.335 (4) Å] in the 1,10-phenanthroline adduct, which has a different hydrogen-bonding arrangement (Ng *et al.*, 1996).

Experimental

The title compound was prepared by heating triphenyltin trifluoro-acetate (0.73 g, 2 mmol), which was synthesized from triphenyltin hydroxide and trifluoroacetic acid, with an equimolar quantity of terpyridine (0.47 g, 2 mmol) in ethanol. The product was obtained as crystals upon evaporation of the solvent (m.p. 409–410 K).

Crystal data

[Sn(C$_2$F$_3$O$_2$)(C$_6$H$_5$)$_3$-(H$_2$O)]·C$_{15}$H$_{11}$N$_3$	$D_x = 1.512$ Mg m^{-3}
$M_r = 714.29$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/n$	Cell parameters from 6202
$a = 10.4257 (7)$ Å	reflections
$b = 10.0510 (7)$ Å	$\theta = 2.0$–26.4°
$c = 30.025 (2)$ Å	$\mu = 0.87$ mm^{-1}
$\beta = 94.265 (1)°$	$T = 158 (2)$ K
$V = 3137.6 (4)$ Å^3	Plate, colorless
$Z = 4$	$0.50 \times 0.24 \times 0.15$ mm

Data collection

Bruker SMART area-detector diffractometer	6320 independent reflections
ω scans	5021 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.051$
	$\theta_{max} = 26.4°$
$T_{min} = 0.744$, $T_{max} = 0.877$	$h = -12 \rightarrow 6$
39984 measured reflections	$k = -12 \rightarrow 12$
	$l = -37 \rightarrow 37$

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.027$	
$wR(F^2) = 0.062$	
$S = 0.95$	$w = 1/[\sigma^2(F_o^2) + (0.0356P)^2]$
6320 reflections	where $P = (F_o^2 + 2F_c^2)/3$
414 parameters	$(\Delta/\sigma)_{max} = 0.001$
	$\Delta\rho_{max} = 0.50$ e Å^{-3}
	$\Delta\rho_{min} = -0.43$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—C1	2.130 (2)	Sn1—O1	2.221 (2)
Sn1—C7	2.126 (2)	Sn1—O1w	2.274 (2)
Sn1—C13	2.126 (2)		
C1—Sn1—C7	118.5 (1)	C7—Sn1—O1	98.4 (1)
C1—Sn1—C13	123.8 (1)	C7—Sn1—O1w	85.8 (1)
C1—Sn1—O1	91.0 (1)	C13—Sn1—O1	87.5 (1)
C1—Sn1—O1w	91.4 (1)	C13—Sn1—O1w	86.0 (1)
C7—Sn1—C13	117.3 (1)	O1—Sn1—O1w	173.4 (1)

The carbon-bound H atoms were positioned geometrically and were allowed to ride on their parent C atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$. The water H atoms were located and refined, subject to O—H = 0.85 (1) Å.
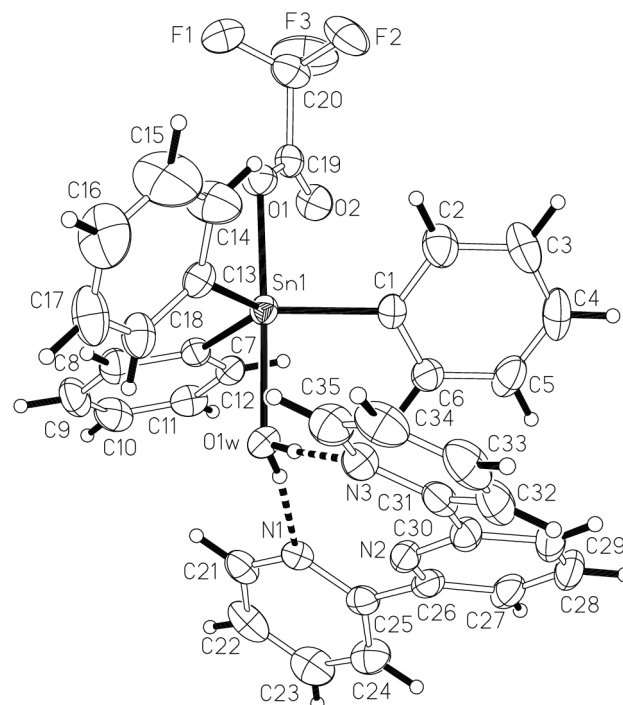

Figure 1
*ORTEP*II (Johnson, 1976) plot of (I), with ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Hydrogen bonds: O1w···N1 = 2.771 (3) Å and O1w···N3 = 2.797 (3) Å.]

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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