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Aquachloridotriphenyltin(IV)–2-[1-(4-pyridylmethyl)-1*H*-imidazol-2-yl]-pyridine (1/1)

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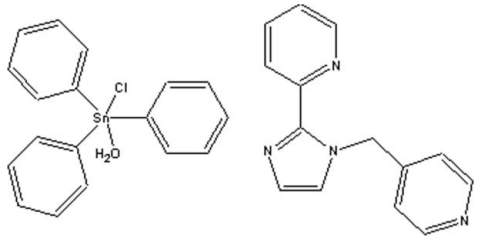
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.041; wR factor = 0.085; data-to-parameter ratio = 18.3.

In the title compound, $[Sn(C_6H_5)_3Cl(H_2O)]\cdot C_{14}H_{12}N_4$, $Ph_3SnCl(H_2O)$ and 2-[1-(4-pyridylmethyl)-1*H*-imidazol-2-yl]-pyridine molecules cocrystallize in the same structure. Each Sn atom displays a distorted trigonal–bipyramidal geometry composed of three phenyl groups, one Cl^- ion and one coordinated water molecule, which links, *via* hydrogen bonding, the $Ph_3SnCl(H_2O)$ molecule to the cocrystallized 2-[1-(4-pyridylmethyl)-1*H*-imidazol-2-yl]pyridine molecule to generate an infinite chain structure.

Related literature

In recent years, there have been many reports of the synthesis and structure determination of various organotin(IV) compounds (Lockhart *et al.*, 1987; Teoh *et al.*, 1997; Basu *et al.*, 2005). Among these, several structures of $Ph_3SnCl(H_2O)$ 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) and [*N*,*N*′-bis(3-methoxysalicylidene)propane-1,3-diamine]nickel(II) (Clarke *et al.*, 1994).



Experimental

Crystal data

$[Sn(C_6H_5)_3Cl(H2O)]\cdot C_{14}H_{12}N_4$
M_r = 639.73
Triclinic, $P\overline{1}$
a = 10.643 (2) Å
b = 11.165 (2) Å
c = 13.196 (3) Å
α = 89.945 (4)°
β = 71.953 (3)°
γ = 79.463 (3)°
V = 1463.2 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 293 (2) K
0.35 × 0.32 × 0.28 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.71, T_{max} = 0.76
9072 measured reflections
6576 independent reflections
4836 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.085
S = 1.02
6576 reflections
360 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.40 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1B···N3	0.85 (3)	1.923 (12)	2.749 (4)	165 (3)
O1—H1A···N1^{i}	0.85 (3)	1.90 (3)	2.751 (4)	174 (3)

Symmetry code: (i) $x, y+1, z$.

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2120).

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supplementary materials

Acta Cryst. (2007). E**63**, m2830 [**doi:10.1107/S1600536807052695**]

Aquachloridotriphenyltin(IV)-2-[1-(4-pyridylmethyl)-1*H*-imidazol-2-yl]pyridine (1/1)

S.-L. Li, G.-J. Ping and J.-F. Ma

Comment

In recent years, there have been many reports on the syntheses and structure determinations of various organotin(IV) compounds (Lockhart *et al.*, 1987; Teoh *et al.*, 1997; Basu *et al.*, 2005). Among them, several structures of $Ph_3SnCl(H_2O)$ 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), *etc*. In all these structures, the coordinated water molecule in $Ph_3SnCl(H_2O)$ is hydrogen bonded to the cocrystallized molecules in the structure.

In the molecular structure of the title compound, $\{[(C_6H_5)_3SnCl(H_2O)](C_{14}H_{12}N_4)\}$ (**I**), the Sn atom is five-coordinated in a slightly distorted trigonal–bipyramidal geometry by three C atoms of three phenyl groups, one Cl^- 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 177.59 (7)°, and the three C—Sn—C angles of 116.65 (13) °, 117.37 (13) ° and 124.52 (13) °. The coordinated water molecule in $Ph_3SnCl(H_2O)$ links the cocrystallized molecules to generate an infinite chain structure through O—H···N hydrogen bonds (Fig. 2 and Table 2).

Experimental

A mixture of Ph_3SnCl (0.385 g, 1 mmol) and 2-(1-(4-pyridylmethyl)-1*H*-imidazol-2-yl)pyridine (0.236 g, 1 mmol) in 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 150 °C 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 49% based on Sn).

Refinement

All H atoms on C atoms were poisitioned geometrically and refined as riding atoms, with C—H = 0.93–0.97 Å, and U_{iso} = 1.2U_{eq} (C). The H atoms of the coordinated water molecule were located in a difference Fourier map and then refined isotropically.

Figures

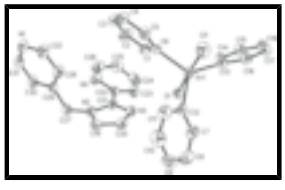


Fig. 1. A view of the molecule of (**I**). Displacement ellipsoids are drawn at the 30% probability level.

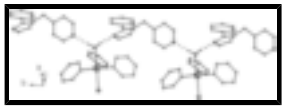


Fig. 2. Ball-stick representation of the infinite chain of (**I**).

Aquachloridotriphenyltin(IV)–2-[1-(4-pyridylmethyl)-1*H*-imidazol-2-yl]pyridine (1/1)

Crystal data

$[Sn(C_6H_5)_3Cl(H2O)]\cdot C_{14}H_{12}N_4$	$Z = 2$
$M_r = 639.73$	$F_{000} = 648$
Triclinic, $P\overline{1}$	$D_x = 1.452$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 10.643$ (2) Å	Cell parameters from 9072 reflections
$b = 11.165$ (2) Å	$\theta = 1.6$–28.3º
$c = 13.196$ (3) Å	$\mu = 1.00$ mm^{-1}
$\alpha = 89.945$ (4)º	$T = 293$ (2) K
$\beta = 71.953$ (3)º	Block, colourless
$\gamma = 79.463$ (3)º	0.35 × 0.32 × 0.28 mm
$V = 1463.2$ (5) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	6576 independent reflections
Radiation source: fine-focus sealed tube	4836 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.019$
$T = 293$(2) K	$\theta_{max} = 28.3$º
ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11\rightarrow14$
$T_{min} = 0.71$, $T_{max} = 0.76$	$k = -12\rightarrow14$
9072 measured reflections	$l = -16\rightarrow17$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.085$	$w = 1/[\sigma^2(F_o^2) + (0.0226P)^2 + 0.8978P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
6576 reflections	$\Delta\rho_{max} = 0.40$ e Å^{-3}
360 parameters	$\Delta\rho_{min} = -0.42$ e Å^{-3}
3 restraints	Extinction correction: none

Primary atom site location: structure-invariant direct methods

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.14373 (2)	0.73666 (2)	0.74054 (2)	0.05096 (9)
C1	0.3501 (4)	0.5030 (4)	0.6384 (3)	0.0708 (12)
H1	0.4123	0.5516	0.6388	0.085*
C2	0.3954 (5)	0.3825 (4)	0.5992 (4)	0.0902 (15)
H2	0.4873	0.3507	0.5745	0.108*
C3	0.3061 (6)	0.3105 (4)	0.5965 (4)	0.0867 (14)
H3	0.3370	0.2293	0.5710	0.104*
C4	0.1720 (5)	0.3569 (4)	0.6312 (4)	0.0771 (12)
H4	0.1111	0.3084	0.6272	0.093*
C5	0.1252 (4)	0.4773 (4)	0.6728 (3)	0.0635 (10)
H5	0.0330	0.5076	0.6982	0.076*
C6	0.2135 (3)	0.5526 (3)	0.6771 (3)	0.0487 (8)
C7	0.1129 (4)	0.8498 (4)	0.9625 (3)	0.0711 (11)
H7	0.1685	0.9000	0.9230	0.085*
C8	0.0711 (5)	0.8622 (5)	1.0732 (4)	0.0886 (14)
H8	0.0973	0.9216	1.1073	0.106*
C9	−0.0080 (5)	0.7878 (5)	1.1320 (4)	0.0894 (15)
H9	−0.0346	0.7952	1.2062	0.107*
C10	−0.0483 (4)	0.7022 (5)	1.0817 (4)	0.0883 (15)
H10	−0.1022	0.6512	1.1218	0.106*
C11	−0.0093 (4)	0.6913 (4)	0.9717 (3)	0.0715 (12)
H11	−0.0390	0.6339	0.9383	0.086*
C12	0.0733 (3)	0.7643 (3)	0.9103 (3)	0.0533 (9)
C13	0.1896 (3)	0.8775 (3)	0.6325 (3)	0.0495 (8)
C14	0.3197 (4)	0.8708 (3)	0.5644 (3)	0.0615 (10)
H14	0.3886	0.8104	0.5718	0.074*
C15	0.3484 (4)	0.9522 (4)	0.4860 (3)	0.0713 (11)
H15	0.4359	0.9452	0.4401	0.086*
C16	0.2496 (5)	1.0429 (4)	0.4750 (4)	0.0735 (12)
H16	0.2694	1.0978	0.4220	0.088*
C17	0.1220 (5)	1.0523 (4)	0.5422 (4)	0.0733 (12)

H17	0.0545	1.1146	0.5354	0.088*
C18	0.0909 (4)	0.9704 (3)	0.6207 (3)	0.0607 (10)
H18	0.0029	0.9780	0.6659	0.073*
C19	0.3493 (4)	0.4092 (4)	1.0023 (3)	0.0626 (10)
H19	0.3018	0.3738	1.0623	0.075*
C20	0.3158 (4)	0.5232 (4)	0.9716 (3)	0.0625 (10)
H20	0.2388	0.5796	1.0077	0.075*
C21	0.5020 (3)	0.4413 (3)	0.8543 (3)	0.0502 (8)
C22	0.6210 (4)	0.4207 (3)	0.7590 (3)	0.0525 (9)
C23	0.6732 (4)	0.5173 (4)	0.7092 (3)	0.0710 (11)
H23	0.6352	0.5971	0.7363	0.085*
C24	0.7829 (5)	0.4929 (5)	0.6184 (4)	0.0846 (14)
H24	0.8215	0.5562	0.5840	0.102*
C25	0.8350 (5)	0.3743 (6)	0.5789 (4)	0.0874 (14)
H25	0.9081	0.3559	0.5169	0.105*
C26	0.7766 (5)	0.2846 (5)	0.6333 (4)	0.0854 (14)
H26	0.8119	0.2043	0.6065	0.102*
C27	0.5463 (4)	0.2360 (3)	0.9335 (3)	0.0664 (11)
H27A	0.5299	0.2193	1.0081	0.080*
H27B	0.6414	0.2375	0.9026	0.080*
C28	0.4026 (4)	0.1447 (4)	0.8450 (4)	0.0734 (12)
H28	0.3443	0.2197	0.8535	0.088*
C29	0.5133 (4)	0.1337 (3)	0.8775 (3)	0.0541 (9)
C30	0.5958 (4)	0.0205 (3)	0.8614 (3)	0.0652 (11)
H30	0.6738	0.0088	0.8808	0.078*
C31	0.5626 (4)	−0.0744 (4)	0.8167 (3)	0.0651 (11)
H31	0.6196	−0.1502	0.8070	0.078*
N1	0.4532 (3)	−0.0648 (3)	0.7861 (3)	0.0664 (9)
Cl1	−0.09058 (10)	0.75149 (10)	0.73063 (10)	0.0815 (3)
C32	0.3762 (4)	0.0448 (4)	0.7993 (4)	0.0767 (12)
H32	0.3006	0.0553	0.7766	0.092*
N2	0.4681 (3)	0.3567 (3)	0.9264 (2)	0.0548 (7)
N3	0.4103 (3)	0.5435 (3)	0.8808 (3)	0.0563 (8)
N4	0.6719 (3)	0.3049 (3)	0.7225 (3)	0.0718 (9)
O1	0.3576 (2)	0.7300 (2)	0.7549 (2)	0.0511 (6)
H1A	0.389 (4)	0.7939 (19)	0.760 (3)	0.083 (15)*
H1B	0.373 (3)	0.683 (2)	0.802 (2)	0.066 (12)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.04668 (14)	0.04605 (15)	0.05895 (16)	−0.00622 (10)	−0.01647 (11)	0.00314 (11)
C1	0.068 (3)	0.064 (3)	0.085 (3)	−0.001 (2)	−0.037 (2)	−0.023 (2)
C2	0.080 (3)	0.075 (3)	0.115 (4)	0.016 (3)	−0.048 (3)	−0.039 (3)
C3	0.117 (4)	0.056 (3)	0.099 (4)	−0.001 (3)	−0.059 (3)	−0.014 (2)
C4	0.104 (4)	0.054 (3)	0.085 (3)	−0.033 (3)	−0.038 (3)	0.006 (2)
C5	0.073 (3)	0.057 (2)	0.064 (3)	−0.021 (2)	−0.020 (2)	0.007 (2)
C6	0.056 (2)	0.047 (2)	0.046 (2)	−0.0089 (17)	−0.0212 (17)	0.0006 (16)

C7	0.066 (3)	0.064 (3)	0.070 (3)	−0.010 (2)	−0.004 (2)	−0.009 (2)
C8	0.082 (3)	0.084 (3)	0.088 (4)	−0.008 (3)	−0.014 (3)	−0.024 (3)
C9	0.091 (4)	0.113 (4)	0.051 (3)	−0.004 (3)	−0.012 (3)	−0.005 (3)
C10	0.066 (3)	0.099 (4)	0.080 (3)	−0.015 (3)	0.006 (3)	0.018 (3)
C11	0.055 (2)	0.072 (3)	0.076 (3)	−0.013 (2)	−0.003 (2)	0.002 (2)
C12	0.0454 (19)	0.053 (2)	0.055 (2)	−0.0035 (17)	−0.0094 (17)	0.0019 (18)
C13	0.055 (2)	0.0420 (19)	0.055 (2)	−0.0073 (16)	−0.0221 (18)	−0.0020 (16)
C14	0.061 (2)	0.058 (2)	0.063 (2)	−0.0031 (19)	−0.021 (2)	0.009 (2)
C15	0.074 (3)	0.071 (3)	0.065 (3)	−0.018 (2)	−0.014 (2)	0.010 (2)
C16	0.101 (3)	0.057 (3)	0.074 (3)	−0.026 (3)	−0.037 (3)	0.016 (2)
C17	0.090 (3)	0.049 (2)	0.088 (3)	−0.004 (2)	−0.043 (3)	0.010 (2)
C18	0.061 (2)	0.051 (2)	0.069 (3)	−0.0010 (18)	−0.025 (2)	0.0017 (19)
C19	0.073 (3)	0.066 (3)	0.055 (2)	−0.022 (2)	−0.024 (2)	0.010 (2)
C20	0.063 (2)	0.060 (3)	0.065 (3)	−0.008 (2)	−0.021 (2)	−0.004 (2)
C21	0.056 (2)	0.042 (2)	0.062 (2)	−0.0138 (17)	−0.0285 (18)	0.0028 (17)
C22	0.056 (2)	0.056 (2)	0.055 (2)	−0.0131 (18)	−0.0300 (18)	0.0059 (18)
C23	0.074 (3)	0.062 (3)	0.081 (3)	−0.018 (2)	−0.027 (2)	0.016 (2)
C24	0.075 (3)	0.109 (4)	0.077 (3)	−0.030 (3)	−0.026 (3)	0.030 (3)
C25	0.063 (3)	0.120 (5)	0.073 (3)	−0.009 (3)	−0.018 (2)	−0.009 (3)
C26	0.073 (3)	0.087 (4)	0.091 (4)	−0.006 (3)	−0.023 (3)	−0.023 (3)
C27	0.086 (3)	0.048 (2)	0.080 (3)	−0.016 (2)	−0.046 (2)	0.016 (2)
C28	0.070 (3)	0.042 (2)	0.119 (4)	−0.008 (2)	−0.047 (3)	0.004 (2)
C29	0.061 (2)	0.044 (2)	0.063 (2)	−0.0142 (18)	−0.0252 (19)	0.0146 (18)
C30	0.059 (2)	0.050 (2)	0.093 (3)	−0.0114 (19)	−0.032 (2)	0.012 (2)
C31	0.066 (3)	0.047 (2)	0.078 (3)	−0.006 (2)	−0.019 (2)	0.012 (2)
N1	0.065 (2)	0.0461 (19)	0.090 (3)	−0.0166 (16)	−0.0234 (19)	0.0061 (17)
Cl1	0.0500 (5)	0.0848 (8)	0.1148 (9)	−0.0104 (5)	−0.0346 (6)	0.0109 (7)
C32	0.070 (3)	0.056 (3)	0.113 (4)	−0.015 (2)	−0.040 (3)	0.003 (2)
N2	0.0636 (19)	0.0428 (17)	0.065 (2)	−0.0126 (15)	−0.0286 (17)	0.0046 (15)
N3	0.0599 (18)	0.0446 (18)	0.068 (2)	−0.0069 (15)	−0.0272 (17)	0.0020 (15)
N4	0.061 (2)	0.062 (2)	0.086 (3)	−0.0059 (17)	−0.0170 (19)	−0.0113 (19)
O1	0.0558 (14)	0.0410 (14)	0.0620 (17)	−0.0114 (13)	−0.0255 (13)	0.0081 (13)

Geometric parameters (Å, °)

Sn1—C6	2.129 (3)	C17—H17	0.9300
Sn1—C12	2.134 (4)	C18—H18	0.9300
Sn1—C13	2.142 (3)	C19—C20	1.354 (5)
Sn1—O1	2.329 (2)	C19—N2	1.375 (5)
Sn1—Cl1	2.5128 (11)	C19—H19	0.9300
C1—C2	1.387 (5)	C20—N3	1.353 (5)
C1—C6	1.388 (5)	C20—H20	0.9300
C1—H1	0.9300	C21—N3	1.326 (4)
C2—C3	1.360 (6)	C21—N2	1.356 (4)
C2—H2	0.9300	C21—C22	1.464 (5)
C3—C4	1.357 (6)	C22—N4	1.335 (4)
C3—H3	0.9300	C22—C23	1.376 (5)
C4—C5	1.395 (5)	C23—C24	1.375 (6)
C4—H4	0.9300	C23—H23	0.9300

C5—C6	1.384 (5)	C24—C25	1.373 (6)
C5—H5	0.9300	C24—H24	0.9300
C7—C12	1.375 (5)	C25—C26	1.362 (6)
C7—C8	1.388 (6)	C25—H25	0.9300
C7—H7	0.9300	C26—N4	1.332 (5)
C8—C9	1.361 (6)	C26—H26	0.9300
C8—H8	0.9300	C27—N2	1.468 (4)
C9—C10	1.365 (6)	C27—C29	1.511 (5)
C9—H9	0.9300	C27—H27A	0.9700
C10—C11	1.380 (6)	C27—H27B	0.9700
C10—H10	0.9300	C28—C29	1.359 (5)
C11—C12	1.384 (5)	C28—C32	1.380 (5)
C11—H11	0.9300	C28—H28	0.9300
C13—C18	1.380 (5)	C29—C30	1.376 (5)
C13—C14	1.387 (5)	C30—C31	1.365 (5)
C14—C15	1.376 (5)	C30—H30	0.9300
C14—H14	0.9300	C31—N1	1.332 (5)
C15—C16	1.362 (5)	C31—H31	0.9300
C15—H15	0.9300	N1—C32	1.321 (5)
C16—C17	1.358 (6)	C32—H32	0.9300
C16—H16	0.9300	O1—H1A	0.85 (3)
C17—C18	1.384 (5)	O1—H1B	0.85 (3)
C6—Sn1—C12	116.65 (13)	C16—C17—H17	119.5
C6—Sn1—C13	117.37 (13)	C18—C17—H17	119.5
C12—Sn1—C13	124.52 (13)	C13—C18—C17	120.5 (4)
C6—Sn1—O1	86.85 (11)	C13—C18—H18	119.8
C12—Sn1—O1	85.73 (11)	C17—C18—H18	119.8
C13—Sn1—O1	85.47 (11)	C20—C19—N2	105.8 (3)
C6—Sn1—Cl1	95.43 (10)	C20—C19—H19	127.1
C12—Sn1—Cl1	92.53 (10)	N2—C19—H19	127.1
C13—Sn1—Cl1	94.16 (10)	N3—C20—C19	110.4 (4)
O1—Sn1—Cl1	177.59 (7)	N3—C20—H20	124.8
C2—C1—C6	121.2 (4)	C19—C20—H20	124.8
C2—C1—H1	119.4	N3—C21—N2	110.3 (3)
C6—C1—H1	119.4	N3—C21—C22	125.2 (3)
C3—C2—C1	120.4 (4)	N2—C21—C22	124.5 (3)
C3—C2—H2	119.8	N4—C22—C23	122.7 (4)
C1—C2—H2	119.8	N4—C22—C21	116.4 (3)
C4—C3—C2	120.0 (4)	C23—C22—C21	120.8 (4)
C4—C3—H3	120.0	C24—C23—C22	118.4 (4)
C2—C3—H3	120.0	C24—C23—H23	120.8
C3—C4—C5	120.1 (4)	C22—C23—H23	120.8
C3—C4—H4	120.0	C25—C24—C23	119.5 (5)
C5—C4—H4	120.0	C25—C24—H24	120.2
C6—C5—C4	121.2 (4)	C23—C24—H24	120.2
C6—C5—H5	119.4	C26—C25—C24	118.1 (5)
C4—C5—H5	119.4	C26—C25—H25	121.0
C5—C6—C1	117.1 (3)	C24—C25—H25	121.0
C5—C6—Sn1	121.7 (3)	N4—C26—C25	123.9 (5)

C1—C6—Sn1	121.2 (3)	N4—C26—H26	118.0
C12—C7—C8	121.0 (4)	C25—C26—H26	118.0
C12—C7—H7	119.5	N2—C27—C29	113.6 (3)
C8—C7—H7	119.5	N2—C27—H27A	108.8
C9—C8—C7	120.2 (5)	C29—C27—H27A	108.8
C9—C8—H8	119.9	N2—C27—H27B	108.8
C7—C8—H8	119.9	C29—C27—H27B	108.8
C8—C9—C10	119.7 (4)	H27A—C27—H27B	107.7
C8—C9—H9	120.1	C29—C28—C32	120.2 (4)
C10—C9—H9	120.1	C29—C28—H28	119.9
C9—C10—C11	120.2 (4)	C32—C28—H28	119.9
C9—C10—H10	119.9	C28—C29—C30	116.9 (4)
C11—C10—H10	119.9	C28—C29—C27	124.0 (3)
C10—C11—C12	121.0 (4)	C30—C29—C27	119.1 (3)
C10—C11—H11	119.5	C31—C30—C29	119.7 (4)
C12—C11—H11	119.5	C31—C30—H30	120.2
C7—C12—C11	117.9 (4)	C29—C30—H30	120.2
C7—C12—Sn1	121.9 (3)	N1—C31—C30	123.8 (4)
C11—C12—Sn1	120.2 (3)	N1—C31—H31	118.1
C18—C13—C14	117.7 (3)	C30—C31—H31	118.1
C18—C13—Sn1	122.0 (3)	C32—N1—C31	116.2 (3)
C14—C13—Sn1	119.9 (3)	N1—C32—C28	123.2 (4)
C15—C14—C13	120.9 (4)	N1—C32—H32	118.4
C15—C14—H14	119.5	C28—C32—H32	118.4
C13—C14—H14	119.5	C21—N2—C19	107.1 (3)
C16—C15—C14	120.6 (4)	C21—N2—C27	128.5 (3)
C16—C15—H15	119.7	C19—N2—C27	124.0 (3)
C14—C15—H15	119.7	C21—N3—C20	106.3 (3)
C17—C16—C15	119.3 (4)	C26—N4—C22	117.4 (4)
C17—C16—H16	120.3	Sn1—O1—H1A	123 (2)
C15—C16—H16	120.3	Sn1—O1—H1B	112 (2)
C16—C17—C18	120.9 (4)	H1A—O1—H1B	108.3 (16)
C6—C1—C2—C3	0.9 (7)	Sn1—C13—C14—C15	172.4 (3)
C1—C2—C3—C4	0.8 (8)	C13—C14—C15—C16	1.3 (6)
C2—C3—C4—C5	−2.1 (7)	C14—C15—C16—C17	−0.1 (7)
C3—C4—C5—C6	1.8 (6)	C15—C16—C17—C18	−0.7 (7)
C4—C5—C6—C1	−0.1 (6)	C14—C13—C18—C17	0.9 (6)
C4—C5—C6—Sn1	−180.0 (3)	Sn1—C13—C18—C17	−173.1 (3)
C2—C1—C6—C5	−1.2 (6)	C16—C17—C18—C13	0.2 (6)
C2—C1—C6—Sn1	178.6 (3)	N2—C19—C20—N3	−1.0 (4)
C12—Sn1—C6—C5	78.9 (3)	N3—C21—C22—N4	−154.8 (3)
C13—Sn1—C6—C5	−114.3 (3)	N2—C21—C22—N4	23.2 (5)
O1—Sn1—C6—C5	162.5 (3)	N3—C21—C22—C23	23.2 (5)
Cl1—Sn1—C6—C5	−16.7 (3)	N2—C21—C22—C23	−158.8 (3)
C12—Sn1—C6—C1	−101.0 (3)	N4—C22—C23—C24	−0.4 (6)
C13—Sn1—C6—C1	65.8 (3)	C21—C22—C23—C24	−178.3 (4)
O1—Sn1—C6—C1	−17.4 (3)	C22—C23—C24—C25	1.4 (6)
Cl1—Sn1—C6—C1	163.4 (3)	C23—C24—C25—C26	−1.2 (7)
C12—C7—C8—C9	1.3 (7)	C24—C25—C26—N4	0.0 (7)

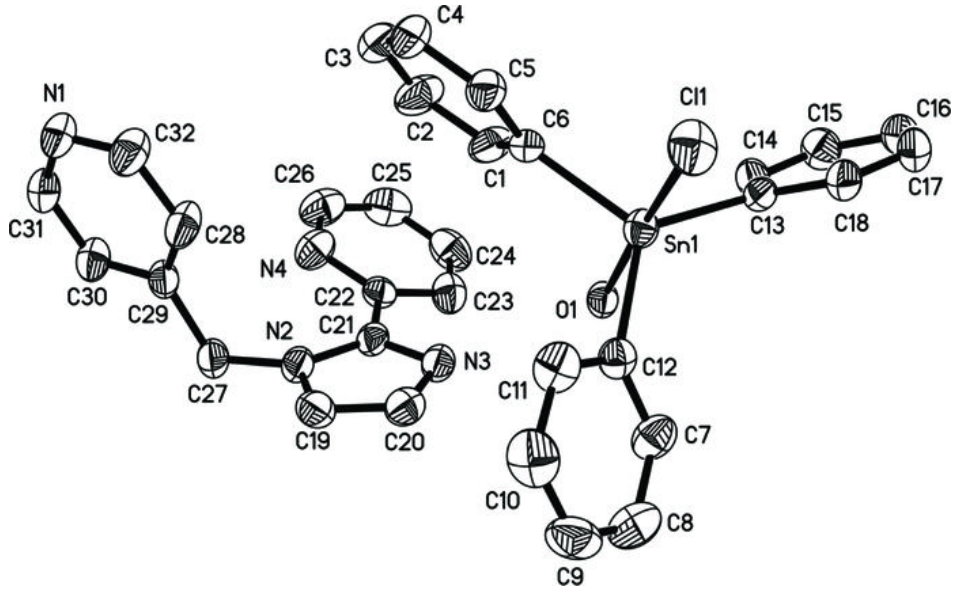
C7—C8—C9—C10	−1.2 (8)	C32—C28—C29—C30	0.7 (6)
C8—C9—C10—C11	−0.2 (8)	C32—C28—C29—C27	−176.6 (4)
C9—C10—C11—C12	1.5 (7)	N2—C27—C29—C28	−14.5 (6)
C8—C7—C12—C11	0.0 (6)	N2—C27—C29—C30	168.2 (3)
C8—C7—C12—Sn1	−176.8 (3)	C28—C29—C30—C31	−1.4 (6)
C10—C11—C12—C7	−1.3 (6)	C27—C29—C30—C31	176.1 (4)
C10—C11—C12—Sn1	175.5 (3)	C29—C30—C31—N1	0.4 (6)
C6—Sn1—C12—C7	132.9 (3)	C30—C31—N1—C32	1.3 (6)
C13—Sn1—C12—C7	−32.9 (4)	C31—N1—C32—C28	−2.1 (6)
O1—Sn1—C12—C7	48.6 (3)	C29—C28—C32—N1	1.1 (7)
Cl1—Sn1—C12—C7	−129.8 (3)	N3—C21—N2—C19	−0.4 (4)
C6—Sn1—C12—C11	−43.8 (3)	C22—C21—N2—C19	−178.6 (3)
C13—Sn1—C12—C11	150.3 (3)	N3—C21—N2—C27	−173.8 (3)
O1—Sn1—C12—C11	−128.1 (3)	C22—C21—N2—C27	7.9 (5)
Cl1—Sn1—C12—C11	53.5 (3)	C20—C19—N2—C21	0.8 (4)
C6—Sn1—C13—C18	125.8 (3)	C20—C19—N2—C27	174.6 (3)
C12—Sn1—C13—C18	−68.5 (3)	C29—C27—N2—C21	−94.1 (4)
O1—Sn1—C13—C18	−150.2 (3)	C29—C27—N2—C19	93.4 (4)
Cl1—Sn1—C13—C18	27.4 (3)	N2—C21—N3—C20	−0.2 (4)
C6—Sn1—C13—C14	−48.1 (3)	C22—C21—N3—C20	178.0 (3)
C12—Sn1—C13—C14	117.6 (3)	C19—C20—N3—C21	0.7 (4)
O1—Sn1—C13—C14	36.0 (3)	C25—C26—N4—C22	1.1 (7)
Cl1—Sn1—C13—C14	−146.4 (3)	C23—C22—N4—C26	−0.8 (6)
C18—C13—C14—C15	−1.7 (6)	C21—C22—N4—C26	177.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1B···N3	0.85 (3)	1.923 (12)	2.749 (4)	165 (3)
O1—H1A···N1^{i}	0.85 (3)	1.90 (3)	2.751 (4)	174 (3)

Symmetry codes: (i) *x*, *y*+1, *z*.

Fig. 1


C4
C3
C5
N1
C2
C6
Cl1
C15
C16
C32
C1
C14
C26
C25
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C28
C13
C18
Sn1
C24
N4
C22
C23
O1
C30
C29
N2
C21
N3
C12
C27
C11
C19
C20
C7
C10
C8
C9

Fig. 2