

Aquatriphenyl(trifluoroacetato)tin– 2,4,6-tris(2-pyridyl)-1,3,5-triazine (1/1)

Chin Fei Chee, Kong Mun Lo and
Seik Weng Ng*

Department of Chemistry, University of Malaya,
50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study

$T = 168$ K

Mean $\sigma(\text{C}-\text{C}) = 0.006$ Å

R factor = 0.040

wR factor = 0.095

Data-to-parameter ratio = 14.4

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

The water-coordinated Sn atom in the title compound, $[\text{Sn}(\text{C}_2\text{F}_3\text{O}_2)(\text{C}_6\text{H}_5)_3(\text{H}_2\text{O})] \cdot \text{C}_{18}\text{H}_{12}\text{N}_6$, forms hydrogen bonds to two of the pyridyl N atoms of the *N*-heterocycle $[\text{O}_{\text{water}} \cdots \text{N} = 2.841(4)$ and $2.826(4)$ Å]. The Sn atom shows *trans*- C_3SnO_2 trigonal bipyramidal coordination.

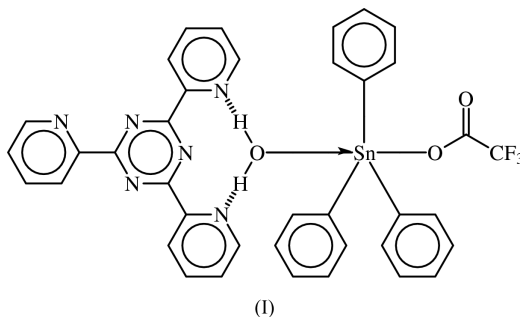
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Comment

The *N*-heterocycle 2,4,6-tris(2-pyridyl)-1,3,5-triazine interacts with the Lewis acceptor bis(triphenyltin) succinate through the coordinated water molecules in the centrosymmetric adduct $[\text{Sn} \leftarrow \text{O}_{\text{water}} = 2.487(3)$ Å in the monoclinic modification and $2.441(3)$ Å in the triclinic modification]. The water molecule forms hydrogen bonds to the N atoms of the pyridyl rings $[\text{O}_{\text{water}} \cdots \text{N} = 2.921(5)$ and $2.999(5)$ Å in the monoclinic modification, and $2.860(5)$ and $2.907(5)$ Å in the triclinic modification] (Ng, 1998). In the the 1/1 adduct, (I), of the same triazine with with triphenyltin trifluoroacetate monohydrate (Fig. 1), a similar hydrogen-bonding scheme is also noted $[\text{O}_{\text{water}} \cdots \text{N} = 2.841(4)$ and $2.826(4)$ Å].



The water donor occupies an apical position of the *trans*- C_3SnO_2 trigonal bipyramidal polyhedron of the Sn atom; owing to the electron-withdrawing capacity of the trifluoromethyl group, the Lewis acidity of the triphenyltin acceptor is enhanced, and this leads to a shortening of the $\text{Sn}-\text{O}_{\text{water}}$ bond $[\text{Sn} \leftarrow \text{O} = 2.311(3)$ Å]. The bond distance is similar to that $[2.335(4)$ Å] found in bis[aquatrifluoroacetatotriphenyltin-1,10-phenanthroline] (Ng *et al.*, 1996); however, this compound features a different hydrogen-bonding scheme.

Experimental

The compound was prepared by heating triphenyltin hydroxide, trifluoroacetic acid and 2,4,6-tris(2-pyridyl)-1,3,5-triazine in a 1:1:1 molar ratio in toluene for 1 h. The product separated as light-yellow cubic blocks when the solvent was removed (m.p. 445–447 K).

Crystal data

$[\text{Sn}(\text{C}_2\text{F}_3\text{O}_2)(\text{C}_6\text{H}_5)_3\text{-(H}_2\text{O)}] \cdot \text{C}_{18}\text{H}_{12}\text{N}_6$
 $M_r = 793.36$
 Triclinic, $P\bar{1}$
 $a = 10.567(1) \text{ \AA}$
 $b = 11.053(1) \text{ \AA}$
 $c = 15.438(1) \text{ \AA}$
 $\alpha = 105.559(2)^\circ$
 $\beta = 97.496(2)^\circ$
 $\gamma = 101.637(2)^\circ$
 $V = 1668.5(2) \text{ \AA}^3$

$Z = 2$
 $D_x = 1.58 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 7791 reflections
 $\theta = 2.0\text{--}26.4^\circ$
 $\mu = 0.83 \text{ mm}^{-1}$
 $T = 168(2) \text{ K}$
 Block, light yellow
 $0.30 \times 0.19 \times 0.10 \text{ mm}$

Data collection

Bruker CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.789$, $T_{\max} = 0.922$
 21865 measured reflections

6720 independent reflections
 5013 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.063$
 $\theta_{\text{max}} = 26.4^\circ$
 $h = -13 \rightarrow 13$
 $k = -13 \rightarrow 7$
 $l = -19 \rightarrow 19$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.095$
 $S = 0.93$
 6720 reflections
 468 parameters

H atoms treated by a mixture of independent and constrained refinement
 $w = 1/[\sigma^2(F_o^2) + (0.0525P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.43 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -1.49 \text{ e \AA}^{-3}$

Table 1

 Selected geometric parameters (\AA , $^\circ$).

Sn1—C1	2.132 (4)	Sn1—O1	2.217 (3)
Sn1—C7	2.135 (3)	Sn1—O1 _w	2.311 (3)
Sn1—C13	2.118 (4)		
C1—Sn1—C13	118.1 (1)	C7—Sn1—O1	86.8 (1)
C1—Sn1—C7	122.7 (1)	C7—Sn1—O1 _w	88.4 (1)
C1—Sn1—O1	97.5 (1)	C13—Sn1—O1	92.6 (1)
C1—Sn1—O1 _w	88.3 (1)	C13—Sn1—O1 _w	86.3 (1)
C7—Sn1—C13	118.8 (1)	O1—Sn1—O1 _w	173.9 (1)

The C-bound H atoms were positioned geometrically ($\text{C—H} = 0.95 \text{ \AA}$) and were allowed to ride on their parent C atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The water H atoms were located and refined, subject to $\text{O—H} = 0.85 \pm 0.01 \text{ \AA}$. A peak/hole larger than 1 e \AA^{-3} was found near Sn1.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve

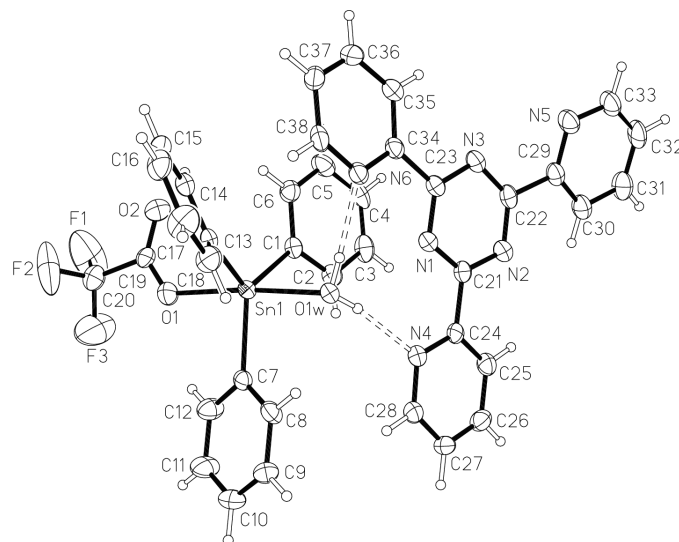


Figure 1

ORTEPII (Johnson, 1976) plot of adduct (I), with ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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