

Shun-Li Li, Jian-Fang Ma\* and  
Ying-Ying LiuDepartment of Chemistry, Northeast Normal  
University, Changchun 130024, People's  
Republic of ChinaCorrespondence e-mail:  
jianfangma@yahoo.com.cn

## Key indicators

Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.019  
 $wR$  factor = 0.049  
Data-to-parameter ratio = 18.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

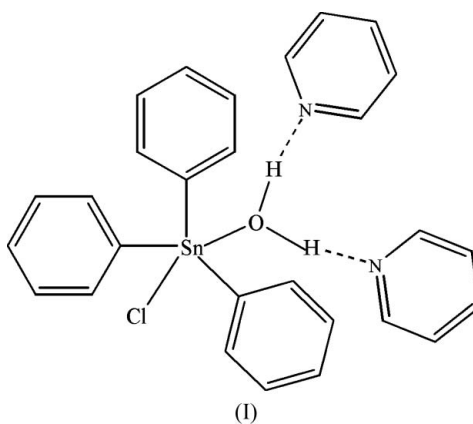
## Aquachlorotriphenyltin(IV) pyridine disolvate

In the structure of the title mononuclear Sn complex,  $[\text{Sn}(\text{C}_6\text{H}_5)_3\text{Cl}(\text{H}_2\text{O})] \cdot 2\text{C}_5\text{H}_5\text{N}$ , the  $\text{Sn}^{\text{IV}}$  atom is coordinated in a slightly distorted trigonal-bipyramidal geometry by three phenyl C atoms, one water molecule and one  $\text{Cl}^-$  anion. Two pyridine molecules are  $\text{O}-\text{H} \cdots \text{N}$  hydrogen bonded to the coordinated water molecule.

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## Comment

In recent years, there have been many reports on the syntheses and structure determinations of various organotin(IV) compounds (*e.g.* Lockhart *et al.*, 1987; Teoh *et al.*, 1997; Basu *et al.*, 2005). These compounds have special applications, such as PVC stabilizers, agricultural biocides, additives for anti-fouling paints, and catalysts for the production of polyurethanes and silicones, and are potential antitumor agents (Thoonen *et al.*, 2004). Furthermore, several structures of  $\text{Ph}_3\text{SnCl}(\text{H}_2\text{O})$  cocrystallized with other molecules have been determined, for example 3-[2-(1,10-phenanthrolyl)]-5,6-diphenyl-1,2,4-triazine (Ladd *et al.*, 1984), 3,4,7,8-tetramethyl-1,10-phenanthroline (Ng & Kumar Das, 1996), [*N,N'*-bis(3-methoxysalicylidene)propane-1,3-diamine]nickel(II) (Clarke *et al.*, 1994), di-2-pyridylketone 2-aminobenzoylhydrazone (Lanelli *et al.*, 1995), *o*-phenanthroline (Ng & Kumar Das, 1996), 2,2':6',2''-terpyridyl (Prasad *et al.*, 1982), 18-crown-6 (Amini *et al.*, 2003), 8-methoxyquinoline (Khoo *et al.*, 2000) and di-2-pyridyl-2-thenoylhydrazone (Carcelli *et al.*, 1995). In these structures, there is hydrogen bonding between the coordinated water molecule of  $\text{Ph}_3\text{SnCl}(\text{H}_2\text{O})$  and the cocrystallized molecule in the structure. In this paper, we report a structure in which two pyridine molecules are hydrogen bonded to  $\text{Ph}_3\text{SnCl}(\text{H}_2\text{O})$ .



bipyramidal geometry by three C atoms of three phenyl groups in the equatorial plane, and by one Cl<sup>-</sup> anion and one water molecule in the axial positions (Fig. 1). The slight distortion from the ideal trigonal-bipyramidal geometry is reflected in the O1—Sn1—Cl1 angle of 175.34 (8)°, and the three C—Sn—C angles of 116.54 (9), 119.84 (7) and 122.39 (7)°. The two pyridine molecules are connected to the coordinated water molecule through O—H...O hydrogen bonds (Fig. 1 and Table 2).

## Experimental

A mixture of Ph<sub>3</sub>SnCl (0.385 g, 0.1 mmol) and pyridine (0.198 g, 0.2 mmol) in 95% ethanol (13 ml) was stirred for 0.5 h. The mixture was then transferred and sealed into an 18 ml Teflon-lined autoclave, which was heated at 393 K for 89 h. After the mixture was cooled to room temperature, colorless blocks of the title complex were filtered off, washed with diethylether and dried at ambient temperature in air (yield 56% based on Sn). Analysis calculated for the title compound: C 59.88, H 4.85, N 4.99%; found: C 59.65, H 4.93, N 5.02%.

### Crystal data

[Sn(C<sub>6</sub>H<sub>5</sub>)<sub>3</sub>Cl(H<sub>2</sub>O)]·2C<sub>5</sub>H<sub>5</sub>N

*M<sub>r</sub>* = 561.66

Orthorhombic, *Pna*2<sub>1</sub>

*a* = 15.492 (5) Å

*b* = 15.925 (5) Å

*c* = 10.885 (5) Å

*V* = 2685.4 (17) Å<sup>3</sup>

*Z* = 4

*D<sub>x</sub>* = 1.389 Mg m<sup>-3</sup>

Mo *K*α radiation

Cell parameters from 8982 reflections

$\theta$  = 2.2–28.2°

$\mu$  = 1.07 mm<sup>-1</sup>

*T* = 293 (2) K

Needle, colorless

0.43 × 0.13 × 0.11 mm

### Data collection

Bruker APEX CCD area-detector diffractometer

$\omega$  scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

*T<sub>min</sub>* = 0.623, *T<sub>max</sub>* = 0.882

15753 measured reflections

5668 independent reflections

5086 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.020

$\theta_{\max}$  = 28.4°

*h* = -14 → 20

*k* = -20 → 20

*l* = -10 → 14

### Refinement

Refinement on *F*<sup>2</sup>

*R* [*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.019

*wR* (*F*<sup>2</sup>) = 0.049

*S* = 1.04

5668 reflections

307 parameters

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2]$

where  $P = (F_o^2 + 2F_c^2)/3$

( $\Delta/\sigma$ )<sub>max</sub> = 0.002

$\Delta\rho_{\max} = 0.30$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -0.22$  e Å<sup>-3</sup>

Extinction correction: SHELXL97

Extinction coefficient: 0.0062 (2)

Absolute structure: Flack (1983),

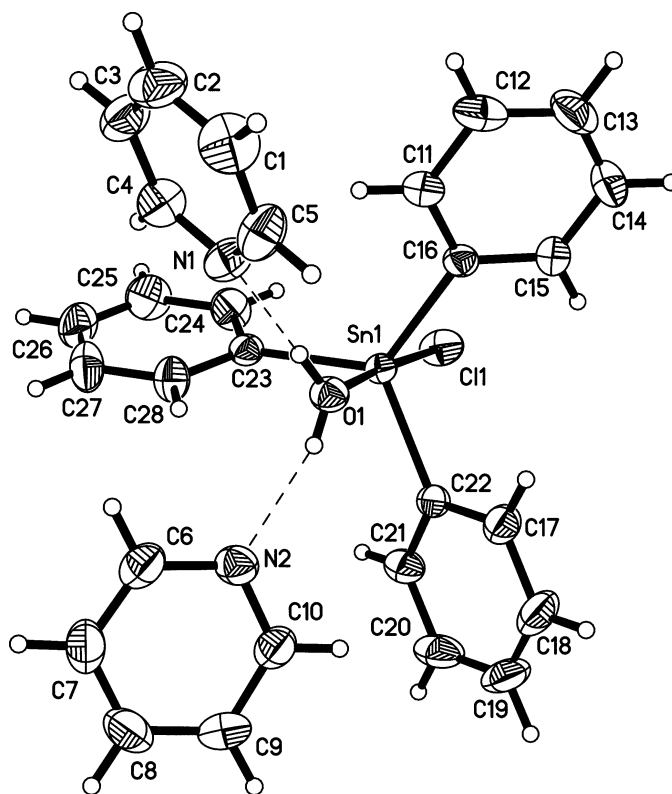
2299 Friedel pairs

Flack parameter: -0.005 (16)

**Table 1**

Selected geometric parameters (Å, °).

C16—Sn1	2.124 (2)	O1—Sn1	2.3469 (14)
C22—Sn1	2.127 (2)	Sn1—Cl1	2.5068 (9)
C23—Sn1	2.145 (3)		
C16—Sn1—C22	116.54 (9)	C23—Sn1—O1	90.01 (9)
C16—Sn1—C23	122.39 (7)	C16—Sn1—Cl1	92.74 (6)
C22—Sn1—C23	119.84 (7)	C22—Sn1—Cl1	93.72 (5)
C16—Sn1—O1	85.41 (7)	C23—Sn1—Cl1	94.59 (7)
C22—Sn1—O1	83.32 (7)	O1—Sn1—Cl1	175.34 (8)



**Figure 1**

View of the structure of (I), showing displacement ellipsoids at the 30% probability level. Dashed lines indicate hydrogen bonds.

**Table 2**

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1A...N1	0.78 (3)	1.96 (3)	2.740 (2)	170 (3)
O1—H1B...N2	0.76 (3)	2.01 (3)	2.745 (2)	164 (6)

All H atoms bonded to C atoms were positioned geometrically and refined as riding atoms with C—H = 0.93 Å and *U*<sub>iso</sub>(H) = 1.2*U*<sub>eq</sub>(C). The H atoms of the coordinated water molecule were located in a difference Fourier map and then refined isotropically.

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1999); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL-Plus (Sheldrick, 1990); software used to prepare material for publication: SHELXL97.

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## References

- Amini, M. M., Foladi, S., Aghabozorg, H., Rare, A. D. & Ng, S. W. (2003). *Chin. J. Struct. Chem.* **22**, 77–83.  
 Basu, B. T. S., Rynfah, W., Rivarola, E., Pettinari, C. & Linden, A. (2005). *J. Organomet. Chem.* **690**, 1413–1421.

- Bruker (1997). *SMART*. Version 5.622. Bruker AXS Inc., Madison, Wisconsin, USA.
- Bruker (1999). *SAINTE*. Version 6.02. Bruker AXS Inc., Madison, Wisconsin, USA.
- Carcelli, M., Pelizzi, C., Pelizzi, G., Mazza, P. & Zani, F. (1995). *J. Organomet. Chem.* **488**, 55–61.
- Clarke, N., Cunningham, D., Higgins, T., McArdle, P., McGinley, J. & O'Gara, M. (1994). *J. Organomet. Chem.* **469**, 33–40.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Khoo, L. E., Ouyang, J., Xu, Y. & Ng, S. W. (2000). *Main Group Metal Chem.* **23**, 723–724.
- Ladd, M. F. C., Povey, D. C. & Smith, F. E. (1984). *J. Crystallogr. Spectrosc. Res.* **14**, 249–259.
- Lanelli, S., Mazza, P., Orcesi, M., Pelizzi, C. & Zani, F. (1995). *J. Inorg. Biochem.* **60**, 89–108.
- Lockhart, T. P., Calabrese, J. C. & Davidson, F. (1987). *Organometallics*, **6**, 2479–2483.
- Ng, S. W. & Kumar Das, V. G. (1996). *J. Organomet. Chem.* **513**, 105–108.
- Prasad, L., Lee, F. L., Le Page, Y. & Smith, F. E. (1982). *Acta Cryst.* **B38**, 259–262.
- Sheldrick, G. M. (1990). *SHELXTL-Plus*. Siemens Analytical X-ray Instrument Inc., Madison, Wisconsin, USA.
- Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Teoh, S. G., Ang, S. H., Looi, E. S., Leok, C. A., Teo, S. B. & Fun, H. K. (1997). *J. Organomet. Chem.* **527**, 15–19.
- Thoonen, S. H. L., Deelman, B.-J. & van Koten, G. (2004). *J. Organomet. Chem.* **689**, 2145–2157.