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fac-(2-Amidoethyl-κ^2C^1,O)aquatrichloridotin(IV) 1,4,7,10,13,16-hexaoxacyclooctadecane (2/1)

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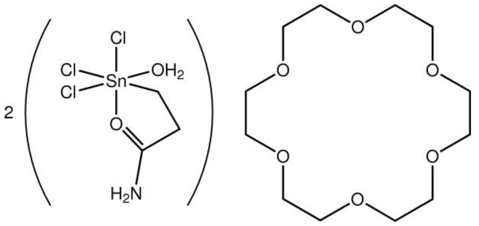
Key indicators: single-crystal X-ray study; *T* = 120 K; mean σ(C–C) = 0.005 Å; *R* factor = 0.030; *wR* factor = 0.090; data-to-parameter ratio = 19.3.

The asymmetric unit of the title compound, $[Sn(C_3H_6NO)Cl_3(H_2O)]_2 \cdot C_{12}H_{24}O_6$, comprises a six-coordinate tin complex and a 18-crown-6 molecule, the latter disposed about a centre of inversion. The tin atom is coordinated by three Cl atoms, that define a facial arrangement, a chelating *C*-,*O*- ligand, and a water molecule. The resulting CCl_3O_2 donor set defines a distorted octahedral geometry. The tin-bound aqua ligand forms O—H$\cdots$O hydrogen bonds to the centrosymmetric 18-crown-6 molecule, resulting in a tri-molecular aggregate. These assemble into a supramolecular chain along the *a* axis being connected by N—H$\cdots$O hydrogen bonds.

Related literature

For background to amidoethyl tin compounds, see: Hutton & Oakes (1976). For the use of organotin compounds as PVC stabilisers, see: Lanigen & Weinberg (1976). For the crystal structures of amidoethyltin compounds, see: Harrison *et al.* (1979); Tiekink *et al.* (2006). For the crystal structures of alkyloxycarbonylethyltin compounds, see: de Lima *et al.* (2009); Milne *et al.* (2005). For a review on tin–crown ether compounds, see: Cusack & Smith (1990). For related structures of organotin(IV) and tin(IV) halide complexes with crown ethers, see: Cusack *et al.* (1983); Amini *et al.* (1984, 2002); Russo *et al.* (1984); Valle *et al.* (1984, 1985); Rivarola *et al.* (1986); Bott *et al.* (1987); Mitra *et al.* (1993); Yap *et al.* (1996); Wolff *et al.* (2009).



Experimental

Crystal data

$[Sn(C_3H_6NO)Cl_3(H_2O)]_2 \cdot C_{12}H_{24}O_6$
M_r = 894.64
Monoclinic, $P2_1/n$
a = 10.1260 (2) Å
b = 10.0893 (3) Å
c = 15.8229 (4) Å
β = 105.814 (2)°
V = 1555.35 (7) Å^3
Z = 2
Mo *Kα* radiation
μ = 2.17 mm^{-1}
T = 120 K
0.20 × 0.18 × 0.02 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
T_{min} = 0.638, T_{max} = 0.746
19526 measured reflections
3555 independent reflections
2981 reflections with $I > 2\sigma(I)$
R_{int} = 0.062

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.090
S = 1.12
3555 reflections
184 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.81 e Å^{-3}
$\Delta\rho_{min}$ = −1.31 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*
O1w—H1w$\cdots$O4	0.84 (2)	1.96 (2)	2.784 (3)	166 (3)
O1w—H2w$\cdots$O2	0.84 (3)	2.01 (3)	2.839 (3)	169 (4)
N1—H1n$\cdots$O3^{i}	0.88 (3)	2.51 (3)	3.061 (4)	121 (2)
N1—H2n$\cdots$Cl1^{ii}	0.88 (3)	2.68 (3)	3.516 (3)	161 (3)

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2997).

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Acta Cryst. (2010). E**66**, m312–m313 Wardell *et al.* • $[Sn(C_3H_6NO)Cl_3(H_2O)]_2 \cdot C_{12}H_{24}O_6$ **m313**

supporting information

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fac-(2-Amidoethyl-κ^2C^1,*O*)aquatrichloridotin(IV) 1,4,7,10,13,16-hexaoxacyclooctadecane (2/1)

Solange M. S. V. Wardell, William T. A. Harrison, Edward R. T. Tiekink, Geraldo M. de Lima and James L. Wardell

S1. Comment

Functionally substituted-alkyl-tin compounds, $X_3SnCR_2CH_2COY$ and $X_2Sn(CR_2CH_2COY)_2$ (X = halide, R = H or alkyl; Y = OR′, R′ or NH_2, R′ = alkyl or aryl), are available from reactions, first reported in the 1970's (Hutton & Oakes, 1976), of R_2C=CHCOY, HX and SnX_2 (for $X_3SnCR_2CH_2COY$ compounds) or HX and tin (for $X_2Sn(CR_2CH_2COY)_2$ compounds). Original interest with these compounds was primarily concerned with their industrial potential as precursors of PVC stabilizers (Lanigen & Weinberg, 1976) but also with regard to their coordination chemistry. Although the potential for use in PVC stabilization has not been realized commercially, the interest in the coordination chemistry, especially of compounds containing $SnCR_2CH_2CO_2R$ moieties, has been maintained over the succeeding decades: of particular interest has been the coordination modes of the CR_2CH_2COY ligands (de Lima *et al.*, 2009; Milne *et al.*, 2005; Harrison *et al.*, 1979). Much less study has been made of amidoethyl-tin species. *i.e.*, tin compounds containing the $CH_2CH_2CONH_2$ group. Only two structures of amidoethyltin derivatives have been previously reported, namely of ($H_2NHCOCH_2CH_2$-*C*,*O*)$_2SnCl_2$ (Harrison *et al.*, 1979) and ($H_2NCOCH_2CH_2$-*C*,*O*)($ClCH_2CH_2CONH_2$-*O*)$SnCl_3$ (Tiekink *et al.*, 2006). We now wish to report the crystal structure of *fac*-aqua-trichloro(2-amidoethyl-*C*,*O*)tin 1,4,7,10,13,16-hexaoxacyclooctadecane (2/1), (I). Crown ether complexes of tin and organotin halides have been variously reported (Cusack *et al.* 1983; Amini *et al.*, 1984; Valle *et al.*, 1984; Russo *et al.*, 1984; Valle *et al.*, 1985; Rivarola *et al.*, 1986; Bott *et al.*, 1987; Cusack & Smith, 1990; Mitra *et al.*, 1993; Yap *et al.*, 1996; Amini *et al.*, 2002; Wolff *et al.*, 2009).

The asymmetric unit of (I) comprises a tin complex and half a 18-crown-6 molecule as the latter is situated about a centre of inversion, Fig. 1. The tin atom is coordinated by three Cl atoms, that define a facial arrangement, a *C*-,*O*-chelating ligand, and an aqua ligand. The resulting CCl_3O_2 donor set defines a distorted octahedral geometry. The Cl atoms *trans* to O-donors form longer Sn–Cl bond distances [Sn–Cl2 = 2.4208 (9) and Sn–Cl3 = 2.4329 (9) Å] than the Cl atom *trans* to the C1 atom [Sn–Cl1 = 2.3800 (9) Å]. The five-membered SnC_3O chelate ring is not planar as seen in the values of the Sn–C1–C2–C3 and C1–C2–C3–O1 torsion angles of 24.0 (4) and -15.9 (5) °, respectively.

The components of the structure are connected via O_{aqua}–H···O_{ether} hydrogen bonds to form a tri-molecular aggregate, Table 1 and Fig. 1. These in turn are connected via N–H···O_{ether} hydrogen bonds so that all ether-O atoms participate in hydrogen bonding interactions, Table 1. The resulting supramolecular aggregate is a linear chain formed along the *a* axis, Fig. 2. These are connected into the 3-D crystal structure via N–H···Cl interactions, Fig. 3.

S2. Experimental

The reaction between $SnCl_2$, $H_2C{=}CHCONH_2$ and gaseous HCl in diethyl ether, as previously reported (Tiekink *et al.*, 2006), produced ($H_2NCOCH_2CH_2$-*C*,*O*)($ClCH_2CH_2CONH_2$-*O*)$SnCl_3$. Solutions of 1,4,7,10,13,16-hexaoxacyclooctadecane (18-crown-6) (0.26 g, 1 mmol) in EtOH (15 ml) and ($H_2NCOCH_2CH_2$-*C*,*O*)($ClCH_2CH_2CONH_2$-*O*)$SnCl_3$ (0.40 g, 1 mmol) in EtOH (20 ml) were mixed and gently heated for 15 min. The reaction mixture was cooled and maintained at room temperature. The crystals which slowly appeared on evaporation of the solvent were harvested after 1 week. M.pt.: partial sublimation at 463 K with complete melting at 469-471 K. IR (KBr, cm^{-1}): 3441, 3349, 3273, 2919(br), 1650, 1573, 1456, 1352, 1297, 1254, 1094, 1037, 958, 915, 844, 702, 564.

S3. Refinement

The C-bound H atoms were geometrically placed (C–H = 0.99 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The O- and N- bound and H atoms were located from difference maps and refined with O–H = 0.84±0.01 Å and N–H = 0.88±0.01 Å, and with $U_{\rm iso}$(H) = 1.5U_{eq}(O, N). The maximum and minimum residual electron density peaks of 0.81 and 1.31 e $Å^{-3}$, respectively, were located 1.29 Å and 0.79 Å from the H4a and Sn atoms, respectively.

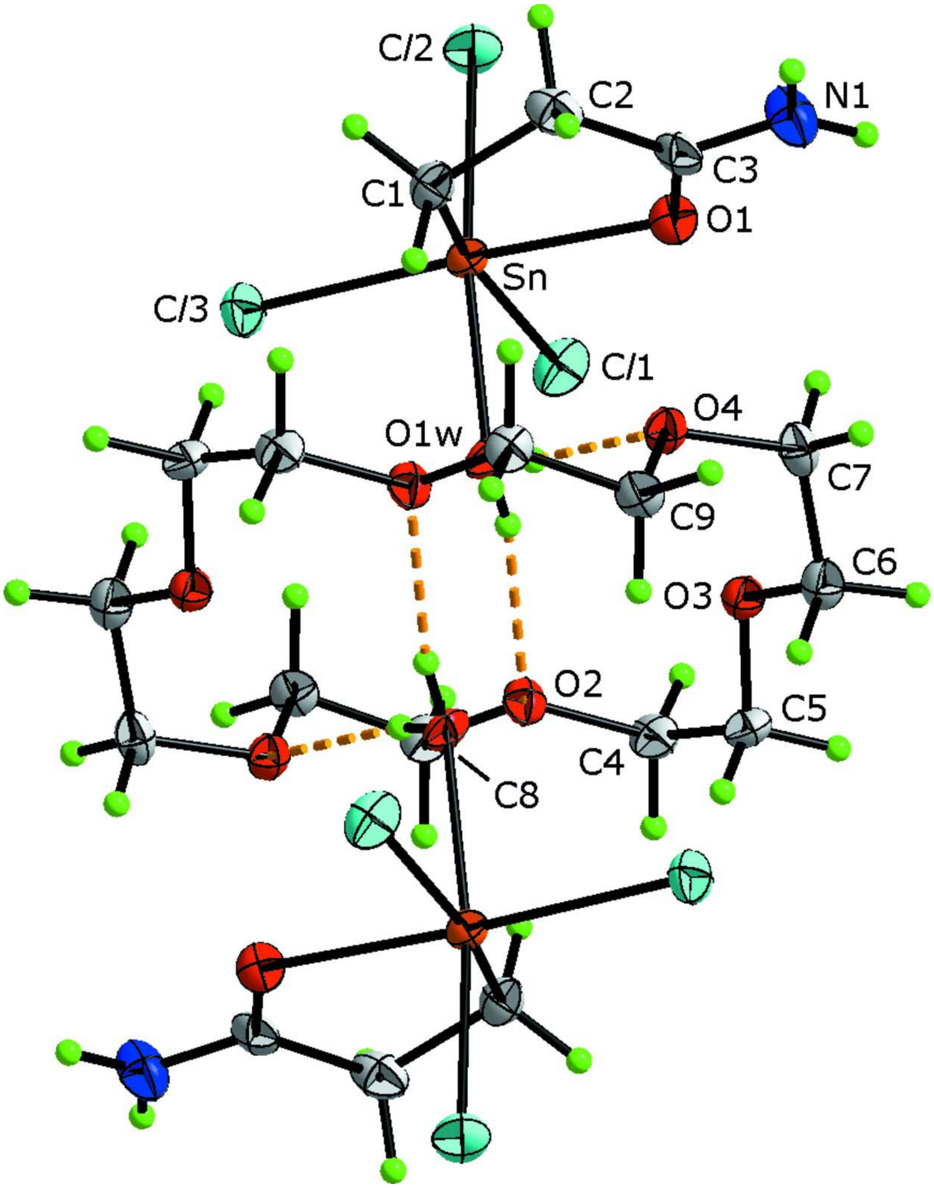

Figure 1

The molecular structure of a tri-molecular aggregate in (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. Dashed lines indicate hydrogen bonds.

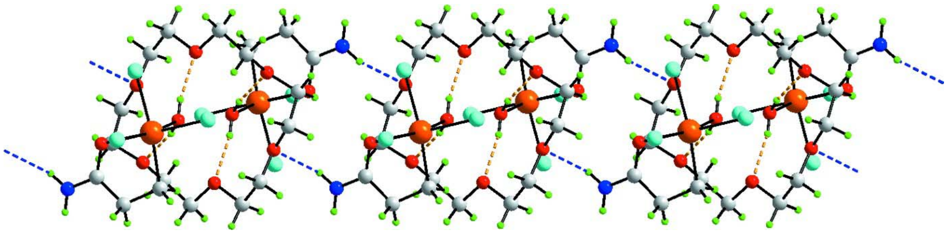

Figure 2

A view of a supramolecular chain in (I), aligned along the *a* axis, whereby the tri-molecular aggregates sustained by O–H···O hydrogen bonds (orange dashed lines) illustrated in Fig. 1, are connected via N–H···O hydrogen bonds (blue dashed lines). Colour code: Sn, orange; Cl, cyan; O, red; N, blue; C, grey; and H, green.

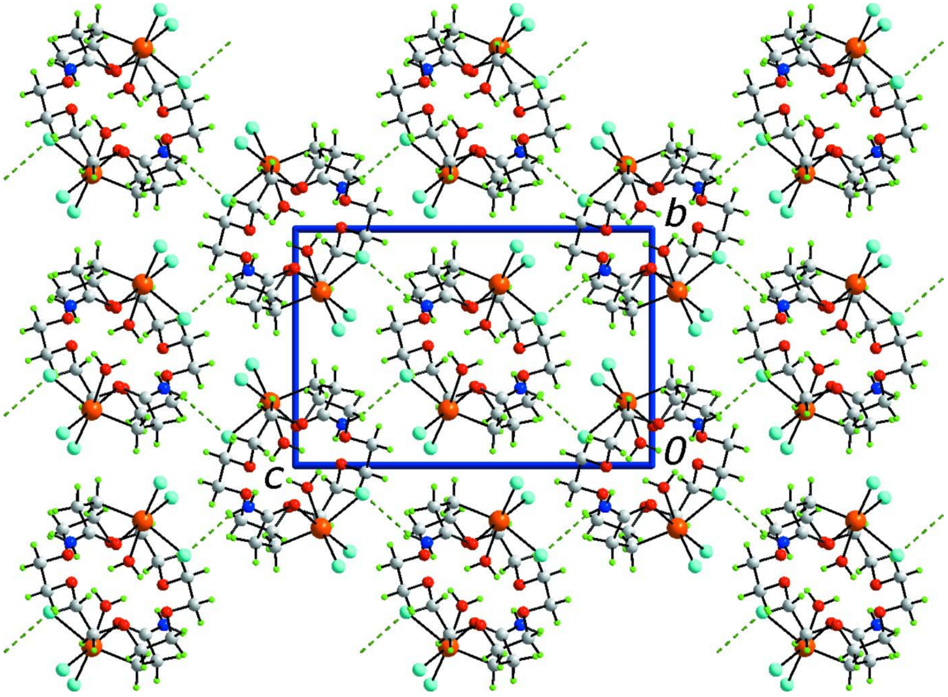

Figure 3

View in projection down the *a* axis of the unit cell contents in (I). The N–H···Cl interactions connecting the supramolecular chains illustrated in Fig. 2 are shown as green dashed lines. Colour code: Sn, orange; Cl, cyan; O, red; N, blue; C, grey; and H, green.

fac-(2-Amidoethyl-κ^2C^1,O)aquatrichloridotin(IV)–1,4,7,10,13,16-hexaoxacyclooctadecane (2/1)

Crystal data

$[Sn(C_3H_6NO)Cl_3(H_2O)]_2\cdot C_{12}H_{24}O_6$	$F(000) = 888$
$M_r = 894.64$	$D_x = 1.910$ Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Hall symbol: -P 2yn	Cell parameters from 9442 reflections
$a = 10.1260$ (2) Å	$\theta = 2.9$–$27.5°$
$b = 10.0893$ (3) Å	$\mu = 2.17$ mm^{-1}
$c = 15.8229$ (4) Å	$T = 120$ K
$\beta = 105.814$ (2)°	Prism, colourless
$V = 1555.35$ (7) Å^3	0.20 × 0.18 × 0.02 mm
$Z = 2$	

Data collection

Nonius KappaCCD area-detector diffractometer
Radiation source: Enraf Nonius FR591 rotating anode
10 cm confocal mirrors monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.638$, $T_{max} = 0.746$
19526 measured reflections
3555 independent reflections
2981 reflections with $I > 2\sigma(I)$
$R_{int} = 0.062$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.0°$
$h = -13 \rightarrow 12$
$k = -13 \rightarrow 13$
$l = -20 \rightarrow 20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.090$
$S = 1.12$
3555 reflections
184 parameters
6 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -1.31$ e Å^{-3}

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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}
Sn	0.78251 (2)	0.23444 (2)	0.571426 (15)	0.01204 (10)
Cl1	0.77631 (9)	0.37992 (9)	0.68869 (6)	0.0199 (2)
Cl2	0.64299 (9)	0.07335 (9)	0.62109 (6)	0.0231 (2)
Cl3	0.99961 (8)	0.13617 (9)	0.65225 (6)	0.0200 (2)
O1	0.5890 (2)	0.3331 (2)	0.49675 (15)	0.0146 (5)
O1W	0.8950 (2)	0.4054 (2)	0.53264 (16)	0.0139 (5)
H1W	0.859 (3)	0.436 (4)	0.4824 (12)	0.021*
H2W	0.922 (4)	0.471 (2)	0.565 (2)	0.021*
N1	0.4259 (3)	0.3257 (3)	0.3687 (2)	0.0217 (7)
H1N	0.377 (3)	0.386 (3)	0.387 (2)	0.033*
H2N	0.396 (4)	0.290 (4)	0.3164 (14)	0.033*
C1	0.7646 (3)	0.1561 (3)	0.4426 (2)	0.0155 (7)
H1A	0.8272	0.2038	0.4148	0.019*
H1B	0.7894	0.0610	0.4465	0.019*
C2	0.6165 (3)	0.1739 (4)	0.3884 (2)	0.0191 (8)

H2A	0.6154	0.1925	0.3267	0.023*
H2B	0.5663	0.0899	0.3890	0.023*
C3	0.5422 (3)	0.2844 (3)	0.4209 (2)	0.0157 (7)
O2	1.0228 (2)	0.6214 (2)	0.63876 (15)	0.0146 (5)
O3	0.7765 (2)	0.6756 (2)	0.51861 (15)	0.0146 (5)
O4	0.7319 (2)	0.4951 (2)	0.37156 (15)	0.0140 (5)
C4	0.9395 (4)	0.7297 (3)	0.6529 (3)	0.0172 (8)
H4A	0.9985	0.8011	0.6861	0.021*
H4B	0.8774	0.6993	0.6877	0.021*
C5	0.8571 (4)	0.7812 (3)	0.5659 (3)	0.0175 (8)
H5A	0.7967	0.8541	0.5745	0.021*
H5B	0.9190	0.8161	0.5323	0.021*
C6	0.7026 (3)	0.7148 (4)	0.4323 (2)	0.0165 (7)
H6A	0.7659	0.7537	0.4012	0.020*
H6B	0.6326	0.7820	0.4349	0.020*
C7	0.6351 (3)	0.5932 (3)	0.3852 (2)	0.0156 (7)
H7A	0.5772	0.5525	0.4195	0.019*
H7B	0.5741	0.6196	0.3274	0.019*
C8	1.1285 (3)	0.5885 (3)	0.7162 (2)	0.0148 (7)
H8A	1.0876	0.5676	0.7648	0.018*
H8B	1.1917	0.6646	0.7342	0.018*
C9	0.7943 (3)	0.5295 (3)	0.3033 (2)	0.0149 (7)
H9A	0.8578	0.6050	0.3223	0.018*
H9B	0.7227	0.5562	0.2498	0.018*

Atomic displacement parameters ($Å^2$)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.01329 (15)	0.01173 (14)	0.01132 (15)	−0.00019 (8)	0.00373 (10)	0.00053 (9)
Cl1	0.0273 (5)	0.0190 (5)	0.0138 (5)	0.0020 (4)	0.0062 (4)	−0.0027 (3)
Cl2	0.0223 (4)	0.0194 (5)	0.0303 (5)	−0.0025 (4)	0.0118 (4)	0.0071 (4)
Cl3	0.0157 (4)	0.0195 (5)	0.0227 (5)	0.0027 (3)	0.0018 (4)	0.0049 (4)
O1	0.0164 (12)	0.0174 (13)	0.0101 (12)	0.0007 (10)	0.0036 (10)	−0.0028 (10)
O1W	0.0189 (12)	0.0094 (12)	0.0121 (13)	0.0002 (10)	0.0023 (10)	0.0026 (10)
N1	0.0165 (15)	0.0297 (19)	0.0176 (17)	0.0027 (14)	0.0023 (13)	−0.0074 (14)
C1	0.0176 (17)	0.0149 (18)	0.0152 (18)	0.0015 (14)	0.0062 (14)	−0.0013 (14)
C2	0.0167 (18)	0.024 (2)	0.017 (2)	−0.0039 (15)	0.0054 (15)	−0.0063 (16)
C3	0.0115 (16)	0.0186 (18)	0.0194 (19)	−0.0020 (14)	0.0084 (14)	0.0025 (15)
O2	0.0135 (11)	0.0160 (12)	0.0129 (13)	0.0015 (9)	0.0011 (9)	−0.0024 (9)
O3	0.0142 (12)	0.0128 (12)	0.0154 (13)	0.0005 (10)	0.0017 (10)	−0.0002 (10)
O4	0.0149 (11)	0.0138 (12)	0.0135 (12)	0.0011 (9)	0.0044 (9)	0.0023 (9)
C4	0.0170 (18)	0.0160 (18)	0.0194 (19)	−0.0013 (14)	0.0060 (15)	−0.0088 (14)
C5	0.0166 (18)	0.0110 (17)	0.025 (2)	−0.0019 (14)	0.0050 (15)	−0.0037 (15)
C6	0.0166 (18)	0.0162 (18)	0.017 (2)	0.0029 (14)	0.0051 (15)	0.0022 (14)
C7	0.0129 (16)	0.0199 (18)	0.0147 (18)	0.0032 (14)	0.0052 (14)	0.0029 (14)
C8	0.0176 (17)	0.0154 (17)	0.0110 (17)	0.0003 (14)	0.0029 (14)	−0.0008 (14)
C9	0.0155 (17)	0.0174 (18)	0.0128 (18)	−0.0002 (14)	0.0058 (14)	0.0035 (14)

Geometric parameters (Å, º)

Sn—C1	2.147 (3)	O3—C6	1.423 (4)
Sn—O1	2.228 (2)	O3—C5	1.424 (4)
Sn—O1W	2.243 (2)	O4—C9	1.434 (4)
Sn—Cl1	2.3800 (9)	O4—C7	1.450 (4)
Sn—Cl2	2.4208 (9)	C4—C5	1.496 (5)
Sn—Cl3	2.4329 (9)	C4—H4A	0.9900
O1—C3	1.263 (4)	C4—H4B	0.9900
O1W—H1W	0.84 (2)	C5—H5A	0.9900
O1W—H2W	0.84 (3)	C5—H5B	0.9900
N1—C3	1.309 (5)	C6—C7	1.500 (5)
N1—H1N	0.88 (3)	C6—H6A	0.9900
N1—H2N	0.88 (3)	C6—H6B	0.9900
C1—C2	1.522 (5)	C7—H7A	0.9900
C1—H1A	0.9900	C7—H7B	0.9900
C1—H1B	0.9900	C8—C9^{i}	1.502 (5)
C2—C3	1.512 (5)	C8—H8A	0.9900
C2—H2A	0.9900	C8—H8B	0.9900
C2—H2B	0.9900	C9—C8^{i}	1.502 (5)
O2—C8	1.429 (4)	C9—H9A	0.9900
O2—C4	1.435 (4)	C9—H9B	0.9900

C1—Sn—O1	80.00 (11)	C6—O3—C5	111.8 (3)
C1—Sn—O1W	86.63 (11)	C9—O4—C7	113.6 (2)
O1—Sn—O1W	87.14 (8)	O2—C4—C5	108.9 (3)
C1—Sn—Cl1	162.49 (10)	O2—C4—H4A	109.9
O1—Sn—Cl1	86.08 (6)	C5—C4—H4A	109.9
O1W—Sn—Cl1	82.09 (6)	O2—C4—H4B	109.9
C1—Sn—Cl2	98.92 (10)	C5—C4—H4B	109.9
O1—Sn—Cl2	88.03 (6)	H4A—C4—H4B	108.3
O1W—Sn—Cl2	171.91 (6)	O3—C5—C4	108.7 (3)
Cl1—Sn—Cl2	91.10 (3)	O3—C5—H5A	110.0
C1—Sn—Cl3	100.34 (10)	C4—C5—H5A	110.0
O1—Sn—Cl3	177.30 (6)	O3—C5—H5B	110.0
O1W—Sn—Cl3	90.20 (6)	C4—C5—H5B	110.0
Cl1—Sn—Cl3	93.07 (3)	H5A—C5—H5B	108.3
Cl2—Sn—Cl3	94.55 (3)	O3—C6—C7	107.4 (3)
C3—O1—Sn	112.2 (2)	O3—C6—H6A	110.2
Sn—O1W—H1W	115 (3)	C7—C6—H6A	110.2
Sn—O1W—H2W	123 (3)	O3—C6—H6B	110.2
H1W—O1W—H2W	106 (4)	C7—C6—H6B	110.2
C3—N1—H1N	120 (2)	H6A—C6—H6B	108.5
C3—N1—H2N	119 (2)	O4—C7—C6	113.4 (3)
H1N—N1—H2N	120.6 (19)	O4—C7—H7A	108.9
C2—C1—Sn	107.9 (2)	C6—C7—H7A	108.9
C2—C1—H1A	110.1	O4—C7—H7B	108.9
Sn—C1—H1A	110.1	C6—C7—H7B	108.9

C2—C1—H1B	110.1	H7A—C7—H7B	107.7
Sn—C1—H1B	110.1	O2—C8—C9^{i}	108.6 (3)
H1A—C1—H1B	108.4	O2—C8—H8A	110.0
C3—C2—C1	113.6 (3)	C9^{i}—C8—H8A	110.0
C3—C2—H2A	108.9	O2—C8—H8B	110.0
C1—C2—H2A	108.9	C9^{i}—C8—H8B	110.0
C3—C2—H2B	108.9	H8A—C8—H8B	108.4
C1—C2—H2B	108.9	O4—C9—C8^{i}	108.9 (3)
H2A—C2—H2B	107.7	O4—C9—H9A	109.9
O1—C3—N1	121.1 (3)	C8^{i}—C9—H9A	109.9
O1—C3—C2	121.2 (3)	O4—C9—H9B	109.9
N1—C3—C2	117.7 (3)	C8^{i}—C9—H9B	109.9
C8—O2—C4	112.2 (3)	H9A—C9—H9B	108.3

C1—Sn—O1—C3	12.0 (2)	Sn—O1—C3—C2	−1.3 (4)
O1W—Sn—O1—C3	99.0 (2)	C1—C2—C3—O1	−15.9 (5)
Cl1—Sn—O1—C3	−178.7 (2)	C1—C2—C3—N1	165.8 (3)
Cl2—Sn—O1—C3	−87.5 (2)	C8—O2—C4—C5	165.3 (3)
O1—Sn—C1—C2	−18.7 (2)	C6—O3—C5—C4	−175.7 (3)
O1W—Sn—C1—C2	−106.4 (2)	O2—C4—C5—O3	57.7 (4)
Cl1—Sn—C1—C2	−56.6 (4)	C5—O3—C6—C7	173.4 (3)
Cl2—Sn—C1—C2	67.6 (2)	C9—O4—C7—C6	−75.0 (4)
Cl3—Sn—C1—C2	164.0 (2)	O3—C6—C7—O4	−65.3 (3)
Sn—C1—C2—C3	24.0 (4)	C4—O2—C8—C9^{i}	177.2 (3)
Sn—O1—C3—N1	177.0 (3)	C7—O4—C9—C8^{i}	−169.7 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H1w···O4	0.84 (2)	1.96 (2)	2.784 (3)	166 (3)
O1w—H2w···O2	0.84 (3)	2.01 (3)	2.839 (3)	169 (4)
N1—H1n···O3^{ii}	0.88 (3)	2.51 (3)	3.061 (4)	121 (2)
N1—H2n···Cl1^{iii}	0.88 (3)	2.68 (3)	3.516 (3)	161 (3)

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