metal-organic compounds

2-(Ethoxycarbonyl)quinolinium butyl-trichlorido(quinoline-2-carboxylato-κ^2N,O)stannate(IV)

Hongyun Wang,[a] Handong Yin[a]* and Yuying Sun[b]

[a]College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China, and [b]Analytical and Testing Center of Beihua University, 132013, People's Republic of China
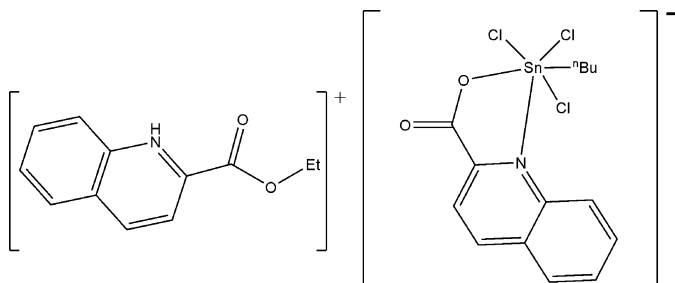Correspondence e-mail: handongyin@163.com

In the title compound, $(C_{12}H_{12}NO_2)[Sn(C_4H_9)(C_{10}H_6NO_2)Cl_3]$, the Sn atom is coordinated by one O and one N atom of a quinolinium-2-carboxylate anion, three Cl atoms and one butyl ligand within a distorted octahedron. Three C atoms of the butyl ligand are disordered and were refined using a split model; the site occupancies are 0.57 and 0.43. The NH group of the cation is involved in intermolecular N—H···O hydrogen bonding.

Related literature

For related literature, see: Xie *et al.* (1991); Ma *et al.* (2006).

Experimental

Crystal data

$(C_{12}H_{12}NO_2)[Sn(C_4H_9)(C_{10}H_6NO_2)Cl_3]$
$M_r = 656.54$
Monoclinic, $P2_1/c$
$a = 13.6828$ (18) Å
$b = 11.0449$ (15) Å
$c = 18.598$ (2) Å
$\beta = 93.898$ (2)°
$V = 2804.1$ (6) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.23$ mm^{-1}
$T = 293$ (2) K
$0.43 \times 0.25 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.620$, $T_{max} = 0.876$
13504 measured reflections
4942 independent reflections
2884 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.132$
$S = 1.00$
4942 reflections
328 parameters
15 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.41$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.079 (4)	Sn1—Cl2	2.4405 (18)
Sn1—C11	2.142 (7)	Sn1—Cl3	2.4482 (18)
Sn1—N1	2.371 (4)	Sn1—Cl1	2.4924 (16)
O1—Sn1—C11	172.6 (2)	N1—Sn1—Cl3	84.64 (12)
O1—Sn1—N1	73.06 (16)	Cl2—Sn1—Cl3	94.28 (6)
C11—Sn1—N1	107.7 (3)	O1—Sn1—Cl1	83.87 (13)
O1—Sn1—Cl2	82.66 (12)	C11—Sn1—Cl1	88.8 (2)
C11—Sn1—Cl2	96.4 (3)	N1—Sn1—Cl1	84.22 (12)
N1—Sn1—Cl2	155.72 (13)	Cl2—Sn1—Cl1	93.73 (6)
O1—Sn1—Cl3	87.93 (13)	Cl3—Sn1—Cl1	167.71 (6)
C11—Sn1—Cl3	99.5 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2—H2···O2^i	0.86	2.26	3.078 (7)	158
N2—H2···O4^i	0.86	2.53	2.990 (6)	114

Symmetry code: (i) $-x + 2, -y, -z + 1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

References

Ma, C. L., Li, J. K., Zhang, R. F. & Wang, D. Q. (2006). *J. Organomet. Chem.* **691**, 1713–1721.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997a). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997b). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Xie, Q. L., Li, S. H., Zhang, D. K., Zhang, Z. G. & Hu, J. M. (1991). *Acta Chim. Sinica*, **49**, 723–728.

supporting information

2-(Ethoxycarbonyl)quinolinium butyltrichlorido(quinoline-2-carboxylato-*κ²N,O*)stannate(IV)

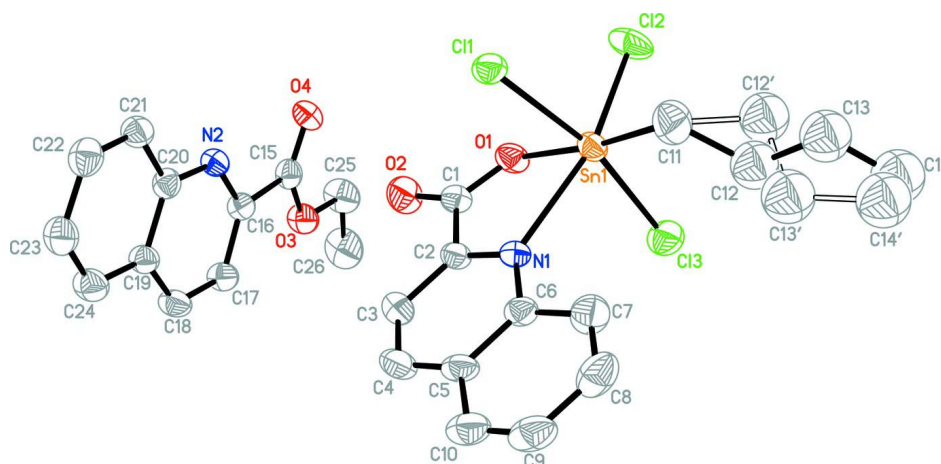### Hongyun Wang, Handong Yin and Yuying Sun

S1. Comment

Organotin esters of carboxylic acids are widely used as biocidesand fungicides and in industry as homogeneous catalysts(Q. *L*. Xie *et al.*, 1991). As a part of our ongoing investigations in this field we have synthesized the title compound and determined its crystal structure. The crystal structure of the title compound consists of discrete [ethyl-(quinolinium-2-carboxylate)] cations and discrete [trichloro-butyl-(quinoline-2-carboxylato)tin(IV)] anions (Fig. 1 and Table 1). The Sn atom is coordinated by one O and one N atom of a quinolinium-2-carboxylate anion, which acts as a chelate ligand, three chloro atoms and one carbon atom of the butyl ligand within a distorted octahedral environment. The Sn1—O1 distance of 2.079 (4)Å and the Sn1—N1 distance of 2.371 (4) Å are comparable to those in similar organotin carboxylates (C. *L*. Ma *et al.*, 2006). The N—H H atom of the [ethyl(quinolinium-2-carboxylate)] cation is involved in intermolecular N—H⋯O hydrogen bonding to O2 of the [ethyl(quinolinium-2-carboxylate)] anion (Table 2). The N—H atom forms an additional very weak hydrogen bond to O4 of a second [ethyl(quinolinium-2-carboxylate)] anion.

S2. Experimental

The reaction was carried out under nitrogen atmosphere. Quinoline-2-carboxylic acid (1 mmol) and sodium ethoxide (1.2 mmol) were added to the solution of ethanol (30 ml) in a Schlenk flask and stirred for 0.5 h. Butyltin trichloride (1 mmol) was added to the Schlenk flask and the reaction mixture was stirred for 12 h at 313 K.The solvent was removed from the clear under reduced pressure. The crew prodcut was recrystallized from a mixture of dichloromethane/methanol (1:1). (yield 76%; m.p. 466 K). Analysis calculated (%) for $C_{26}H_{27}Cl_3N_2O_4Sn$ (Mr = 656.54): C, 47.56; H, 4.14; N, 4.27. found: C, 47.49; H, 4.21; N, 4.32.

S3. Refinement

The C—H and N—H H atoms were positioned with idealized geometry and were refined isotropic $U_{iso}(H) = 1.5\ U_{eq}$ for methyl H atoms and $U_{iso}(H) = 1.2\ U_{eq}$ for all other H atoms using a riding model with with N—H = 0.86 Å and C—H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, The carbon atoms C12, C13, and C14 of the butyl ligand are disordered and were refined using a split model. In the first refinements the site-occupancy factors were refined using fixed isotropic displacement parameters and in the final refinement they were fixed at 0.57 for C12, C13 and C14 and to 0.43 for C12′, C13′ and C14′. The atoms with higher occupancy were refined anisotropic and those of lower occupancy were refined only isotropic.

Figure 1

Crystal structure of the title compound with labeling and displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity and the two orientations of the disordered butyl ligand is shown as closed and open lines.

2-(Ethoxycarbonyl)quinolinium butyltrichlorido(quinoline-2-carboxylato-$\kappa^2 N,O$)tin(IV)

Crystal data

$(C_{12}H_{12}NO_2)[Sn(C_4H_9)(C_{10}H_6NO_2)Cl_3]$	$F(000) = 1320$
$M_r = 656.54$	$D_x = 1.555$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 13.6828$ (18) Å	Cell parameters from 2742 reflections
$b = 11.0449$ (15) Å	$\theta = 2.2$–20.4°
$c = 18.598$ (2) Å	$\mu = 1.23$ mm^{-1}
$\beta = 93.898$ (2)°	$T = 293$ K
$V = 2804.1$ (6) Å^3	Block, colourless
$Z = 4$	$0.43 \times 0.25 \times 0.11$ mm

Data collection

Bruker SMART CCD area-detector diffractometer	13504 measured reflections
Radiation source: fine-focus sealed tube	4942 independent reflections
Graphite monochromator	2884 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.050$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$\theta_{max} = 25.0°$, $\theta_{min} = 1.5°$
	$h = -16 \rightarrow 12$
	$k = -13 \rightarrow 13$
$T_{min} = 0.620$, $T_{max} = 0.877$	$l = -18 \rightarrow 22$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.046$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.132$	
$S = 1.00$	H-atom parameters constrained
4942 reflections	$w = 1/[\sigma^2(F_o^2) + (0.064P)^2]$
328 parameters	where $P = (F_o^2 + 2F_c^2)/3$
15 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.64$ e Å^{-3}
	$\Delta\rho_{min} = -0.41$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.69831 (3)	0.03081 (4)	0.28168 (2)	0.04929 (18)	
Cl1	0.74131 (13)	−0.15041 (15)	0.35719 (8)	0.0612 (5)	
Cl2	0.82158 (17)	−0.01177 (16)	0.19623 (10)	0.0823 (7)	
Cl3	0.65882 (15)	0.23171 (16)	0.23224 (10)	0.0769 (6)	
O1	0.8168 (3)	0.1091 (4)	0.3402 (2)	0.0581 (12)	
O2	0.8843 (4)	0.1604 (5)	0.4467 (3)	0.0805 (15)	
N1	0.6386 (4)	0.1089 (4)	0.3890 (2)	0.0458 (12)	
C1	0.8125 (5)	0.1382 (5)	0.4063 (4)	0.0512 (16)	
C2	0.7123 (5)	0.1434 (5)	0.4343 (3)	0.0470 (15)	
C3	0.6989 (6)	0.1831 (6)	0.5037 (3)	0.0617 (18)	
H3	0.7526	0.2064	0.5339	0.074*	
C4	0.6076 (6)	0.1880 (6)	0.5275 (4)	0.072 (2)	
H4	0.5983	0.2139	0.5742	0.087*	
C5	0.5276 (5)	0.1540 (6)	0.4815 (4)	0.0591 (18)	
C6	0.5443 (5)	0.1167 (5)	0.4111 (3)	0.0497 (16)	
C7	0.4649 (5)	0.0865 (7)	0.3630 (4)	0.076 (2)	
H7	0.4755	0.0634	0.3161	0.092*	
C8	0.3722 (6)	0.0909 (8)	0.3852 (5)	0.093 (3)	
H8	0.3195	0.0703	0.3533	0.112*	
C9	0.3554 (7)	0.1265 (8)	0.4561 (6)	0.093 (3)	
H9	0.2921	0.1281	0.4714	0.111*	
C10	0.4302 (7)	0.1574 (7)	0.5005 (5)	0.082 (3)	
H10	0.4178	0.1827	0.5468	0.099*	
C11	0.5827 (6)	−0.0718 (7)	0.2273 (4)	0.093 (3)	
H11A	0.6106	−0.1407	0.2037	0.111*	0.57
H11B	0.5396	−0.1023	0.2625	0.111*	0.57
H11C	0.6017	−0.1564	0.2288	0.111*	0.43
H11D	0.5249	−0.0640	0.2544	0.111*	0.43
C12	0.5211 (17)	0.0064 (16)	0.1694 (10)	0.120 (6)*	0.57
H12A	0.4823	0.0644	0.1943	0.144*	0.57
H12B	0.5659	0.0516	0.1414	0.144*	0.57
C13	0.4535 (16)	−0.0666 (17)	0.1185 (10)	0.144 (7)*	0.57
H13A	0.3999	−0.1010	0.1433	0.173*	0.57
H13B	0.4887	−0.1313	0.0962	0.173*	0.57
C14	0.4166 (18)	0.0265 (18)	0.0631 (12)	0.148 (9)*	0.57
H14A	0.3730	−0.0118	0.0274	0.222*	0.57
H14B	0.4712	0.0606	0.0402	0.222*	0.57
H14C	0.3824	0.0895	0.0865	0.222*	0.57
C12′	0.553 (2)	−0.038 (3)	0.1457 (10)	0.147 (12)*	0.43
H12C	0.5956	0.0233	0.1271	0.176*	0.43
H12D	0.5502	−0.1082	0.1143	0.176*	0.43
C13′	0.451 (2)	0.011 (3)	0.1610 (18)	0.196 (16)*	0.43
H13C	0.4580	0.0926	0.1803	0.235*	0.43
H13D	0.4235	−0.0390	0.1974	0.235*	0.43
C14′	0.379 (2)	0.014 (3)	0.0927 (17)	0.155 (13)*	0.43

H14D	0.3172	0.0466	0.1048	0.232*	0.43
H14E	0.3694	−0.0671	0.0746	0.232*	0.43
H14F	0.4057	0.0633	0.0564	0.232*	0.43
O3	1.0771 (3)	0.3148 (4)	0.5369 (2)	0.0624 (12)	
O4	1.0959 (3)	0.1229 (4)	0.4993 (2)	0.0598 (12)	
N2	0.9935 (4)	0.0470 (4)	0.6118 (2)	0.0461 (12)	
H2	1.0216	−0.0030	0.5844	0.055*	
C15	1.0645 (5)	0.1969 (6)	0.5387 (3)	0.0506 (16)	
C16	1.0041 (4)	0.1641 (5)	0.5998 (3)	0.0429 (14)	
C17	0.9592 (5)	0.2459 (6)	0.6425 (3)	0.0542 (17)	
H17	0.9642	0.3284	0.6335	0.058 (18)*	
C18	0.9077 (5)	0.2060 (6)	0.6975 (3)	0.0593 (18)	
H18	0.8796	0.2622	0.7272	0.07 (2)*	
C19	0.8962 (5)	0.0835 (5)	0.7110 (3)	0.0487 (15)	
C20	0.9409 (5)	0.0006 (5)	0.6651 (3)	0.0473 (16)	
C21	0.9317 (5)	−0.1241 (6)	0.6754 (3)	0.0571 (18)	
H21	0.9631	−0.1785	0.6465	0.07 (2)*	
C22	0.8756 (5)	−0.1650 (7)	0.7282 (4)	0.068 (2)	
H22	0.8660	−0.2477	0.7337	0.08 (2)*	
C23	0.8330 (6)	−0.0833 (7)	0.7743 (4)	0.072 (2)	
H23	0.7978	−0.1129	0.8116	0.07 (2)*	
C24	0.8416 (5)	0.0365 (7)	0.7658 (4)	0.067 (2)	
H24	0.8115	0.0890	0.7966	0.10 (3)*	
C25	1.1392 (6)	0.3627 (7)	0.4834 (4)	0.084 (2)	
H25A	1.1096	0.3482	0.4353	0.101*	
H25B	1.2028	0.3236	0.4876	0.101*	
C26	1.1503 (7)	0.4927 (7)	0.4965 (5)	0.107 (3)	
H26A	1.0869	0.5301	0.4945	0.161*	
H26B	1.1884	0.5276	0.4603	0.161*	
H26C	1.1829	0.5056	0.5432	0.161*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0565 (3)	0.0507 (3)	0.0415 (3)	0.0008 (2)	0.00965 (19)	−0.0027 (2)
Cl1	0.0690 (12)	0.0592 (10)	0.0573 (10)	0.0150 (9)	0.0176 (8)	0.0050 (8)
Cl2	0.1224 (18)	0.0624 (11)	0.0690 (11)	0.0002 (11)	0.0563 (12)	−0.0073 (9)
Cl3	0.0952 (16)	0.0634 (11)	0.0731 (12)	0.0124 (11)	0.0122 (10)	0.0132 (9)
O1	0.048 (3)	0.071 (3)	0.058 (3)	0.000 (2)	0.015 (2)	−0.012 (2)
O2	0.053 (3)	0.109 (4)	0.079 (3)	−0.004 (3)	−0.007 (3)	−0.020 (3)
N1	0.042 (3)	0.049 (3)	0.047 (3)	0.009 (3)	0.008 (2)	−0.005 (2)
C1	0.047 (4)	0.049 (4)	0.058 (4)	0.001 (3)	0.008 (3)	−0.004 (3)
C2	0.050 (4)	0.046 (4)	0.046 (4)	0.004 (3)	0.008 (3)	−0.004 (3)
C3	0.073 (5)	0.066 (5)	0.046 (4)	0.000 (4)	0.005 (4)	−0.009 (3)
C4	0.098 (7)	0.067 (5)	0.055 (4)	0.011 (5)	0.023 (5)	−0.017 (4)
C5	0.065 (5)	0.053 (4)	0.063 (4)	0.016 (4)	0.031 (4)	0.004 (3)
C6	0.047 (4)	0.053 (4)	0.052 (4)	0.009 (3)	0.017 (3)	0.009 (3)
C7	0.052 (5)	0.106 (6)	0.072 (5)	0.000 (5)	0.010 (4)	0.009 (4)

C8	0.042 (5)	0.129 (7)	0.107 (7)	0.008 (5)	0.002 (5)	0.038 (6)
C9	0.058 (6)	0.096 (7)	0.128 (8)	0.024 (5)	0.044 (6)	0.030 (6)
C10	0.080 (7)	0.068 (5)	0.105 (7)	0.027 (5)	0.047 (6)	0.016 (5)
C11	0.098 (7)	0.083 (5)	0.093 (6)	−0.010 (5)	−0.028 (5)	−0.015 (5)
O3	0.075 (3)	0.054 (3)	0.061 (3)	−0.003 (3)	0.027 (2)	0.011 (2)
O4	0.065 (3)	0.069 (3)	0.047 (3)	0.000 (3)	0.012 (2)	−0.009 (2)
N2	0.048 (3)	0.049 (3)	0.042 (3)	0.002 (3)	0.006 (2)	−0.004 (2)
C15	0.043 (4)	0.064 (5)	0.045 (4)	−0.004 (3)	0.002 (3)	0.006 (3)
C16	0.037 (4)	0.044 (4)	0.048 (4)	−0.001 (3)	0.007 (3)	0.004 (3)
C17	0.056 (4)	0.044 (4)	0.064 (4)	−0.001 (3)	0.020 (3)	0.007 (3)
C18	0.071 (5)	0.048 (4)	0.062 (4)	0.006 (4)	0.028 (4)	−0.001 (3)
C19	0.053 (4)	0.044 (4)	0.050 (4)	0.001 (3)	0.011 (3)	0.000 (3)
C20	0.049 (4)	0.048 (4)	0.045 (4)	−0.002 (3)	0.004 (3)	0.007 (3)
C21	0.070 (5)	0.044 (4)	0.057 (4)	−0.003 (4)	0.005 (4)	−0.003 (3)
C22	0.078 (6)	0.057 (5)	0.069 (5)	−0.009 (4)	0.003 (4)	0.012 (4)
C23	0.088 (6)	0.070 (5)	0.060 (5)	−0.006 (5)	0.023 (4)	0.018 (4)
C24	0.074 (5)	0.064 (5)	0.066 (5)	0.001 (4)	0.027 (4)	0.006 (4)
C25	0.100 (7)	0.072 (5)	0.087 (6)	−0.021 (5)	0.045 (5)	0.012 (4)
C26	0.127 (9)	0.102 (7)	0.098 (6)	−0.028 (6)	0.042 (6)	0.026 (5)

Geometric parameters (Å, º)

Sn1—O1	2.079 (4)	C14—H14B	0.9600
Sn1—C11	2.142 (7)	C14—H14C	0.9600
Sn1—N1	2.371 (4)	C12′—C13′	1.547 (17)
Sn1—Cl2	2.4405 (18)	C12′—H12C	0.9700
Sn1—Cl3	2.4482 (18)	C12′—H12D	0.9700
Sn1—Cl1	2.4924 (16)	C13′—C14′	1.555 (17)
O1—C1	1.275 (7)	C13′—H13C	0.9700
O2—C1	1.221 (7)	C13′—H13D	0.9700
N1—C2	1.325 (7)	C14′—H14D	0.9600
N1—C6	1.383 (7)	C14′—H14E	0.9600
C1—C2	1.500 (8)	C14′—H14F	0.9600
C2—C3	1.386 (8)	O3—C15	1.315 (7)
C3—C4	1.355 (9)	O3—C25	1.452 (7)
C3—H3	0.9300	O4—C15	1.197 (7)
C4—C5	1.394 (10)	N2—C16	1.322 (7)
C4—H4	0.9300	N2—C20	1.363 (7)
C5—C10	1.403 (10)	N2—H2	0.8600
C5—C6	1.407 (8)	C15—C16	1.494 (8)
C6—C7	1.398 (9)	C16—C17	1.375 (8)
C7—C8	1.361 (10)	C17—C18	1.355 (8)
C7—H7	0.9300	C17—H17	0.9298
C8—C9	1.411 (11)	C18—C19	1.387 (8)
C8—H8	0.9300	C18—H18	0.9300
C9—C10	1.316 (11)	C19—C24	1.403 (8)
C9—H9	0.9300	C19—C20	1.419 (8)
C10—H10	0.9300	C20—C21	1.397 (8)

C11—C12	1.579 (13)	C21—C22	1.364 (8)
C11—C12′	1.587 (16)	C21—H21	0.9305
C11—H11A	0.9700	C22—C23	1.398 (9)
C11—H11B	0.9700	C22—H22	0.9295
C11—H11C	0.9700	C23—C24	1.339 (9)
C11—H11D	0.9700	C23—H23	0.9303
C12—C13	1.511 (14)	C24—H24	0.9306
C12—H12A	0.9700	C25—C26	1.463 (9)
C12—H12B	0.9700	C25—H25A	0.9699
C13—C14	1.518 (15)	C25—H25B	0.9699
C13—H13A	0.9700	C26—H26A	0.9600
C13—H13B	0.9700	C26—H26B	0.9600
C14—H14A	0.9600	C26—H26C	0.9600
O1—Sn1—C11	172.6 (2)	C14—C13—H13A	111.2
O1—Sn1—N1	73.06 (16)	C12—C13—H13B	111.2
C11—Sn1—N1	107.7 (3)	C14—C13—H13B	111.2
O1—Sn1—Cl2	82.66 (12)	H13A—C13—H13B	109.1
C11—Sn1—Cl2	96.4 (3)	C13—C14—H14A	109.5
N1—Sn1—Cl2	155.72 (13)	C13—C14—H14B	109.5
O1—Sn1—Cl3	87.93 (13)	H14A—C14—H14B	109.5
C11—Sn1—Cl3	99.5 (2)	C13—C14—H14C	109.5
N1—Sn1—Cl3	84.64 (12)	H14A—C14—H14C	109.5
Cl2—Sn1—Cl3	94.28 (6)	H14B—C14—H14C	109.5
O1—Sn1—Cl1	83.87 (13)	C13′—C12′—C11	94.6 (19)
C11—Sn1—Cl1	88.8 (2)	C13′—C12′—H12C	112.8
N1—Sn1—Cl1	84.22 (12)	C11—C12′—H12C	112.8
Cl2—Sn1—Cl1	93.73 (6)	C13′—C12′—H12D	112.8
Cl3—Sn1—Cl1	167.71 (6)	C11—C12′—H12D	112.8
C1—O1—Sn1	121.6 (4)	H12C—C12′—H12D	110.3
C2—N1—C6	118.7 (5)	C12′—C13′—C14′	113 (3)
C2—N1—Sn1	110.4 (4)	C12′—C13′—H13C	109.0
C6—N1—Sn1	130.8 (4)	C14′—C13′—H13C	109.0
O2—C1—O1	123.7 (6)	C12′—C13′—H13D	109.0
O2—C1—C2	119.7 (6)	C14′—C13′—H13D	109.0
O1—C1—C2	116.6 (6)	H13C—C13′—H13D	107.8
N1—C2—C3	122.6 (6)	C13′—C14′—H14D	109.5
N1—C2—C1	116.2 (5)	C13′—C14′—H14E	109.5
C3—C2—C1	121.2 (6)	H14D—C14′—H14E	109.5
C4—C3—C2	120.0 (7)	C13′—C14′—H14F	109.5
C4—C3—H3	120.0	H14D—C14′—H14F	109.5
C2—C3—H3	120.0	H14E—C14′—H14F	109.5
C3—C4—C5	119.4 (6)	C15—O3—C25	117.5 (5)
C3—C4—H4	120.3	C16—N2—C20	124.1 (5)
C5—C4—H4	120.3	C16—N2—H2	118.0
C4—C5—C10	123.9 (7)	C20—N2—H2	118.0
C4—C5—C6	118.8 (6)	O4—C15—O3	127.4 (6)
C10—C5—C6	117.3 (7)	O4—C15—C16	122.7 (6)

N1—C6—C7	119.7 (6)	O3—C15—C16	109.9 (6)
N1—C6—C5	120.5 (6)	N2—C16—C17	119.1 (5)
C7—C6—C5	119.8 (6)	N2—C16—C15	116.0 (5)
C8—C7—C6	119.8 (7)	C17—C16—C15	124.9 (6)
C8—C7—H7	120.1	C18—C17—C16	119.9 (6)
C6—C7—H7	120.1	C18—C17—H17	120.2
C7—C8—C9	120.5 (8)	C16—C17—H17	119.9
C7—C8—H8	119.8	C17—C18—C19	121.7 (6)
C9—C8—H8	119.8	C17—C18—H18	119.1
C10—C9—C8	119.4 (8)	C19—C18—H18	119.2
C10—C9—H9	120.3	C18—C19—C24	124.4 (6)
C8—C9—H9	120.3	C18—C19—C20	117.5 (6)
C9—C10—C5	123.1 (8)	C24—C19—C20	118.1 (6)
C9—C10—H10	118.4	N2—C20—C21	121.8 (6)
C5—C10—H10	118.4	N2—C20—C19	117.7 (5)
C12—C11—Sn1	112.1 (8)	C21—C20—C19	120.4 (6)
C12′—C11—Sn1	117.2 (12)	C22—C21—C20	119.1 (6)
C12—C11—H11A	109.2	C22—C21—H21	120.5
C12′—C11—H11A	80.4	C20—C21—H21	120.5
Sn1—C11—H11A	109.2	C21—C22—C23	120.4 (7)
C12—C11—H11B	109.2	C21—C22—H22	119.7
C12′—C11—H11B	126.9	C23—C22—H22	119.9
Sn1—C11—H11B	109.2	C24—C23—C22	121.5 (7)
H11A—C11—H11B	107.9	C24—C23—H23	119.3
C12—C11—H11C	132.5	C22—C23—H23	119.2
C12′—C11—H11C	107.6	C23—C24—C19	120.4 (7)
Sn1—C11—H11C	108.0	C23—C24—H24	119.8
H11B—C11—H11C	79.6	C19—C24—H24	119.8
C12—C11—H11D	83.6	O3—C25—C26	107.6 (6)
C12′—C11—H11D	108.3	O3—C25—H25A	110.2
Sn1—C11—H11D	108.0	C26—C25—H25A	110.3
H11A—C11—H11D	131.6	O3—C25—H25B	110.3
H11C—C11—H11D	107.3	C26—C25—H25B	110.0
C13—C12—C11	114.3 (14)	H25A—C25—H25B	108.5
C13—C12—H12A	108.7	C25—C26—H26A	109.5
C11—C12—H12A	108.7	C25—C26—H26B	109.5
C13—C12—H12B	108.7	H26A—C26—H26B	109.5
C11—C12—H12B	108.7	C25—C26—H26C	109.5
H12A—C12—H12B	107.6	H26A—C26—H26C	109.5
C12—C13—C14	103.0 (16)	H26B—C26—H26C	109.5
C12—C13—H13A	111.2		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2[i]	0.86	2.26	3.078 (7)	158

| N2—H2···O4[i] | 0.86 | 2.53 | 2.990 (6) | 114 |

Symmetry code: (i) $-x+2$, $-y$, $-z+1$.