

Aqua(trifluoroacetato)triphenyltin–  
2,2'-bipyridine (2/2)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

In the title compound,  $[\text{Sn}(\text{C}_6\text{H}_5)_3(\text{C}_2\text{O}_2\text{F}_3)(\text{H}_2\text{O})]_2 \cdot 2\text{C}_{10}\text{H}_8\text{N}_2$ , the coordinated water molecule forms a hydrogen bond to the N atom of each of the two N-heterocycles [ $\text{O}_{\text{water}} \cdots \text{N} = 2.754(3)$  and  $2.795(3)$  Å]; the pyridyl rings of the N-heterocycle are twisted by  $34.2(1)^\circ$ . The Sn atom is five-coordinate in a *trans*- $\text{C}_3\text{SnO}_2$  trigonal-bipyramidal geometry.

Received 14 March 2003

Accepted 24 March 2003

Online 31 March 2003

## Key indicators

Single-crystal X-ray study

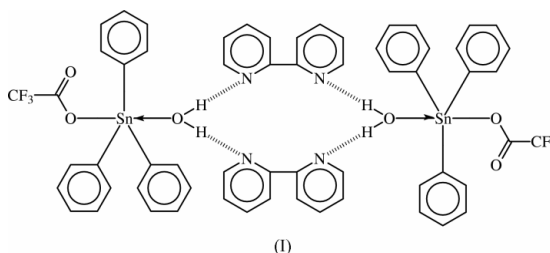
 $T = 168$  KMean  $\sigma(\text{C}-\text{C}) = 0.005$  Å $R$  factor = 0.028 $wR$  factor = 0.077

Data-to-parameter ratio = 15.2

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

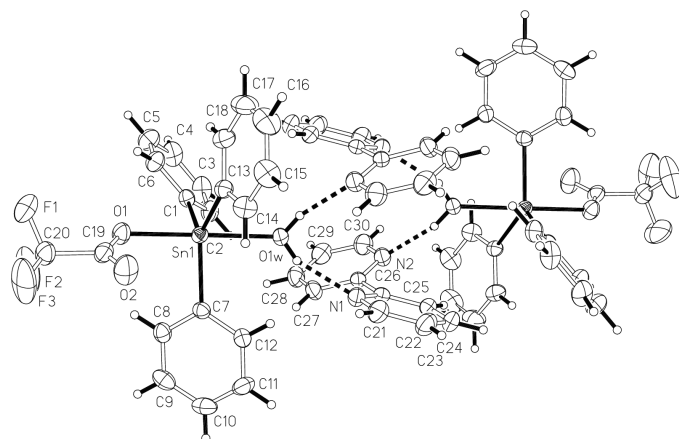
## Comment

The aquatrifluoroacetatotriphenyltin entity forms a dinuclear hydrogen-bonded complex with 1,10-phenanthroline (Ng *et al.*, 1996) and a mononuclear complex with 2,2':6'2''-terpyridine (Chee *et al.*, 2003). The formation of a mononuclear complex in the case of the fused-ring heterocycle can probably be attributed to the inability of the ligand to form two hydrogen bonds to the water molecule owing to its small 'bite'. The water molecule in the 2,2'-bipyridine analog, (I), is similarly unable to interact with the potentially bidentate ligand. Instead, it interacts with a second ligand to furnish a centrosymmetric dinuclear complex (Fig. 1). The pyridyl rings are twisted by  $34.2(1)^\circ$ ; the large twist apparently allows the acceptor N atoms to approach the water molecule [ $\text{O}_{\text{water}} \cdots \text{N} = 2.754(3)$  and  $2.795(3)$  Å] (Fig. 2); the hydrogen-bonding distances are somewhat shorter than those [2.809(6) and 2.814(6) Å] found in the 1,10-phenanthroline complex [ $\text{Sn} \leftarrow \text{O}_{\text{water}} = 2.335(4)$  Å] (Ng *et al.*, 1996). In the terpyridine complex, the two outer rings are twisted with respect to the central pyridyl ring for their N atoms to form hydrogen bonds to the water molecule.

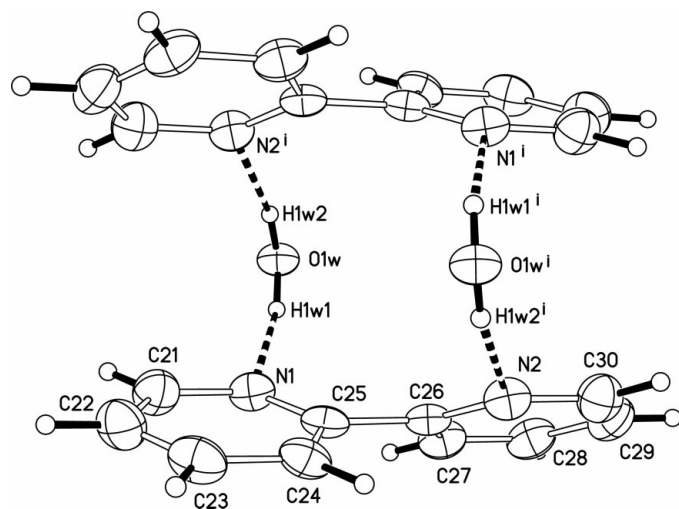


## Experimental

The title compound was obtained by heating triphenyltin trifluoroacetate (2.31 g, 5 mol) and 2,2'-bipyridine (0.78 g, 5 mmol) in a small volume of acetone. The compound was recrystallized from ethanol (m.p. 388–390 K).



**Figure 1**  
ORTEPII (Johnson, 1976) plot of the title adduct, with ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. The unlabeled part of the hydrogen-bonded dimer is related to the labeled part by the symmetry code  $(1-x, 1-y, 1-z)$ .



**Figure 2**  
ORTEPII (Johnson, 1976) plot of the diaquabis(2,2'-bipyridine) moiety, with ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.  $O1w \cdots N1 = 2.795$  (3) and  $O1w \cdots N2^i = 2.754$  (3) Å, and  $O1w-H1w1 \cdots N1 = 153$  (2) and  $O1w-H1w2 \cdots N2^i = 164$  (3)°. [Symmetry code: (i)  $1-x, 1-y, 1-z$ .]

#### Crystal data

$[Sn(C_6H_5)_3(C_2O_2F_3)(H_2O)]_2 \cdot 2C_{10}H_8N_2$   
 $M_r = 1274.42$   
 Triclinic,  $P1$   
 $a = 11.556$  (1) Å  
 $b = 11.662$  (1) Å  
 $c = 12.387$  (1) Å  
 $\alpha = 101.524$  (1)°  
 $\beta = 101.037$  (1)°  
 $\gamma = 117.313$  (1)°  
 $V = 1374.3$  (2) Å<sup>3</sup>

$Z = 1$   
 $D_x = 1.540$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 Cell parameters from 6120 reflections  
 $\theta = 1.8$ – $26.4$ °  
 $\mu = 0.98$  mm<sup>-1</sup>  
 $T = 168$  (2) K  
 Block, colorless  
 $0.60 \times 0.29 \times 0.10$  mm

#### Data collection

Bruker AXS area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{min} = 0.767$ ,  $T_{max} = 0.906$   
 17712 measured reflections

5484 independent reflections  
 4816 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.040$   
 $\theta_{max} = 26.4$ °  
 $h = -14 \rightarrow 13$   
 $k = -14 \rightarrow 14$   
 $l = -15 \rightarrow 15$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.028$   
 $wR(F^2) = 0.077$   
 $S = 1.02$   
 5484 reflections  
 360 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0494P)^2]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} = 0.001$   
 $\Delta\rho_{max} = 0.74$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.89$  e Å<sup>-3</sup>

**Table 1**

Selected geometric parameters (Å, °).

Sn1–C7	2.120 (3)	Sn1–O1	2.189 (2)
Sn1–C1	2.133 (3)	Sn1–O1w	2.335 (2)
Sn1–C13	2.115 (3)		
C1–Sn1–C13	114.0 (1)	C7–Sn1–O1	93.5 (1)
C1–Sn1–C7	114.1 (1)	C7–Sn1–O1w	86.0 (1)
C1–Sn1–O1	89.3 (1)	C13–Sn1–O1	98.2 (1)
C1–Sn1–O1w	89.3 (1)	C13–Sn1–O1w	83.6 (1)
C7–Sn1–C13	130.5 (1)	O1–Sn1–O1w	178.1 (1)

The water H atoms were located and refined, subject to the restraints  $O-H = 0.85$  (1) Å and  $H \cdots H = 1.39$  (1) Å. The aromatic H atoms were positioned geometrically, and were allowed to ride on their parent C atoms, with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

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

The authors thank Dr Jan Wikaira of the University of Canterbury for the diffraction measurements, and the University of Malaya (Nos. F0146/2002B and F0717/2002A) for supporting this work.

#### References

- Bruker (1997). SAINT and SMART. Bruker AXS Inc., Madison, Wisconsin, USA.  
 Chee, C. F., Lo, K. M. & Ng, S. W. (2003). *Acta Cryst.* **E59**, m174–m175.  
 Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.  
 Ng, S. W., Kumar Das, V. G. & Kennard, C. H. L. (1996). *Main Group Met. Chem.* **19**, 107–111.  
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.  
 Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.