Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(Dimethylamino)pyridinium tetrachlorido(quinoline-2-carboxylato-κ^2N,O)stannate(IV)

Ezzatollah Najafi,[a] Mostafa M. Amini[a] and Seik Weng Ng[b,c]*

[a]Department of Chemistry, General Campus, Shahid Beheshti University, Tehran 1983963113, Iran, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

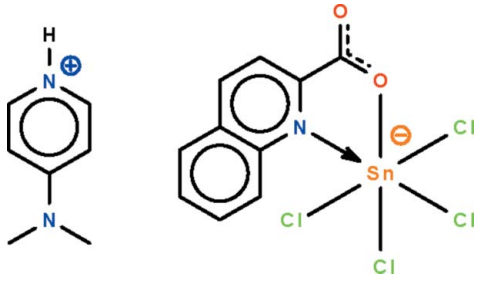
Received 1 August 2011; accepted 4 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.021; wR factor = 0.047; data-to-parameter ratio = 18.4.

In the title salt, $(C_7H_{11}N_2)[SnCl_4(C_{10}H_6NO_2)]$, the Sn^{IV} atom is chelated by the N,O-bidentate carboxylate ions and four chloride ions, showing a distorted octahedral $SnNOCl_4$ coordination. In the crystal, the cation and anion are linked by a pyridinium–carboxylate N—H···O hydrogen bond.

Related literature

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



Experimental

Crystal data

$(C_7H_{11}N_2)[SnCl_4(C_{10}H_6NO_2)]$
M_r = 555.83
Triclinic, $P\overline{1}$
a = 8.6681 (3) Å
b = 8.8407 (4) Å
c = 14.4447 (5) Å
α = 96.721 (3)°
β = 91.924 (3)°
γ = 108.038 (4)°
V = 1042.43 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.76 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.10 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.621, T_{max} = 0.844
8056 measured reflections
4610 independent reflections
4202 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.047
S = 1.06
4610 reflections
250 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.52 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1	0.87 (1)	1.98 (1)	2.816 (2)	160 (2)

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; 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: *publCIF* (Westrip, 2010).

We thank Shahid Beheshti University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5284).

References

Agilent (2010). *CrysAlis PRO*. Agilent Technologies, Yarnton, England.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Najafi, E., Amini, M. M. & Ng, S. W. (2011). *Acta Cryst.* E**67**, m351.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supplementary materials

Acta Cryst. (2011). E**67**, m1224 [**doi:10.1107/S1600536811031473**]

4-(Dimethylamino)pyridinium tetrachlorido(quinoline-2-carboxylato-κ^2N,O)stannate(IV)

E. Najafi, M. M. Amini and S. W. Ng

Comment

We have recently synthesized some ammonium tetrachlorido(carboxylato)stannates; in a recent study, we reacted stannic chloride with pyridine-2-carboxylic acid and triethylamine to yield the chelated stannate salt (Najafi *et al.*, 2011). The use of quinoline-2-carboxylic acid and 4-dimethyaminopyridine yielded the expected dimethylaminopyridinium stannate in which the amine is protonated on the aromatic nitrogen atom (Scheme I, Fig. 1). The Sn^{IV} atom is chelated by the *N*,*O*-bidentate carboxylate ligand and four chloride ions, and shows octahedral $SnNOCl_4$ coordination at the metal atom. The cation and anion are linked an $N–H_{pyridinium}\cdots O$ hydrogen bond (Table 1).

Experimental

Stannic chloride pentahydrate (1 mmol), quinoline-2-carboxylic acid (1 mmol) and 4-dimethylaminopyridine (1 mmol) were loaded into a convection tube and the tube was filled with dry methanol and kept at 333 K. Colorless crystals were collected from the side arm after several days.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, U_{iso}(H) 1.2 to 1.5U_{eq}(C)] and were included in the refinement in the riding model approximation.

The ammonium H-atom was located in a difference Fourier map, and was refined with a distance restraint of N–H 0.88±0.01 Å; its temperature factor was refined.

Omitted from the refinement was the (0 1 0) reflection.

Figures

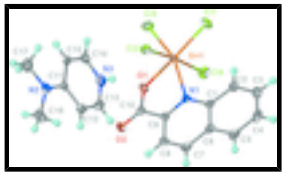


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $(C_7H_{11}N_2)[SnCl_4(C_{10}H_6NO_2)]$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

4-(Dimethylamino)pyridinium tetrachlorido(quinoline-2-carboxylato-κ^2*N*,*O*)stannate(IV)

Crystal data

$(C_7H_{11}N_2)[SnCl_4(C_{10}H_6NO_2)]$ $Z = 2$

M_r = 555.83	F(000) = 548
Triclinic, $P\overline{1}$	D_x = 1.771 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation, λ = 0.71073 Å
a = 8.6681 (3) Å	Cell parameters from 5833 reflections
b = 8.8407 (4) Å	θ = 2.4–29.2°
c = 14.4447 (5) Å	μ = 1.76 mm^{-1}
α = 96.721 (3)°	T = 100 K
β = 91.924 (3)°	Block, colorless
γ = 108.038 (4)°	0.30 × 0.20 × 0.10 mm
V = 1042.43 (7) Å^3	

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	4610 independent reflections
Radiation source: SuperNova (Mo) X-ray Source	4202 reflections with $I > 2\sigma(I)$
Mirror	R_{int} = 0.022
Detector resolution: 10.4041 pixels mm^{-1}	θ_{max} = 27.5°, θ_{min} = 2.5°
ω scans	h = −8→11
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)	k = −11→11
T_{min} = 0.621, T_{max} = 0.844	l = −18→18
8056 measured reflections	

Refinement

Refinement on F^2	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)]$ = 0.021	Hydrogen site location: inferred from neighbouring sites
$wR(F^2)$ = 0.047	H atoms treated by a mixture of independent and constrained refinement
S = 1.06	$w = 1/[\sigma^2(F_o^2) + (0.0181P)^2 + 0.127P]$ where $P = (F_o^2 + 2F_c^2)/3$
4610 reflections	$(\Delta/\sigma)_{max}$ = 0.001
250 parameters	$\Delta\rho_{max}$ = 0.52 e Å^{-3}
1 restraint	$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Sn1	0.361135 (16)	0.258730 (15)	0.271428 (9)	0.01232 (5)
Cl1	0.16903 (6)	0.37830 (6)	0.33361 (4)	0.02211 (12)
Cl2	0.13953 (6)	0.04597 (6)	0.18599 (3)	0.01824 (11)
Cl3	0.41373 (6)	0.41174 (6)	0.14341 (4)	0.02133 (11)
Cl4	0.58090 (6)	0.44245 (6)	0.37084 (4)	0.02246 (12)
O1	0.51697 (17)	0.14313 (16)	0.21142 (9)	0.0165 (3)

O2	0.57573 (18)	−0.08559 (17)	0.19327 (10)	0.0207 (3)
N1	0.36250 (19)	0.06808 (18)	0.36458 (10)	0.0124 (3)
N2	1.0685 (2)	0.3405 (2)	−0.12106 (11)	0.0173 (4)
N3	0.7058 (2)	0.2281 (2)	0.05939 (12)	0.0203 (4)
H3	0.629 (2)	0.206 (3)	0.0979 (13)	0.024 (6)*
C1	0.2921 (2)	0.0400 (2)	0.44784 (13)	0.0134 (4)
C2	0.2404 (2)	0.1582 (2)	0.49972 (13)	0.0173 (4)
H2	0.2535	0.2582	0.4777	0.021*
C3	0.1712 (3)	0.1279 (3)	0.58221 (14)	0.0203 (5)
H3A	0.1369	0.2080	0.6172	0.024*
C4	0.1499 (3)	−0.0194 (3)	0.61614 (14)	0.0219 (5)
H4	0.0987	−0.0389	0.6726	0.026*
C5	0.2022 (2)	−0.1341 (3)	0.56843 (14)	0.0194 (5)
H5	0.1888	−0.2327	0.5923	0.023*
C6	0.2768 (2)	−0.1071 (2)	0.48305 (13)	0.0158 (4)
C7	0.3379 (2)	−0.2201 (2)	0.43302 (14)	0.0172 (4)
H7	0.3269	−0.3199	0.4550	0.021*
C8	0.4130 (2)	−0.1860 (2)	0.35297 (13)	0.0164 (4)
H8	0.4577	−0.2598	0.3196	0.020*
C9	0.4230 (2)	−0.0400 (2)	0.32101 (13)	0.0133 (4)
C10	0.5114 (2)	0.0037 (2)	0.23433 (13)	0.0145 (4)
C11	0.9504 (2)	0.3054 (2)	−0.06169 (13)	0.0143 (4)
C12	0.9714 (3)	0.2416 (2)	0.02178 (14)	0.0184 (4)
H12	1.0717	0.2248	0.0375	0.022*
C13	0.8486 (3)	0.2047 (2)	0.07897 (14)	0.0205 (5)
H13	0.8638	0.1612	0.1344	0.025*
C14	0.6811 (3)	0.2898 (2)	−0.01880 (14)	0.0199 (5)
H14	0.5797	0.3062	−0.0316	0.024*
C15	0.7983 (2)	0.3288 (2)	−0.07943 (14)	0.0166 (4)
H15	0.7784	0.3720	−0.1341	0.020*
C16	1.2127 (3)	0.2906 (3)	−0.10898 (16)	0.0242 (5)
H16A	1.2761	0.3488	−0.0511	0.036*
H16B	1.2794	0.3146	−0.1621	0.036*
H16C	1.1793	0.1750	−0.1057	0.036*
C17	1.0413 (3)	0.3978 (3)	−0.20898 (14)	0.0258 (5)
H17A	0.9928	0.4840	−0.1971	0.039*
H17B	0.9676	0.3091	−0.2522	0.039*
H17C	1.1454	0.4388	−0.2367	0.039*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01240 (7)	0.01035 (8)	0.01461 (8)	0.00357 (6)	0.00258 (5)	0.00280 (5)
Cl1	0.0238 (3)	0.0179 (3)	0.0275 (3)	0.0104 (2)	0.0071 (2)	0.0023 (2)
Cl2	0.0183 (3)	0.0146 (2)	0.0197 (2)	0.0034 (2)	−0.0038 (2)	0.00033 (19)
Cl3	0.0229 (3)	0.0214 (3)	0.0235 (3)	0.0086 (2)	0.0061 (2)	0.0125 (2)
Cl4	0.0208 (3)	0.0168 (3)	0.0243 (3)	−0.0010 (2)	−0.0032 (2)	0.0012 (2)
O1	0.0185 (7)	0.0168 (7)	0.0173 (7)	0.0084 (6)	0.0074 (6)	0.0045 (6)

O2	0.0244 (8)	0.0229 (8)	0.0197 (8)	0.0145 (7)	0.0054 (6)	0.0025 (6)
N1	0.0110 (8)	0.0117 (8)	0.0134 (8)	0.0021 (7)	0.0000 (7)	0.0015 (6)
N2	0.0155 (9)	0.0163 (9)	0.0181 (9)	0.0026 (7)	0.0042 (7)	0.0005 (7)
N3	0.0200 (10)	0.0245 (10)	0.0175 (9)	0.0072 (8)	0.0089 (8)	0.0042 (7)
C1	0.0110 (9)	0.0149 (10)	0.0122 (9)	0.0010 (8)	−0.0007 (8)	0.0027 (8)
C2	0.0167 (10)	0.0170 (11)	0.0171 (10)	0.0039 (9)	−0.0004 (8)	0.0024 (8)
C3	0.0164 (11)	0.0256 (12)	0.0177 (10)	0.0062 (9)	0.0013 (9)	−0.0013 (9)
C4	0.0159 (11)	0.0329 (13)	0.0134 (10)	0.0027 (10)	0.0022 (8)	0.0030 (9)
C5	0.0159 (10)	0.0194 (11)	0.0183 (10)	−0.0027 (9)	−0.0010 (9)	0.0075 (9)
C6	0.0126 (10)	0.0164 (10)	0.0155 (10)	0.0006 (8)	−0.0029 (8)	0.0032 (8)
C7	0.0187 (11)	0.0117 (10)	0.0187 (10)	0.0012 (9)	−0.0048 (9)	0.0034 (8)
C8	0.0166 (10)	0.0146 (10)	0.0169 (10)	0.0052 (9)	−0.0034 (8)	−0.0013 (8)
C9	0.0113 (9)	0.0139 (10)	0.0136 (10)	0.0033 (8)	−0.0012 (8)	0.0003 (8)
C10	0.0120 (10)	0.0171 (10)	0.0136 (10)	0.0039 (8)	−0.0016 (8)	0.0019 (8)
C11	0.0157 (10)	0.0098 (9)	0.0154 (10)	0.0021 (8)	0.0023 (8)	−0.0022 (7)
C12	0.0170 (10)	0.0204 (11)	0.0193 (10)	0.0084 (9)	0.0006 (9)	0.0020 (8)
C13	0.0245 (12)	0.0204 (11)	0.0179 (10)	0.0077 (10)	0.0017 (9)	0.0062 (8)
C14	0.0178 (11)	0.0230 (12)	0.0198 (11)	0.0096 (9)	0.0000 (9)	−0.0020 (9)
C15	0.0195 (11)	0.0174 (10)	0.0143 (10)	0.0086 (9)	−0.0002 (8)	0.0002 (8)
C16	0.0132 (10)	0.0261 (12)	0.0317 (12)	0.0054 (9)	0.0070 (9)	−0.0015 (10)
C17	0.0333 (13)	0.0236 (12)	0.0204 (11)	0.0065 (10)	0.0118 (10)	0.0068 (9)

Geometric parameters (Å, °)

Sn1—O1	2.0848 (13)	C4—H4	0.9500
Sn1—N1	2.2790 (16)	C5—C6	1.422 (3)
Sn1—Cl1	2.3802 (5)	C5—H5	0.9500
Sn1—Cl4	2.3840 (5)	C6—C7	1.409 (3)
Sn1—Cl3	2.3912 (5)	C7—C8	1.365 (3)
Sn1—Cl2	2.4106 (5)	C7—H7	0.9500
O1—C10	1.301 (2)	C8—C9	1.400 (3)
O2—C10	1.213 (2)	C8—H8	0.9500
N1—C9	1.333 (2)	C9—C10	1.516 (3)
N1—C1	1.381 (2)	C11—C15	1.416 (3)
N2—C11	1.343 (2)	C11—C12	1.419 (3)
N2—C17	1.459 (3)	C12—C13	1.353 (3)
N2—C16	1.460 (3)	C12—H12	0.9500
N3—C13	1.343 (3)	C13—H13	0.9500
N3—C14	1.348 (3)	C14—C15	1.353 (3)
N3—H3	0.869 (9)	C14—H14	0.9500
C1—C2	1.408 (3)	C15—H15	0.9500
C1—C6	1.421 (3)	C16—H16A	0.9800
C2—C3	1.369 (3)	C16—H16B	0.9800
C2—H2	0.9500	C16—H16C	0.9800
C3—C4	1.406 (3)	C17—H17A	0.9800
C3—H3A	0.9500	C17—H17B	0.9800
C4—C5	1.360 (3)	C17—H17C	0.9800
O1—Sn1—N1	75.24 (5)	C7—C6—C5	122.27 (19)
O1—Sn1—Cl1	176.27 (4)	C1—C6—C5	118.72 (19)

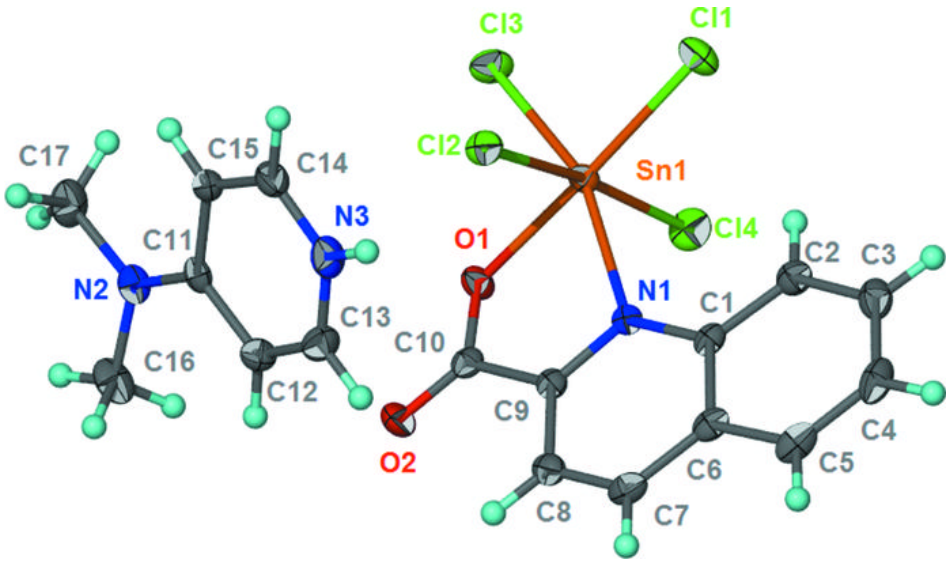
N1—Sn1—Cl1	104.74 (4)	C8—C7—C6	119.87 (18)
O1—Sn1—Cl4	90.93 (4)	C8—C7—H7	120.1
N1—Sn1—Cl4	88.46 (4)	C6—C7—H7	120.1
Cl1—Sn1—Cl4	92.797 (19)	C7—C8—C9	118.64 (19)
O1—Sn1—Cl3	85.08 (4)	C7—C8—H8	120.7
N1—Sn1—Cl3	160.21 (4)	C9—C8—H8	120.7
Cl1—Sn1—Cl3	94.762 (18)	N1—C9—C8	123.44 (17)
Cl4—Sn1—Cl3	93.991 (19)	N1—C9—C10	116.83 (17)
O1—Sn1—Cl2	87.29 (4)	C8—C9—C10	119.70 (17)
N1—Sn1—Cl2	83.40 (4)	O2—C10—O1	124.30 (18)
Cl1—Sn1—Cl2	89.002 (18)	O2—C10—C9	120.59 (18)
Cl4—Sn1—Cl2	171.852 (17)	O1—C10—C9	115.05 (17)
Cl3—Sn1—Cl2	93.779 (18)	N2—C11—C15	121.88 (18)
C10—O1—Sn1	118.81 (12)	N2—C11—C12	121.52 (19)
C9—N1—C1	119.22 (16)	C15—C11—C12	116.60 (18)
C9—N1—Sn1	110.22 (12)	C13—C12—C11	119.88 (19)
C1—N1—Sn1	129.82 (13)	C13—C12—H12	120.1
C11—N2—C17	120.69 (18)	C11—C12—H12	120.1
C11—N2—C16	120.42 (17)	N3—C13—C12	121.67 (19)
C17—N2—C16	117.65 (17)	N3—C13—H13	119.2
C13—N3—C14	120.35 (18)	C12—C13—H13	119.2
C13—N3—H3	120.3 (15)	N3—C14—C15	121.2 (2)
C14—N3—H3	119.4 (15)	N3—C14—H14	119.4
N1—C1—C2	120.50 (17)	C15—C14—H14	119.4
N1—C1—C6	119.72 (17)	C14—C15—C11	120.29 (19)
C2—C1—C6	119.74 (17)	C14—C15—H15	119.9
C3—C2—C1	119.50 (19)	C11—C15—H15	119.9
C3—C2—H2	120.2	N2—C16—H16A	109.5
C1—C2—H2	120.2	N2—C16—H16B	109.5
C2—C3—C4	121.3 (2)	H16A—C16—H16B	109.5
C2—C3—H3A	119.3	N2—C16—H16C	109.5
C4—C3—H3A	119.3	H16A—C16—H16C	109.5
C5—C4—C3	120.29 (19)	H16B—C16—H16C	109.5
C5—C4—H4	119.9	N2—C17—H17A	109.5
C3—C4—H4	119.9	N2—C17—H17B	109.5
C4—C5—C6	120.34 (19)	H17A—C17—H17B	109.5
C4—C5—H5	119.8	N2—C17—H17C	109.5
C6—C5—H5	119.8	H17A—C17—H17C	109.5
C7—C6—C1	119.00 (17)	H17B—C17—H17C	109.5
N1—Sn1—O1—C10	17.16 (14)	C4—C5—C6—C1	−1.4 (3)
Cl4—Sn1—O1—C10	105.32 (14)	C1—C6—C7—C8	1.2 (3)
Cl3—Sn1—O1—C10	−160.75 (14)	C5—C6—C7—C8	−177.90 (19)
Cl2—Sn1—O1—C10	−66.72 (14)	C6—C7—C8—C9	−1.9 (3)
O1—Sn1—N1—C9	−16.03 (12)	C1—N1—C9—C8	2.9 (3)
Cl1—Sn1—N1—C9	160.11 (12)	Sn1—N1—C9—C8	−168.24 (16)
Cl4—Sn1—N1—C9	−107.40 (12)	C1—N1—C9—C10	−174.97 (16)
Cl3—Sn1—N1—C9	−9.9 (2)	Sn1—N1—C9—C10	13.9 (2)
Cl2—Sn1—N1—C9	72.90 (12)	C7—C8—C9—N1	−0.2 (3)
O1—Sn1—N1—C1	174.03 (17)	C7—C8—C9—C10	177.68 (17)

Cl1—Sn1—N1—C1	−9.83 (16)	Sn1—O1—C10—O2	167.37 (15)
Cl4—Sn1—N1—C1	82.65 (16)	Sn1—O1—C10—C9	−15.3 (2)
Cl3—Sn1—N1—C1	−179.84 (11)	N1—C9—C10—O2	176.83 (18)
Cl2—Sn1—N1—C1	−97.05 (16)	C8—C9—C10—O2	−1.1 (3)
C9—N1—C1—C2	174.22 (18)	N1—C9—C10—O1	−0.6 (3)
Sn1—N1—C1—C2	−16.6 (3)	C8—C9—C10—O1	−178.61 (17)
C9—N1—C1—C6	−3.6 (3)	C17—N2—C11—C15	−2.8 (3)
Sn1—N1—C1—C6	165.62 (14)	C16—N2—C11—C15	−169.76 (18)
N1—C1—C2—C3	−179.86 (18)	C17—N2—C11—C12	176.65 (18)
C6—C1—C2—C3	−2.1 (3)	C16—N2—C11—C12	9.6 (3)
C1—C2—C3—C4	−0.3 (3)	N2—C11—C12—C13	−178.67 (19)
C2—C3—C4—C5	1.8 (3)	C15—C11—C12—C13	0.8 (3)
C3—C4—C5—C6	−0.9 (3)	C14—N3—C13—C12	0.0 (3)
N1—C1—C6—C7	1.6 (3)	C11—C12—C13—N3	−0.5 (3)
C2—C1—C6—C7	−176.23 (18)	C13—N3—C14—C15	0.3 (3)
N1—C1—C6—C5	−179.32 (17)	N3—C14—C15—C11	−0.1 (3)
C2—C1—C6—C5	2.9 (3)	N2—C11—C15—C14	178.95 (19)
C4—C5—C6—C7	177.70 (19)	C12—C11—C15—C14	−0.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1	0.87 (1)	1.98 (1)	2.816 (2)	160 (2)

Fig. 1


Cl3
Cl1
Cl2
Sn1
Cl4
C17
C15
C14
N3
C11
O1
C2
C3
N2
N1
C1
C13
C10
C16
C12
C9
C4
O2
C6
C5
C8
C7