metal-organic compounds

Tetramethylammonium aquatrichlorido-oxalatostannate(IV) monohydrate

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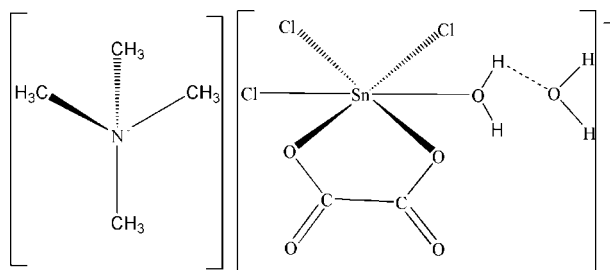Correspondence e-mail: yayasow81@yahoo.fr

The Sn^{IV} atom in the title compound, $[(CH_3)_4N][Sn(C_2O_4)Cl_3(H_2O)]\cdot H_2O$, obtained from the reaction between $SnCl_4$ and $[(CH_3)_4N]_2C_2O_4\cdot2H_2O$, is six-coordinated by three Cl atoms, an O atom of a water molecule and two O atoms from an asymmetrically chelating oxalate anion. The environment around the Sn^{IV} atom is distorted octahedral. The anions are connected by the lattice water molecule through O—H···O hydrogen bonds, leading to a layered structure parallel to (010). The cations are located between these layers and besides Coulombic forces are connected to the anionic layers through weak C—H···O and C—H···Cl interactions.

Related literature

For background to halogentin(IV) chemistry, see: Hausen *et al.* (1986); Koutsantonis *et al.* (2003); Mahon *et al.* (2004); Patt-Siebel *et al.* (1986); Szymanska-Buzar *et al.* (2001); Tudela *et al.* (1986). For tin compounds containing an Sn—Cl bond in a *cis*- or *trans*-position, see: Fernandez *et al.* (2002); Hazell *et al.* (1998); Sow *et al.* (2010). For tin compounds containing carboxylate moieties, see: Ng & Kumar Das (1993); Xu *et al.* (2003).

Experimental

Crystal data

$(C_4H_{12}N)[Sn(C_2O_4)Cl_3(H_2O)]\cdot H_2O$
$M_r = 423.24$
Monoclinic, $P2_1/n$
$a = 7.2458$ (1) Å
$b = 22.2812$ (2) Å
$c = 9.6019$ (1) Å
$\beta = 98.015$ (1)°
$V = 1535.04$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 2.20$ mm^{-1}
$T = 150$ K
$0.15 \times 0.15 \times 0.13$ mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.734$, $T_{max} = 0.763$
35849 measured reflections
4445 independent reflections
3855 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.062$
$S = 1.08$
4445 reflections
175 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.92$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O5—H50A···O6	0.86 (2)	1.66 (2)	2.511 (2)	173 (3)
O5—H50B···O4^i	0.85 (2)	1.78 (2)	2.6120 (19)	168 (3)
O6—H60A···O3^{ii}	0.84 (2)	1.99 (2)	2.792 (2)	160 (3)
O6—H60A···O3^{iii}	0.84 (2)	1.95 (2)	2.7840 (19)	172 (3)
O6—H60B···O4^{ii}	0.84 (2)	2.47 (3)	2.993 (2)	122 (3)
C6—H6B···O6^i	0.98	2.54	3.411 (3)	148
C6—H6A···Cl3^{iv}	0.98	2.91	3.762 (3)	146

Symmetry codes: (i) $-x+2, -y, -z+1$; (ii) $x-1, y, z$; (iii) $-x+2, -y, -z+2$; (iv) $x, y, z-1$.

Data collection: *COLLECT* (Nonius, 1999); cell refinement: *DENZO* and *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 2012); software used to prepare material for publication: *WinGX* (Farrugia, 2012).

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supporting information

Tetramethylammonium aquatrichloridooxalatostannate(IV) monohydrate

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S1. Comment

Numerous crystal structures of SnX_4 adducts (X = halogen) containing tin(IV) in an octahedral environment have been reported up to date, e.g. Hausen *et al.* (1986); Koutsantonis *et al.* (2003); Mahon *et al.* (2004); Patt-Siebel *et al.* (1986); Szymanska-Buzar *et al.* (2001); Tudela *et al.* (1986). Our group has previously reported the crystal structure of ((n-$C_3H_7)_2NH_2)_2[Sn(C_2O_4)Cl_4]$ which contains a chelating oxalate anion, and the environment of tin(IV) being likewise octahedral (Sow *et al.*, 2010). In the context of our search for new SnX_4 adducts we report here the study of the reaction between $((CH_3)_4N)_2C_2O_4{\cdot}2H_2O$ and $SnCl_4$ which has yielded the title compound, $((CH_3)_4N)[Sn(C_2O_4)Cl_3(H_2O)]{\cdot}H_2O$. While many SnX_4 adducts have been reported (see above), a complex with a $[SnCl_3]$-containing residue is reported here.

The octahedral geometry around the tin(IV) atom is defined by three Cl atoms, two oxygen atoms from the chelating oxalate anion and the oxygen atom of a water molecule (Fig. 1). The two oxygen atoms from the oxalate anion and two of the Cl atoms are in the equatorial plane while the remaining Cl atom and the oxygen atom of the H_2O molecule are in axial positions.

The $[Sn(C_2O_4)Cl_3(H_2O)]^-$ anions are connected to the lattice water molecule through $H-O-H{\cdots}OH_2$ hydrogen bonds. The water molecule bonded to the tin(IV) atom is also hydrogen-bonded to the O4 atom of a neighbour complex-anion. The lattice water molecule O6 is bonded to O3 and O4 of the same oxalate anion through a bifurcated hydrogen bond and to a O3 atom of a neighbouring oxalate anion, leading to a layered structure extending parallel to (010). The cations are located between the anionic planes (Figs. 2,3). In the crystal packing, $C-H{\cdots}O$ and $C-H{\cdots}Cl$ interactions between cations and anions are also observed (Table 1).

The angle O5—Sn—Cl3 [170.75°(5)] deviates from linearity. The two Sn—Cl bond lengths in the equatorial plane are very similar [Sn—Cl2 = 2.3598 (5), Sn—Cl1 = 2.3627 (5) Å], but different from the one *trans* to the water molecule [Sn—Cl3 = 2.3926 (5) Å], pointing to a weak *trans*-effect involving the latter. The Sn—O5 bond of 2.0781 (15) Å involving the water molecule is shorter than the Sn—O bonds distances involving the oxalate anion [Sn—O1 = 2.0980 (13); Sn—O2 = 2.1025 (13) Å], whereby these two last Sn—O distances are very close. The dimensions of Sn—O bonds and Sn—Cl bonds are in the range of Sn—O and Sn—Cl bonds reported for O_2SnCl_4 containing adducts with *cis*- or *trans*-geometry (Fernandez *et al.*, 2002; Hazell *et al.*, 1998; Sow *et al.*, 2010).

The C—O distances [O1—C1 = 1.285 (2); O2—C2 = 1.288 (2) Å; O3—C1 = 1.219 (2) Å; O4—C2 = 1.223 (2) Å] are in the typical range of C—O and C=O bonds (Ng & Kumar Das, 1993; Xu *et al.*, 2003).

S2. Experimental

All chemicals were purchased from Aldrich (Germany) and used without any further purification. $((CH_3)_4N)_2C_2O_4{\cdot}2H_2O$ has been obtained on allowing $((CH_3)_4N)OH$ as a 20% water solution to react with oxalic acid in a 2:1 ratio. A powder is obtained after evaporation of water at 333 K. On allowing the oxalic acid salt to react with $SnCl_4$ in a 1:1 ratio in ethanol, a colorless solution is obtained, which gives, after slow solvent evaporation, crystals suitable for X-ray determination .

The reaction equation of the title compound is: $((CH_3)_4N)_2C_2O_4 \cdot 2H_2O + SnCl_4 \rightarrow ((CH_3)_4N)Cl + ((CH_3)_4N)$
$[Sn(C_2O_4)Cl_3H_2O] \cdot H_2O$

S3. Refinement

Water molecule hydrogen atoms have been located in the difference fourier map and were refined with an idealized bond lenght of 0.85 Å. The other hydrogen atoms have been placed onto calculated position and were refined using a riding model, with C—H distances of 0.98 Å and $U_{iso}(H) = 1.5U_{eq}(C)$.
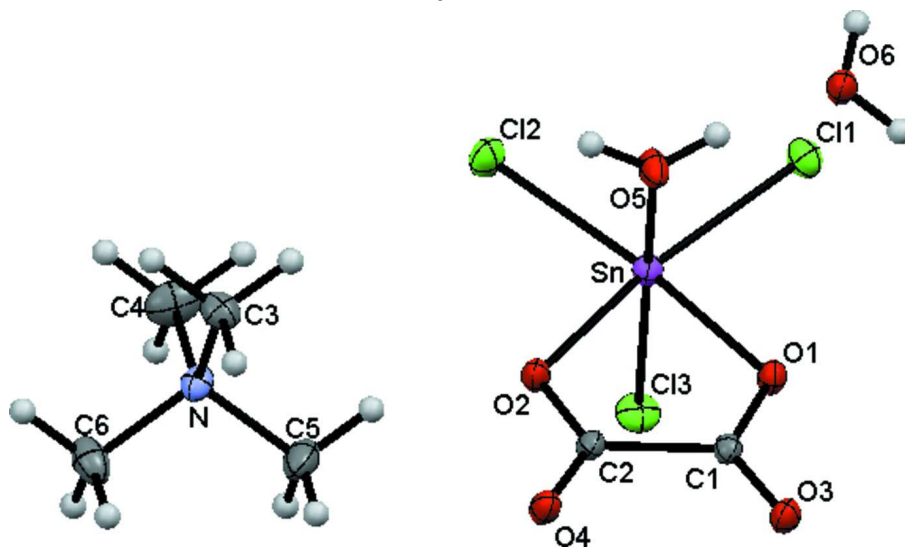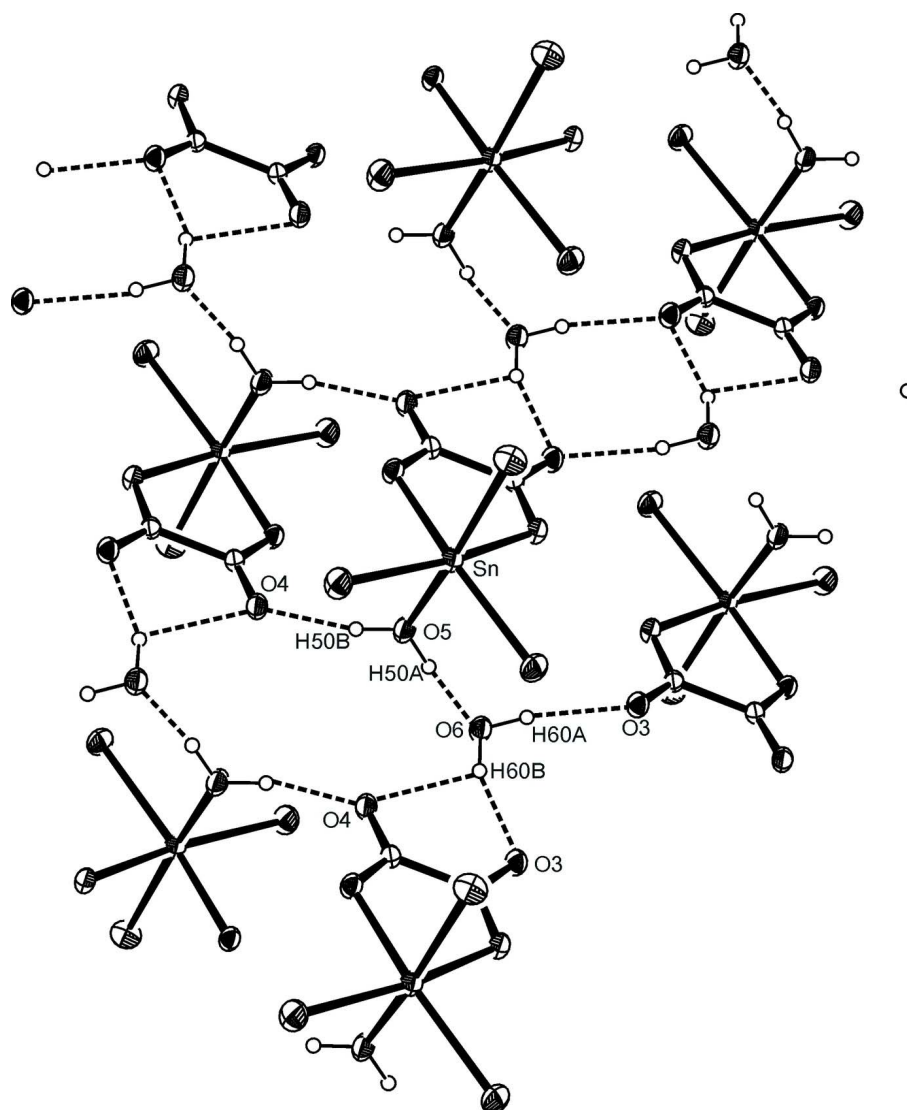

Figure 1
The asymmetric unit showing the numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Figure 2

The layered structure of the anions and the lattice water molecule parallel to (010). O—H···O hydrogen bonding interactions are shown as dashed lines.
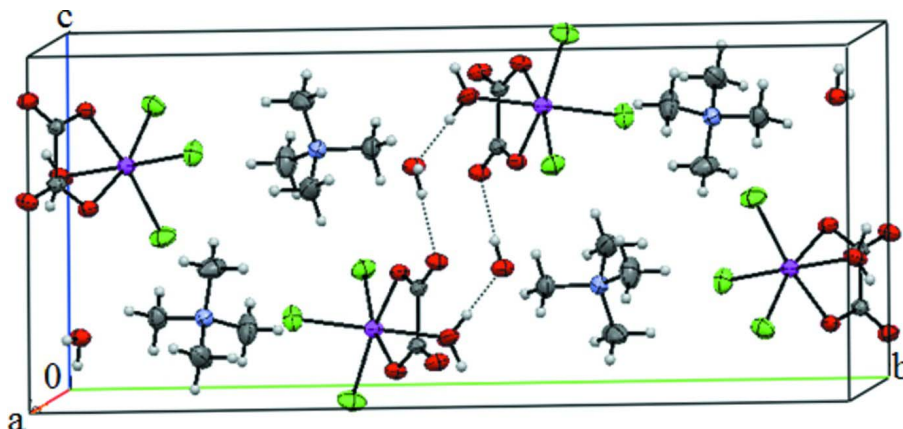
Figure 3

The packing of the structure showing O—H···O hydrogen bonding interactions as dashed lines [C—H···O and C—H···Cl contacts are omitted for clarity].

Tetramethylammonium aquatrichloridooxalatostannate(IV) monohydrate

Crystal data

$(C_4H_{12}N)[Sn(C_2O_4)Cl_3(H_2O)]\cdot H_2O$	$F(000) = 832$
$M_r = 423.24$	$D_x = 1.831$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 29534 reflections
$a = 7.2458$ (1) Å	$\theta = 2.9$–30.0°
$b = 22.2812$ (2) Å	$\mu = 2.20$ mm^{-1}
$c = 9.6019$ (1) Å	$T = 150$ K
$\beta = 98.015$ (1)°	Irregular, colourless
$V = 1535.04$ (3) Å^3	$0.15 \times 0.15 \times 0.13$ mm
$Z = 4$	

Data collection

Nonius KappaCCD diffractometer	35849 measured reflections
Radiation source: fine-focus sealed tube	4445 independent reflections
Graphite monochromator	3855 reflections with $I > 2\sigma(I)$
461 1.3 degree images with ω scans	$R_{int} = 0.042$
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)	$\theta_{max} = 30.0°$, $\theta_{min} = 4.2°$
$T_{min} = 0.734$, $T_{max} = 0.763$	$h = -10 \rightarrow 10$
	$k = -28 \rightarrow 31$
	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.026$	
$wR(F^2) = 0.062$	$w = 1/[\sigma^2(F_o^2) + (0.0322P)^2 + 0.5616P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.08$	
4445 reflections	$(\Delta/\sigma)_{max} = 0.001$
175 parameters	$\Delta\rho_{max} = 0.92$ e Å^{-3}
4 restraints	$\Delta\rho_{min} = -0.79$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Secondary atom site location: difference Fourier map	Extinction coefficient: 0.0124 (5)

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 $F^2 > \sigma(F^2)$ 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 (Å²)

	x	*y*	*z*	$U_{iso}*/U_{eq}$
Sn	0.834510 (17)	0.112222 (6)	0.679281 (12)	0.02693 (6)
Cl1	0.61541 (8)	0.13476 (3)	0.83233 (5)	0.03867 (12)
Cl2	0.66559 (8)	0.14793 (3)	0.46760 (5)	0.04369 (14)
Cl3	1.01222 (8)	0.20243 (2)	0.72319 (6)	0.04152 (13)
O5	0.7216 (2)	0.02693 (7)	0.64413 (15)	0.0372 (3)
O1	1.00588 (18)	0.07154 (6)	0.84708 (13)	0.0278 (3)
O3	1.2565 (2)	0.01364 (6)	0.89271 (13)	0.0310 (3)
O4	1.28776 (19)	0.01308 (7)	0.61246 (13)	0.0323 (3)
O2	1.04412 (18)	0.07556 (6)	0.57415 (13)	0.0285 (3)
O6	0.5915 (2)	−0.03357 (7)	0.82856 (15)	0.0320 (3)
N	1.0670 (2)	0.16827 (7)	0.20003 (17)	0.0298 (3)
C1	1.1444 (2)	0.04194 (8)	0.81171 (17)	0.0241 (3)
C2	1.1635 (3)	0.04294 (8)	0.65224 (18)	0.0249 (3)
C3	0.9820 (3)	0.10701 (9)	0.1966 (3)	0.0370 (5)
H3A	0.8911	0.1053	0.2632	0.055*
H3B	1.0798	0.0771	0.2228	0.055*
H3C	0.9192	0.0985	0.1015	0.055*
C4	0.9184 (4)	0.21327 (11)	0.1570 (3)	0.0561 (7)
H4A	0.8558	0.2036	0.0624	0.084*
H4B	0.9739	0.2534	0.1566	0.084*
H4C	0.8274	0.2125	0.2235	0.084*
C5	1.1603 (4)	0.18245 (13)	0.3445 (2)	0.0500 (6)
H5A	1.2132	0.2230	0.3458	0.075*
H5B	1.2601	0.1533	0.3721	0.075*
H5C	1.0689	0.1804	0.4106	0.075*
C6	1.2081 (4)	0.17066 (11)	0.0997 (3)	0.0491 (6)
H6A	1.1482	0.1599	0.0051	0.074*
H6B	1.3090	0.1423	0.1300	0.074*
H6C	1.2592	0.2113	0.0984	0.074*
H50B	0.703 (4)	0.0121 (13)	0.562 (2)	0.058 (8)*
H60B	0.481 (3)	−0.0227 (14)	0.829 (3)	0.057 (9)*
H60A	0.647 (4)	−0.0270 (13)	0.909 (2)	0.053 (8)*
H50A	0.668 (4)	0.0068 (12)	0.704 (3)	0.059 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.02791 (9)	0.02922 (8)	0.02369 (8)	0.00383 (4)	0.00368 (5)	0.00042 (4)
Cl1	0.0382 (3)	0.0436 (3)	0.0363 (3)	0.0062 (2)	0.0124 (2)	−0.0069 (2)
Cl2	0.0376 (3)	0.0596 (3)	0.0325 (3)	0.0146 (2)	0.0002 (2)	0.0094 (2)
Cl3	0.0423 (3)	0.0295 (2)	0.0520 (3)	−0.0019 (2)	0.0039 (2)	0.0029 (2)
O5	0.0468 (9)	0.0414 (8)	0.0256 (7)	−0.0136 (7)	0.0122 (6)	−0.0087 (6)
O1	0.0321 (7)	0.0308 (6)	0.0208 (6)	0.0045 (5)	0.0048 (5)	−0.0001 (5)
O3	0.0316 (7)	0.0376 (7)	0.0230 (6)	0.0047 (6)	0.0014 (5)	0.0034 (5)
O4	0.0291 (7)	0.0442 (8)	0.0230 (6)	0.0069 (6)	0.0018 (5)	−0.0051 (5)
O2	0.0287 (7)	0.0362 (7)	0.0209 (6)	0.0051 (5)	0.0040 (5)	0.0033 (5)
O6	0.0323 (8)	0.0396 (8)	0.0239 (7)	0.0062 (6)	0.0031 (6)	0.0003 (5)
N	0.0361 (9)	0.0254 (7)	0.0272 (8)	−0.0021 (6)	0.0018 (6)	−0.0007 (6)
C1	0.0268 (9)	0.0247 (8)	0.0205 (8)	−0.0031 (6)	0.0024 (7)	−0.0013 (6)
C2	0.0260 (9)	0.0281 (8)	0.0199 (8)	−0.0025 (7)	0.0014 (6)	−0.0014 (6)
C3	0.0409 (12)	0.0269 (9)	0.0445 (12)	−0.0048 (8)	0.0106 (10)	−0.0014 (8)
C4	0.0539 (15)	0.0325 (12)	0.0774 (19)	0.0084 (10)	−0.0061 (13)	0.0040 (11)
C5	0.0551 (15)	0.0598 (15)	0.0319 (11)	−0.0207 (12)	−0.0052 (10)	0.0029 (10)
C6	0.0646 (16)	0.0399 (12)	0.0477 (13)	−0.0152 (11)	0.0249 (12)	−0.0067 (10)

Geometric parameters (Å, º)

Sn—O5	2.0781 (15)	N—C3	1.496 (2)
Sn—O1	2.0980 (13)	N—C6	1.500 (3)
Sn—O2	2.1025 (13)	C1—C2	1.557 (2)
Sn—Cl2	2.3598 (5)	C3—H3A	0.9800
Sn—Cl1	2.3627 (5)	C3—H3B	0.9800
Sn—Cl3	2.3926 (5)	C3—H3C	0.9800
O5—H50B	0.850 (17)	C4—H4A	0.9800
O5—H50A	0.859 (17)	C4—H4B	0.9800
O1—C1	1.285 (2)	C4—H4C	0.9800
O3—C1	1.219 (2)	C5—H5A	0.9800
O4—C2	1.223 (2)	C5—H5B	0.9800
O2—C2	1.288 (2)	C5—H5C	0.9800
O6—H60B	0.836 (17)	C6—H6A	0.9800
O6—H60A	0.836 (17)	C6—H6B	0.9800
N—C4	1.488 (3)	C6—H6C	0.9800
N—C5	1.490 (3)		
O5—Sn—O1	84.67 (6)	O1—C1—C2	115.63 (15)
O5—Sn—O2	82.02 (6)	O4—C2—O2	126.11 (16)
O1—Sn—O2	79.11 (5)	O4—C2—C1	118.03 (16)
O5—Sn—Cl2	91.33 (5)	O2—C2—C1	115.85 (15)
O1—Sn—Cl2	170.93 (4)	N—C3—H3A	109.5
O2—Sn—Cl2	92.30 (4)	N—C3—H3B	109.5
O5—Sn—Cl1	90.68 (4)	H3A—C3—H3B	109.5
O1—Sn—Cl1	89.50 (4)	N—C3—H3C	109.5

O2—Sn—Cl1	166.95 (4)	H3A—C3—H3C	109.5
Cl2—Sn—Cl1	98.70 (2)	H3B—C3—H3C	109.5
O5—Sn—Cl3	170.75 (5)	N—C4—H4A	109.5
O1—Sn—Cl3	88.93 (4)	N—C4—H4B	109.5
O2—Sn—Cl3	90.23 (4)	H4A—C4—H4B	109.5
Cl2—Sn—Cl3	94.03 (2)	N—C4—H4C	109.5
Cl1—Sn—Cl3	95.95 (2)	H4A—C4—H4C	109.5
Sn—O5—H50B	121 (2)	H4B—C4—H4C	109.5
Sn—O5—H50A	125 (2)	N—C5—H5A	109.5
H50B—O5—H50A	113 (3)	N—C5—H5B	109.5
C1—O1—Sn	114.77 (11)	H5A—C5—H5B	109.5
C2—O2—Sn	114.29 (11)	N—C5—H5C	109.5
H60B—O6—H60A	107 (3)	H5A—C5—H5C	109.5
C4—N—C5	109.4 (2)	H5B—C5—H5C	109.5
C4—N—C3	109.18 (18)	N—C6—H6A	109.5
C5—N—C3	110.24 (17)	N—C6—H6B	109.5
C4—N—C6	109.2 (2)	H6A—C6—H6B	109.5
C5—N—C6	109.25 (18)	N—C6—H6C	109.5
C3—N—C6	109.49 (16)	H6A—C6—H6C	109.5
O3—C1—O1	124.90 (16)	H6B—C6—H6C	109.5
O3—C1—C2	119.47 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O5—H50*A*···O6	0.86 (2)	1.66 (2)	2.511 (2)	173 (3)
O5—H50*B*···O4[i]	0.85 (2)	1.78 (2)	2.6120 (19)	168 (3)
O6—H60*B*···O3[ii]	0.84 (2)	1.99 (2)	2.792 (2)	160 (3)
O6—H60*A*···O3[iii]	0.84 (2)	1.95 (2)	2.7840 (19)	172 (3)
O6—H60*B*···O4[ii]	0.84 (2)	2.47 (3)	2.993 (2)	122 (3)
C6—H6*B*···O6[i]	0.98	2.54	3.411 (3)	148
C6—H6*A*···Cl3[iv]	0.98	2.91	3.762 (3)	146

Symmetry codes: (i) −*x*+2, −*y*, −*z*+1; (ii) *x*−1, *y*, *z*; (iii) −*x*+2, −*y*, −*z*+2; (iv) *x*, *y*, *z*−1.