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Triethylammonium tetrachlorido-(pyridine-2-carboxylato- κ^2 N,O)-stannate(IV)

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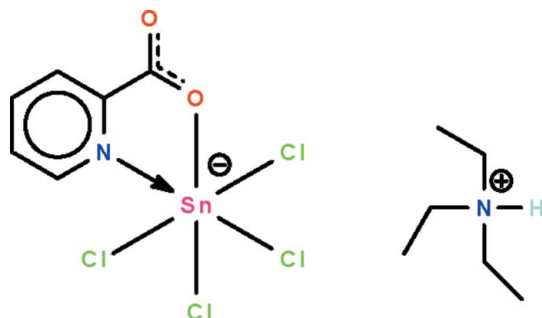
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 Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; disorder in main residue; R factor = 0.019; wR factor = 0.048; data-to-parameter ratio = 18.0.

The cation and the anion in the title salt, $(\text{C}_6\text{H}_{16}\text{N})(\text{SnCl}_4(\text{C}_6\text{H}_4\text{NO}_2))$, are linked by an $\text{N}-\text{H}\cdots\text{O}$ hydrogen bond. The Sn^{IV} atom in the stannate anion is chelated by the pyridine-2-carboxylate group and exists in a *cis*- SnCl_4NO octahedral geometry. The cation is disordered over two positions in a 0.564 (1):0.436 (1) ratio.

Related literature

 For another ammonium tetrachlorido(pyridine-2-carboxylato)stannate, see: Najafi *et al.* (2011).


Experimental

Crystal data

 $(\text{C}_6\text{H}_{16}\text{N})(\text{SnCl}_4(\text{C}_6\text{H}_4\text{NO}_2))$
 $M_r = 484.79$
 Monoclinic, $P2_1/n$
 $a = 11.6310$ (7) Å
 $b = 10.4912$ (6) Å
 $c = 16.4452$ (9) Å
 $\beta = 109.672$ (1)°

 $V = 1889.57$ (19) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 1.92$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.25 \times 0.05$ mm

Data collection

 Bruker SMART APEX
 diffractometer
 Absorption correction: multi-scan
 (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.596$, $T_{\text{max}} = 0.910$

 17476 measured reflections
 4344 independent reflections
 3896 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.019$
 $wR(F^2) = 0.048$
 $S = 1.01$
 4344 reflections
 242 parameters

 25 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.41$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.39$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N2}-\text{H2}\cdots\text{O2}$	0.88	1.95	2.828 (4)	172
$\text{N2}'-\text{H2}'\cdots\text{O2}$	0.88	2.02	2.895 (5)	173

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *pubCIF* (Westrip, 2010).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SI2335).

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
 Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Najafi, E., Amini, M. M. & Ng, S. W. (2011). *Acta Cryst.* **E67**, m239.
 Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2011). E67, m351 [doi:10.1107/S1600536811005460]

Triethylammonium tetrachlorido(pyridine-2-carboxylato- κ^2N,O)stannate(IV)

Ezzatollah Najafi, Mostafa M. Amini and Seik Weng Ng

S1. Comment

In the reaction of pyridine-2-carboxylic acid and stannic chloride in methanol, one equivalent of the carboxylic acid is protonated at the amino site and is also esterified, the reaction yielding the salt, $(C_7H_8NO_2)^+ [SnCl_4(C_6H_4NO_2)]^-$. The Sn^{IV} atom in the anion is *N,O*-chelated by the pyridine-2-carboxylate in a *cis*- $SnNOCl_4$ octahedral geometry (Najafi *et al.*, 2011). In the present study, triethylamine was added to function as proton abstractor. The reaction affords a similar salt, $(Et_3NH)^+ [SnCl_4(C_6H_4NO_2)]^-$ (Scheme I, Fig. 1). The tin atom in the stannate is chelated by the pyridine-2-carboxylate group and it exists in a *cis*- $SnCl_4NO$ octahedral geometry.

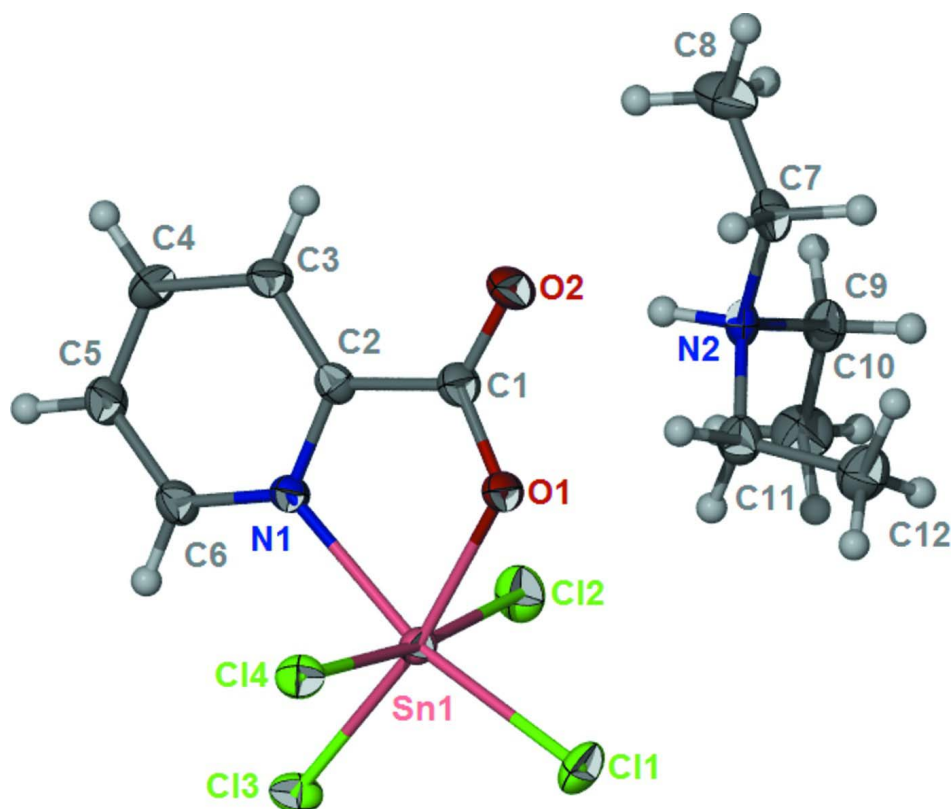
S2. Experimental

The reaction was carried out under a nitrogen atmosphere. Pyridine-2-carboxylic acid (1.0 mmol, 0.12 g) and the triethylamine (1.0 mmol, 0.10 g) were dissolved in dry methanol (20 ml). Stannic chloride ((1.0 mmol, 0.35 g) was added to the mixture and stirred for 12 h. Suitable crystals were obtained by slow evaporation of the solvent.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.95 to 0.99, N—H 0.88 Å) and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 to 1.5 $U(C)$.

The triethylammonium cation is disordered over two positions in a 56.4 (1): 43.6 (1) ratio. The N—C distances were restrained to within 0.01 Å of each other, as were the C—C distances. Because the C11' atom is close to the C11 atom (the C12' atom is also close to the C12 atom), the temperature factors of the C11' atom were restrained to those of the C11 atom; those of the C12' atom were set to those of the C12 atom.

**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $(\text{Et}_3\text{NH})^+ [\text{SnCl}_4(\text{C}_6\text{H}_4\text{NO}_2)]^-$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder in the cation is not shown.

Triethylammonium tetrachlorido(pyridine-2-carboxylato- $\kappa^2\text{N},\text{O}$)stannate(IV)

Crystal data

$(\text{C}_6\text{H}_{16}\text{N})[\text{SnCl}_4(\text{C}_6\text{H}_4\text{NO}_2)]$

$M_r = 484.79$

Monoclinic, $P2_1/n$

Hall symbol: $-P\ 2_1/n$

$a = 11.6310\ (7)\ \text{\AA}$

$b = 10.4912\ (6)\ \text{\AA}$

$c = 16.4452\ (9)\ \text{\AA}$

$\beta = 109.672\ (1)^\circ$

$V = 1889.57\ (19)\ \text{\AA}^3$

$Z = 4$

$F(000) = 960$

$D_x = 1.704\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 8286 reflections

$\theta = 2.3\text{--}28.3^\circ$

$\mu = 1.92\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Prism, colorless

$0.30 \times 0.25 \times 0.05\ \text{mm}$

Data collection

Bruker SMART APEX
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

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

$T_{\min} = 0.596$, $T_{\max} = 0.910$

17476 measured reflections

4344 independent reflections

3896 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.033$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.3^\circ$

$h = -15 \rightarrow 15$

$k = -13 \rightarrow 13$

$l = -19 \rightarrow 21$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.019$

$wR(F^2) = 0.048$

$S = 1.01$

4344 reflections

242 parameters

25 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0213P)^2 + 0.5451P]$

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

$(\Delta/\sigma)_{\max} = 0.001$

$\Delta\rho_{\max} = 0.41 \text{ e } \text{\AA}^{-3}$

$\Delta\rho_{\min} = -0.39 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.563342 (11)	0.304590 (11)	0.743404 (8)	0.01440 (5)	
Cl1	0.37811 (4)	0.38342 (5)	0.64455 (3)	0.02443 (11)	
Cl2	0.47250 (5)	0.23860 (5)	0.84821 (3)	0.02561 (11)	
Cl3	0.56293 (4)	0.08950 (4)	0.69586 (3)	0.01948 (10)	
Cl4	0.67771 (4)	0.36886 (4)	0.65317 (3)	0.01872 (10)	
O1	0.59288 (12)	0.48336 (12)	0.80497 (8)	0.0200 (3)	
O2	0.69627 (13)	0.58704 (13)	0.92554 (9)	0.0263 (3)	
N1	0.74369 (14)	0.28596 (14)	0.84631 (10)	0.0150 (3)	
C1	0.68201 (17)	0.49487 (17)	0.87734 (12)	0.0187 (4)	
C2	0.77238 (17)	0.38638 (17)	0.90022 (11)	0.0151 (4)	
C3	0.87950 (17)	0.39107 (17)	0.96906 (12)	0.0183 (4)	
H3	0.8968	0.4612	1.0079	0.022*	
C4	0.96192 (18)	0.29127 (18)	0.98084 (12)	0.0207 (4)	
H4	1.0377	0.2933	1.0269	0.025*	
C5	0.93224 (19)	0.18882 (18)	0.92456 (12)	0.0208 (4)	
H5	0.9873	0.1195	0.9317	0.025*	
C6	0.82192 (18)	0.18857 (17)	0.85810 (12)	0.0189 (4)	
H6	0.8009	0.1178	0.8199	0.023*	
N2	0.5100 (3)	0.7717 (3)	0.8635 (2)	0.0168 (8)	0.564 (3)
H2	0.5718	0.7181	0.8804	0.020*	0.564 (3)
C7	0.5607 (4)	0.9017 (4)	0.8956 (3)	0.0209 (9)	0.564 (3)
H7A	0.6002	0.9376	0.8559	0.025*	0.564 (3)
H7B	0.4927	0.9589	0.8948	0.025*	0.564 (3)
C8	0.6523 (4)	0.8976 (4)	0.9858 (3)	0.0289 (9)	0.564 (3)
H8A	0.6834	0.9837	1.0035	0.043*	0.564 (3)
H8B	0.7203	0.8416	0.9868	0.043*	0.564 (3)
H8C	0.6130	0.8648	1.0256	0.043*	0.564 (3)
C9	0.4203 (3)	0.7295 (3)	0.9059 (2)	0.0227 (8)	0.564 (3)
H9A	0.3543	0.7936	0.8941	0.027*	0.564 (3)
H9B	0.4623	0.7263	0.9691	0.027*	0.564 (3)
C10	0.3642 (5)	0.6008 (5)	0.8754 (4)	0.0307 (12)	0.564 (3)
H10A	0.3067	0.5791	0.9053	0.046*	0.564 (3)
H10B	0.4286	0.5361	0.8882	0.046*	0.564 (3)
H10C	0.3207	0.6036	0.8130	0.046*	0.564 (3)

C11	0.4630 (14)	0.7685 (17)	0.7665 (4)	0.0215 (11)	0.564 (3)
H11A	0.4388	0.6801	0.7472	0.026*	0.564 (3)
H11B	0.5297	0.7934	0.7450	0.026*	0.564 (3)
C12	0.3551 (13)	0.8558 (13)	0.7272 (9)	0.0279 (18)	0.564 (3)
H12A	0.3340	0.8565	0.6643	0.042*	0.564 (3)
H12B	0.3762	0.9423	0.7497	0.042*	0.564 (3)
H12C	0.2852	0.8250	0.7422	0.042*	0.564 (3)
N2'	0.4707 (4)	0.7281 (4)	0.8540 (3)	0.0178 (10)	0.436 (3)
H2'	0.5376	0.6845	0.8801	0.021*	0.436 (3)
C7'	0.4711 (4)	0.8380 (4)	0.9124 (3)	0.0232 (11)	0.436 (3)
H7'A	0.4561	0.8058	0.9645	0.028*	0.436 (3)
H7'B	0.4036	0.8968	0.8822	0.028*	0.436 (3)
C8'	0.5902 (5)	0.9107 (6)	0.9395 (5)	0.0281 (14)	0.436 (3)
H8'A	0.5857	0.9819	0.9770	0.042*	0.436 (3)
H8'B	0.6050	0.9438	0.8882	0.042*	0.436 (3)
H8'C	0.6570	0.8537	0.9711	0.042*	0.436 (3)
C9'	0.3664 (5)	0.6386 (5)	0.8450 (4)	0.0206 (12)	0.436 (3)
H9'A	0.3600	0.5777	0.7977	0.025*	0.436 (3)
H9'B	0.2895	0.6881	0.8289	0.025*	0.436 (3)
C10'	0.3807 (5)	0.5650 (5)	0.9267 (4)	0.0288 (12)	0.436 (3)
H10D	0.3119	0.5061	0.9166	0.043*	0.436 (3)
H10E	0.3822	0.6245	0.9730	0.043*	0.436 (3)
H10F	0.4572	0.5167	0.9435	0.043*	0.436 (3)
C11'	0.4774 (19)	0.765 (2)	0.7673 (6)	0.0215 (11)	0.44
H11C	0.4877	0.6871	0.7366	0.026*	0.436 (3)
H11D	0.5502	0.8194	0.7762	0.026*	0.436 (3)
C12'	0.3646 (18)	0.8367 (19)	0.7110 (11)	0.0279 (18)	0.44
H12D	0.3698	0.8490	0.6533	0.042*	0.436 (3)
H12E	0.3603	0.9198	0.7370	0.042*	0.436 (3)
H12F	0.2913	0.7872	0.7066	0.042*	0.436 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01336 (7)	0.01342 (7)	0.01478 (7)	0.00074 (5)	0.00259 (5)	-0.00027 (5)
Cl1	0.0152 (2)	0.0307 (3)	0.0233 (2)	0.00400 (19)	0.00109 (19)	0.00435 (19)
Cl2	0.0271 (3)	0.0307 (3)	0.0228 (2)	0.0027 (2)	0.0133 (2)	0.0037 (2)
Cl3	0.0254 (2)	0.0132 (2)	0.0181 (2)	-0.00356 (17)	0.00515 (18)	-0.00112 (17)
Cl4	0.0195 (2)	0.0163 (2)	0.0205 (2)	-0.00436 (17)	0.00697 (18)	-0.00023 (17)
O1	0.0195 (7)	0.0164 (6)	0.0194 (7)	0.0054 (5)	0.0005 (6)	-0.0035 (5)
O2	0.0283 (8)	0.0197 (7)	0.0251 (7)	0.0066 (6)	0.0015 (6)	-0.0080 (6)
N1	0.0164 (8)	0.0141 (7)	0.0131 (7)	0.0015 (6)	0.0033 (6)	-0.0008 (6)
C1	0.0198 (10)	0.0157 (9)	0.0197 (9)	0.0019 (7)	0.0054 (8)	-0.0004 (7)
C2	0.0180 (9)	0.0149 (8)	0.0139 (9)	0.0008 (7)	0.0072 (7)	0.0005 (7)
C3	0.0204 (10)	0.0179 (9)	0.0146 (9)	0.0006 (7)	0.0033 (7)	-0.0012 (7)
C4	0.0187 (10)	0.0236 (10)	0.0159 (9)	0.0029 (8)	0.0008 (8)	0.0029 (7)
C5	0.0234 (10)	0.0183 (9)	0.0191 (10)	0.0073 (8)	0.0049 (8)	0.0024 (7)
C6	0.0221 (10)	0.0152 (9)	0.0192 (9)	0.0031 (7)	0.0069 (8)	-0.0005 (7)

N2	0.0134 (19)	0.018 (2)	0.0199 (17)	0.0040 (13)	0.0071 (15)	0.0005 (15)
C7	0.021 (2)	0.0159 (18)	0.028 (2)	0.0027 (15)	0.012 (2)	-0.0004 (19)
C8	0.036 (3)	0.028 (2)	0.026 (2)	-0.0108 (19)	0.015 (2)	-0.0077 (18)
C9	0.0178 (17)	0.0273 (19)	0.0266 (19)	-0.0008 (14)	0.0120 (15)	-0.0011 (15)
C10	0.030 (2)	0.027 (3)	0.038 (4)	-0.012 (2)	0.015 (3)	-0.003 (2)
C11	0.021 (3)	0.0250 (13)	0.0191 (10)	0.0037 (17)	0.0075 (11)	0.0019 (8)
C12	0.026 (2)	0.029 (4)	0.026 (5)	0.004 (2)	0.006 (2)	0.005 (3)
N2'	0.015 (3)	0.018 (3)	0.022 (2)	0.0004 (17)	0.009 (2)	0.0004 (19)
C7'	0.021 (2)	0.019 (2)	0.030 (3)	-0.0010 (18)	0.010 (2)	-0.0072 (19)
C8'	0.030 (4)	0.023 (3)	0.032 (4)	-0.005 (3)	0.012 (3)	-0.009 (3)
C9'	0.020 (3)	0.018 (3)	0.027 (3)	-0.002 (2)	0.013 (2)	-0.001 (2)
C10'	0.036 (3)	0.027 (3)	0.027 (3)	-0.005 (2)	0.016 (3)	0.001 (2)
C11'	0.021 (3)	0.0250 (13)	0.0191 (10)	0.0037 (17)	0.0075 (11)	0.0019 (8)
C12'	0.026 (2)	0.029 (4)	0.026 (5)	0.004 (2)	0.006 (2)	0.005 (3)

Geometric parameters (Å, °)

Sn1—O1	2.1039 (13)	C10—H10A	0.9800
Sn1—N1	2.2163 (15)	C10—H10B	0.9800
Sn1—C11	2.3686 (5)	C10—H10C	0.9800
Sn1—C13	2.3876 (5)	C11—C12	1.512 (8)
Sn1—C14	2.3990 (5)	C11—H11A	0.9900
Sn1—C12	2.4066 (5)	C11—H11B	0.9900
O1—C1	1.294 (2)	C12—H12A	0.9800
O2—C1	1.226 (2)	C12—H12B	0.9800
N1—C6	1.338 (2)	C12—H12C	0.9800
N1—C2	1.345 (2)	N2'—C7'	1.499 (5)
C1—C2	1.509 (2)	N2'—C9'	1.501 (5)
C2—C3	1.374 (3)	N2'—C11'	1.504 (7)
C3—C4	1.388 (3)	N2'—H2'	0.8800
C3—H3	0.9500	C7'—C8'	1.511 (6)
C4—C5	1.384 (3)	C7'—H7'A	0.9900
C4—H4	0.9500	C7'—H7'B	0.9900
C5—C6	1.377 (3)	C8'—H8'A	0.9800
C5—H5	0.9500	C8'—H8'B	0.9800
C6—H6	0.9500	C8'—H8'C	0.9800
N2—C11	1.503 (6)	C9'—C10'	1.509 (6)
N2—C9	1.503 (4)	C9'—H9'A	0.9900
N2—C7	1.508 (5)	C9'—H9'B	0.9900
N2—H2	0.8800	C10'—H10D	0.9800
C7—C8	1.508 (5)	C10'—H10E	0.9800
C7—H7A	0.9900	C10'—H10F	0.9800
C7—H7B	0.9900	C11'—C12'	1.524 (13)
C8—H8A	0.9800	C11'—H11C	0.9900
C8—H8B	0.9800	C11'—H11D	0.9900
C8—H8C	0.9800	C12'—H12D	0.9800
C9—C10	1.510 (5)	C12'—H12E	0.9800
C9—H9A	0.9900	C12'—H12F	0.9800

C9—H9B	0.9900		
O1—Sn1—N1	75.63 (5)	C9—C10—H10A	109.5
O1—Sn1—Cl1	89.00 (4)	C9—C10—H10B	109.5
N1—Sn1—Cl1	164.42 (4)	H10A—C10—H10B	109.5
O1—Sn1—Cl3	169.14 (4)	C9—C10—H10C	109.5
N1—Sn1—Cl3	93.66 (4)	H10A—C10—H10C	109.5
Cl1—Sn1—Cl3	101.778 (17)	H10B—C10—H10C	109.5
O1—Sn1—Cl4	90.71 (4)	N2—C11—C12	113.1 (11)
N1—Sn1—Cl4	85.28 (4)	N2—C11—H11A	108.9
Cl1—Sn1—Cl4	92.462 (18)	C12—C11—H11A	108.9
Cl3—Sn1—Cl4	90.200 (16)	N2—C11—H11B	108.9
O1—Sn1—Cl2	87.23 (4)	C12—C11—H11B	108.9
N1—Sn1—Cl2	87.63 (4)	H11A—C11—H11B	107.8
Cl1—Sn1—Cl2	94.290 (18)	C11—C12—H12A	109.5
Cl3—Sn1—Cl2	90.554 (18)	C11—C12—H12B	109.5
Cl4—Sn1—Cl2	172.905 (17)	H12A—C12—H12B	109.5
C1—O1—Sn1	118.44 (11)	C11—C12—H12C	109.5
C6—N1—C2	119.80 (16)	H12A—C12—H12C	109.5
C6—N1—Sn1	126.91 (12)	H12B—C12—H12C	109.5
C2—N1—Sn1	113.29 (12)	C7'—N2'—C9'	111.9 (4)
O2—C1—O1	124.09 (17)	C7'—N2'—C11'	114.7 (10)
O2—C1—C2	120.18 (17)	C9'—N2'—C11'	111.5 (10)
O1—C1—C2	115.73 (16)	C7'—N2'—H2'	106.0
N1—C2—C3	121.77 (16)	C9'—N2'—H2'	106.0
N1—C2—C1	115.42 (16)	C11'—N2'—H2'	106.0
C3—C2—C1	122.75 (16)	N2'—C7'—C8'	112.5 (4)
C2—C3—C4	118.69 (17)	N2'—C7'—H7'A	109.1
C2—C3—H3	120.7	C8'—C7'—H7'A	109.1
C4—C3—H3	120.7	N2'—C7'—H7'B	109.1
C5—C4—C3	119.16 (18)	C8'—C7'—H7'B	109.1
C5—C4—H4	120.4	H7'A—C7'—H7'B	107.8
C3—C4—H4	120.4	C7'—C8'—H8'A	109.5
C6—C5—C4	119.22 (17)	C7'—C8'—H8'B	109.5
C6—C5—H5	120.4	H8'A—C8'—H8'B	109.5
C4—C5—H5	120.4	C7'—C8'—H8'C	109.5
N1—C6—C5	121.32 (17)	H8'A—C8'—H8'C	109.5
N1—C6—H6	119.3	H8'B—C8'—H8'C	109.5
C5—C6—H6	119.3	N2'—C9'—C10'	112.9 (5)
C11—N2—C9	115.1 (7)	N2'—C9'—H9'A	109.0
C11—N2—C7	110.6 (8)	C10'—C9'—H9'A	109.0
C9—N2—C7	110.8 (3)	N2'—C9'—H9'B	109.0
C11—N2—H2	106.6	C10'—C9'—H9'B	109.0
C9—N2—H2	106.6	H9'A—C9'—H9'B	107.8
C7—N2—H2	106.6	C9'—C10'—H10D	109.5
C8—C7—N2	112.4 (4)	C9'—C10'—H10E	109.5
C8—C7—H7A	109.1	H10D—C10'—H10E	109.5
N2—C7—H7A	109.1	C9'—C10'—H10F	109.5

C8—C7—H7B	109.1	H10D—C10'—H10F	109.5
N2—C7—H7B	109.1	H10E—C10'—H10F	109.5
H7A—C7—H7B	107.8	N2'—C11'—C12'	113.2 (14)
C7—C8—H8A	109.5	N2'—C11'—H11C	108.9
C7—C8—H8B	109.5	C12'—C11'—H11C	108.9
H8A—C8—H8B	109.5	N2'—C11'—H11D	108.9
C7—C8—H8C	109.5	C12'—C11'—H11D	108.9
H8A—C8—H8C	109.5	H11C—C11'—H11D	107.7
H8B—C8—H8C	109.5	C11'—C12'—H12D	109.5
N2—C9—C10	113.6 (3)	C11'—C12'—H12E	109.5
N2—C9—H9A	108.8	H12D—C12'—H12E	109.5
C10—C9—H9A	108.8	C11'—C12'—H12F	109.5
N2—C9—H9B	108.8	H12D—C12'—H12F	109.5
C10—C9—H9B	108.8	H12E—C12'—H12F	109.5
H9A—C9—H9B	107.7		
N1—Sn1—O1—C1	-11.42 (13)	O1—C1—C2—N1	-5.5 (2)
Cl1—Sn1—O1—C1	171.18 (14)	O2—C1—C2—C3	-7.3 (3)
Cl3—Sn1—O1—C1	-1.6 (3)	O1—C1—C2—C3	171.81 (17)
Cl4—Sn1—O1—C1	-96.37 (14)	N1—C2—C3—C4	2.5 (3)
Cl2—Sn1—O1—C1	76.84 (14)	C1—C2—C3—C4	-174.58 (18)
O1—Sn1—N1—C6	-171.97 (17)	C2—C3—C4—C5	-1.8 (3)
Cl1—Sn1—N1—C6	-162.25 (12)	C3—C4—C5—C6	0.2 (3)
Cl3—Sn1—N1—C6	9.87 (16)	C2—N1—C6—C5	-0.2 (3)
Cl4—Sn1—N1—C6	-80.03 (15)	Sn1—N1—C6—C5	179.52 (14)
Cl2—Sn1—N1—C6	100.27 (16)	C4—C5—C6—N1	0.8 (3)
O1—Sn1—N1—C2	7.73 (12)	C11—N2—C7—C8	-156.5 (7)
Cl1—Sn1—N1—C2	17.5 (2)	C9—N2—C7—C8	74.7 (4)
Cl3—Sn1—N1—C2	-170.42 (12)	C11—N2—C9—C10	52.6 (8)
Cl4—Sn1—N1—C2	99.68 (12)	C7—N2—C9—C10	179.0 (4)
Cl2—Sn1—N1—C2	-80.02 (12)	C9—N2—C11—C12	61.6 (14)
Sn1—O1—C1—O2	-167.96 (16)	C7—N2—C11—C12	-64.9 (13)
Sn1—O1—C1—C2	12.9 (2)	C9'—N2'—C7'—C8'	166.0 (5)
C6—N1—C2—C3	-1.5 (3)	C11'—N2'—C7'—C8'	-65.8 (10)
Sn1—N1—C2—C3	178.74 (14)	C7'—N2'—C9'—C10'	-69.7 (6)
C6—N1—C2—C1	175.77 (17)	C11'—N2'—C9'—C10'	160.4 (10)
Sn1—N1—C2—C1	-4.0 (2)	C7'—N2'—C11'—C12'	-66.1 (18)
O2—C1—C2—N1	175.38 (18)	C9'—N2'—C11'—C12'	62.3 (19)

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2 \cdots O2	0.88	1.95	2.828 (4)	172
N2'—H2' \cdots O2	0.88	2.02	2.895 (5)	173