



# A new organic–inorganic compound, ethylenediammonium hexachloridostannate(IV) *p*-anisaldehyde disolvate

Adrienne Ndiolene,<sup>a\*</sup> Tidiane Diop,<sup>a</sup> Mouhamadou Sembène Boye,<sup>b</sup> Aminata Diasse-Sarr<sup>a</sup> and Ulli Englert<sup>c</sup>

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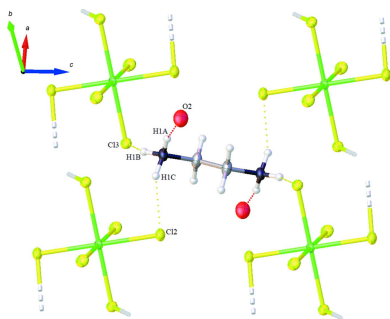
<sup>a</sup>Laboratoire de Chimie Minérale et Analytique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, <sup>b</sup>Département de Physique Chimie, Faculté des Sciences et Technologies de l'Éducation et de la Formation, Université Cheikh Anta Diop, Boulevard Habib, Bourguiba, BP 5036 Fann-Dakar, Senegal, and <sup>c</sup>Institute of Inorganic Chemistry, RWTH Aachen University, Landoltweg 1, 52056 Aachen, Germany.

\*Correspondence e-mail: andiolene@gmail.com

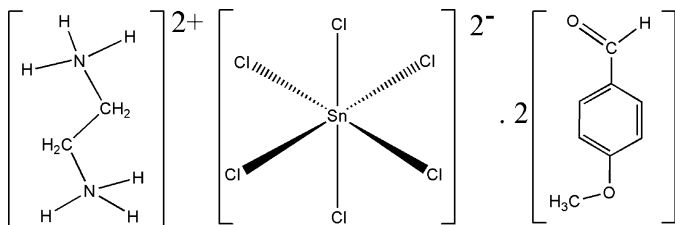
The asymmetric unit of the title organic–inorganic hybrid complex [systematic name: ethane-1,2-diaminium hexachloridostannate(IV)–4-methoxybenzaldehyde (1/2)], (C<sub>2</sub>H<sub>10</sub>N<sub>2</sub>)[SnCl<sub>6</sub>]<sub>2</sub>·2C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>, contains one half of an ethylenediammonium cation, one half of an [SnCl<sub>6</sub>]<sup>2−</sup> anion and one *p*-anisaldehyde molecule. Both the organic cation and the quasi-regular octahedral inorganic anion are located about inversion centres. The organic cations and [SnCl<sub>6</sub>]<sup>2−</sup> anions lie in layers parallel to the *ac* plane with *p*-anisaldehyde molecules occupying the space between the layers. A network of classical N–H···Cl and N–H···O hydrogen bonds exists between the ethylenediammonium cations and the [SnCl<sub>6</sub>]<sup>2−</sup> anions and *p*-anisaldehyde molecules. These interactions, together with non-classical C–H···O interactions between the ethylenediammonium cations and the *p*-anisaldehyde molecules, serve to hold the structure together. The crystal studied was refined as a two-component twin.

## 1. Chemical context

The combination of organic and inorganic components to form organic–inorganic hybrid materials has attracted considerable attention owing to the generation of new properties that are absent in type either of building block (Boopathi *et al.*, 2017; Newman *et al.*, 1989; Chun & Jung, 2009; Bouchene *et al.*, 2018). Hybrid functional materials, containing both inorganic and organic components, are considered to be potential platforms for applications in extremely diverse fields, such as optics, micro-electronics, magnetism, vibrational spectroscopy, transportation, health, energy, energy storage, diagnosis, housing and the environment (Masteri-Farahani *et al.*, 2012; Kim *et al.*, 2020; Manser *et al.*, 2016; Rademeyer *et al.*, 2007). Moreover, halogenostannate hybrid compounds containing protonated amine cations have recently received considerable attention because of their interesting physical and chemical properties, such as magnetism, electroluminescence, photoluminescence and conductivity, which may lead to technological innovations (Aruta *et al.*, 2005; Chouaib & Kamoun, 2015; Papavassiliou *et al.*, 1999; Yin & Yo, 1998). The structures of these hybrid materials have been shown to contain isolated or connected chains or clusters of SnX<sub>6</sub> octahedra separated by amine cations (Zhou

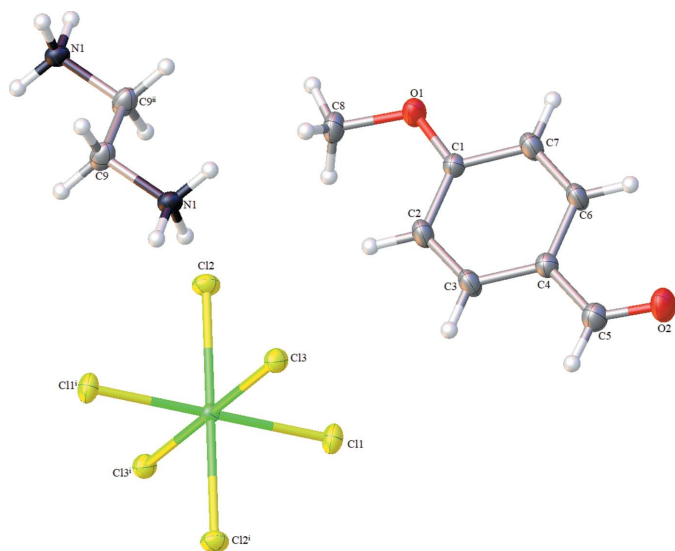


& Liu, 2012; Shahzadi *et al.*, 2008; Liu, 2012; Diop *et al.*, 2020). In this category of materials, the organic moieties, which balance the negative charge on the inorganic units, may also act as structure-directing agents and greatly affect the structure and dimensionality of the supramolecular framework formed (Díaz *et al.*, 2006; Hannon *et al.*, 2002). In the present study, we report the synthesis and structural analysis of a new organic–inorganic hybrid complex,  $(C_2H_{10}N_2)[SnCl_6] \cdot 2C_8H_8O_2$ .



## 2. Structural commentary

The asymmetric unit comprises of one half of an ethylenediammonium cation, one half of a hexachlorostannate(IV) dianion,  $[SnCl_6]^{2-}$ , both of which lie on centres of inversion, and one molecule of *p*-anisaldehyde (Fig. 1). The environment around the tin atom in the  $[SnCl_6]^{2-}$  dianion is an almost undistorted octahedron in which the Sn–Cl bond lengths lie in the range 2.4100 (12) to 2.4322 (11) Å and the *cis* Cl–Sn–Cl bond angles lie in the range 89.36 (4) to 90.20 (4)°. The Sn–Cl2 bond involved in hydrogen bonding is slightly longer, at 2.4322 (11) Å, than the other Sn–Cl bonds [Sn–Cl1 = 2.4100 (12) Å and Sn–Cl3 = 2.4220 (11) Å]. These results are comparable to those reported by other research groups (van Megen *et al.*, 2013; Ali *et al.*, 2008; Xue & Kong 2014).



**Figure 1**  
The atom-numbering for the asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry codes: (i)  $-x, -y, -z$ ; (ii)  $-x + 1, -y, -z + 1$ .]

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$C6-H6 \cdots Cl1^i$	0.95	3.05	3.596 (5)	118
$N1-H1A \cdots O2^i$	0.90 (2)	1.89 (3)	2.763 (6)	162 (6)
$N1-H1B \cdots Cl1^{ii}$	0.92 (2)	2.71 (5)	3.312 (4)	124 (5)
$N1-H1B \cdots Cl3^{iii}$	0.92 (2)	2.62 (4)	3.404 (4)	144 (5)
$N1-H1C \cdots Cl2$	0.92 (2)	2.44 (3)	3.315 (5)	158 (6)
$N1-H1C \cdots Cl3$	0.92 (2)	2.75 (6)	3.292 (4)	119 (5)
$C9-H9B \cdots O2^{iv}$	0.99	2.62	3.319 (7)	128

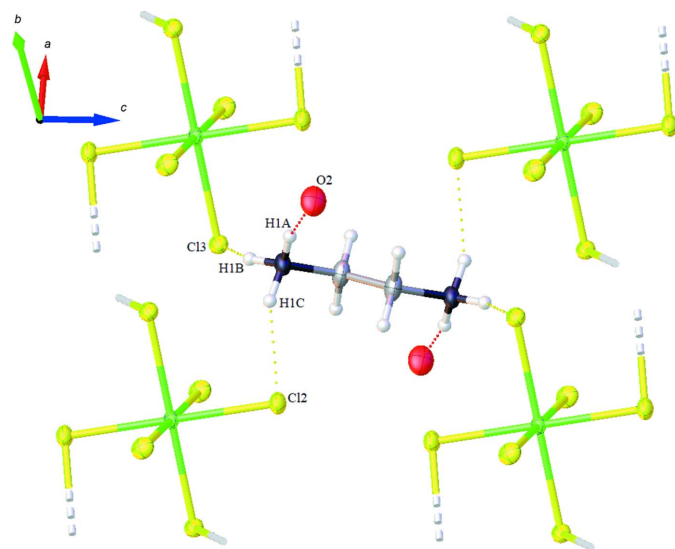
Symmetry codes: (i)  $x + \frac{1}{2}, -y + \frac{1}{2}, z + \frac{1}{2}$ ; (ii)  $x + 1, y, z$ ; (iii)  $-x + 1, -y, -z$ ; (iv)  $-x + \frac{1}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$ .

## 3. Supramolecular features

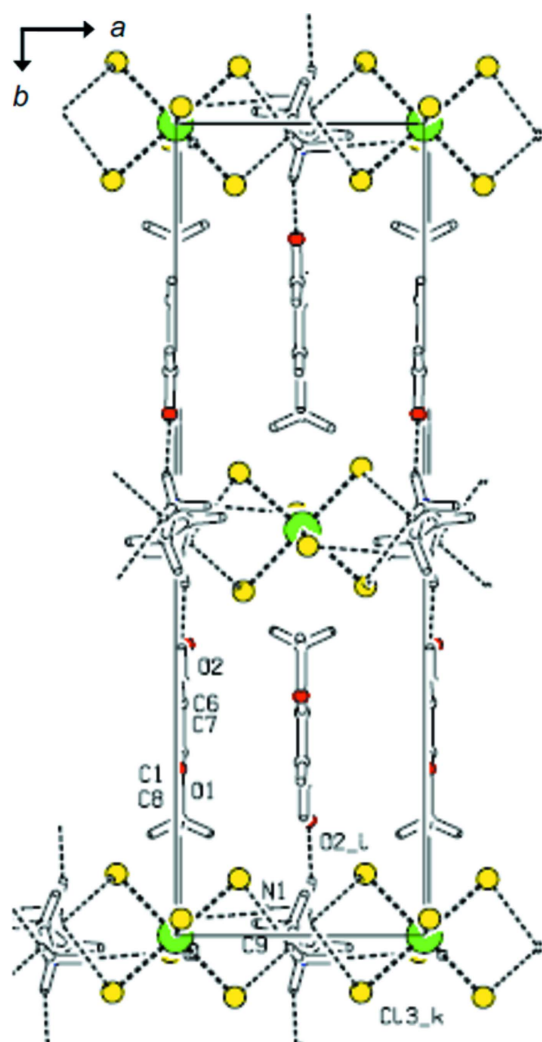
The packed crystal structure contains sheets lying parallel to the *ac* plane in which each  $[SnCl_6]^{2-}$  dianion is surrounded by four ethylenediammonium cations (Fig. 2). The *p*-anisaldehyde molecules are located in the otherwise empty space between the sheets (Fig. 3). The crystal packing of the complex is supported by  $N-H \cdots Cl$  and  $N-H \cdots O$  hydrogen-bonding interactions (Table 1). The  $NH_3^+$  groups of the ethylenediammonium cation act as the hydrogen-bonding donors. The  $D \cdots A$  distances involving the  $NH_3^+$  group and either the *p*-anisaldehyde molecule or the  $[SnCl_6]^{2-}$  units range from 2.763 (6) Å for  $N1 \cdots O2^i$  to 3.404 (4) Å for  $N1 \cdots Cl3^v$ . Non-classical interactions between the *p*-anisaldehyde molecules and the ethylenediammonium cations,  $C9-H9 \cdots O2^{vi}$  at 2.62 Å, further serve to hold the structure together.

## 4. Database survey

Organic–inorganic hybrid compounds with structures most similar to that of the title compound include:  $(C_6H_{22}N_4)[SnCl_6]Cl_2 \cdot 2H_2O$  and  $(C_8H_{24}N_4)[SnCl_6]Cl_2 \cdot 2H_2O$  (Bouchene *et al.* 2018),  $(C_5H_5BrN_2)[SnCl_6]$  (Ali *et al.*, 2008),



**Figure 2**  
The arrangement of the  $(C_2H_{10}N_2)^{2+}$  and  $[SnCl_6]^{2-}$  units of the title compound in the *ac* plane showing the  $N1-H1C \cdots Cl2$  and  $N1-H1A \cdots O2$  hydrogen bonds as dashed lines.



**Figure 3**  
View of the title compound along the  $c$  axis showing the organic cation-inorganic anion layers separated by  $p$ -anisaldehyde molecules. Hydrogen bonds are indicated by dashed lines.

$(C_5H_7N_2)_2[SnCl_6]$ , and  $(C_7H_{10}N)_2[SnCl_6]$  (Rademeyer *et al.*, 2007) and  $(C_8H_{12}N)_3SnBr_6 \cdot Br$  (Chouaib & Kamoun, 2015). These structures contain isolated or connected chains or

clusters of  $SnX_6$  octahedra separated by the organic cations. A variety of intermolecular hydrogen bonds,  $N-H \cdots O$ ,  $N-H \cdots Cl$  and  $O-H \cdots O$ , together with  $C-H \cdots \pi$  interactions, serve to consolidate the molecular structures.

## 5. Synthesis and crystallization

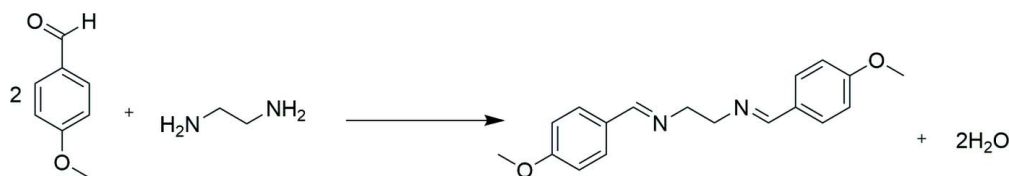
Chemicals [ $p$ -anisaldehyde, ethylenediamine and tin(II)] were purchased from Sigma-Aldrich and were used without any further purification. The solvent use for the synthesis was ethanol (96%).

### Synthesis of $N,N'$ -bis(4-methoxybenzylidene)ethylenediamine

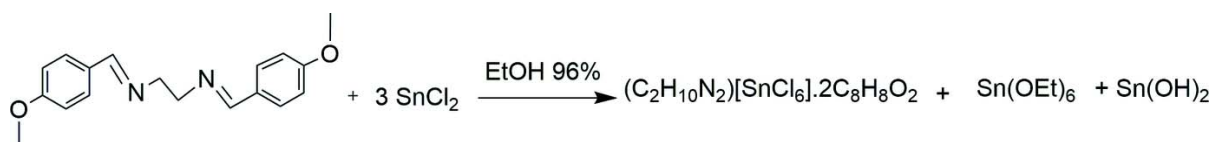
The Schiff base  $N,N'$ -bis(4-methoxybenzylidene)ethylenediamine was prepared by condensing  $p$ -anisaldehyde (10 g; 0.0734 mol) with ethylenediamine (2.205 g; 0.0367 mol) in ethanol (30 ml) (Fig. 4). The resulting mixture was heated under reflux for 6 h, filtered and left to evaporate at ambient temperature. (The reaction between  $p$ -anisaldehyde and ethylenediamine gave the same product whatever the proportions of reactants used). After a few days of slow evaporation, 4.511 g of crystals were obtained, corresponding to a yield of 82%. The compound was characterized by FT-IR ( $cm^{-1}$ : 1639.05 (C=N); 1603, 1505, 1461 and 1448 (C=C, aromatic); 1019 (C-O, ether).

### Synthesis of the title compound

0.3 g (0.00168 mol) of  $N,N'$ -bis(4-methoxybenzylidene)ethylenediamine were dissolved in 30 ml of ethanol in a round-bottomed flask, followed by the addition of  $SnCl_2$  (0.638 g; 0.00168 mol) to form a yellow solution (Fig. 5). The mixture was refluxed for 7 h at 353 K, filtered to remove  $Sn(OEt)_6$  and  $Sn(OH)_2$  and the resulting solution was allowed to evaporate slowly. After a few days of evaporation, light-yellow block-shaped crystals suitable for single-crystal X-ray analysis were obtained in a yield of 31%. The presence of water molecules in the solvent (EtOH, 96%) causes hydrolysis of the Schiff base and oxidation of tin(II) to tin(IV). The hydrolysis reaction leads to the formation of two molecules of  $p$ -anisaldehyde and one ethylenediammonium cation.



**Figure 4**  
Synthesis of the intermediate  $N,N'$ -bis(4-methoxybenzylidene)ethylenediamine.



**Figure 5**  
Synthesis of the title compound.

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	(C <sub>2</sub> H <sub>10</sub> N <sub>2</sub> )[SnCl <sub>6</sub> ]·2C <sub>8</sub> H <sub>8</sub> O <sub>2</sub>
<i>M<sub>r</sub></i>	665.80
Crystal system, space group	Monoclinic, <i>P</i> 2 <sub>1</sub> / <i>n</i>
Temperature (K)	100
<i>a</i> , <i>b</i> , <i>c</i> (Å)	6.9762 (12), 22.806 (4), 8.0394 (13)
$\beta$ (°)	90.948 (4)
<i>V</i> (Å <sup>3</sup> )	1278.9 (4)
<i>Z</i>	2
Radiation type	Mo <i>K</i> $\alpha$
$\mu$ (mm <sup>-1</sup> )	1.65
Crystal size (mm)	0.17 × 0.17 × 0.13
Data collection	
Diffractometer	Bruker D8 goniometer with APEX CCD detector
Absorption correction	Multi-scan ( <i>SADABS</i> ; Krause <i>et al.</i> , 2015)
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	3929, 3929, 3182
<i>R</i> <sub>int</sub>	0.112
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.723
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2 $\sigma$ ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.062, 0.164, 1.07
No. of reflections	3929
No. of parameters	154
No. of restraints	3
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$ , $\Delta\rho_{\min}$ (e Å <sup>-3</sup> )	2.91, -2.69

Computer programs: *SMART* (Bruker, 2002), *SAINT* (Bruker, 2009), *SHELXT* (Sheldrick 2015a), *SHELXL2018/3* (Sheldrick, 2015b) and *PLATON* (Spek, 2020).

The crystalline product was characterized by FT-IR (cm<sup>-1</sup>: 1659 (C=O); 3290 (N-H); 2801 (C-H, aldehyde); 1596, 1570 and 1556 (C=C, phenyl); 1259 (C-O, ether).

## 6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. (C<sub>2</sub>H<sub>10</sub>N<sub>2</sub>)[SnCl<sub>6</sub>]·2C<sub>8</sub>H<sub>8</sub>O<sub>2</sub> crystallizes in the space group *P*2<sub>1</sub>/*n* with the monoclinic angle,  $\beta$ , close to 90°. The crystals formed as non-merohedral twins with about one quarter of reflections overlapping. The twin law corresponds to rotation about *c*\*. For the crystal investigated, the relative domain sizes amounted to 0.790 (4):0.210 (4). The structure was solved by intrinsic phasing (Sheldrick, 2015a). The twin law was identified from reflections with *I*<sub>obs</sub> >> *I*<sub>calc</sub>, and *PLATON* (Spek, 2020) was used to generate a suitable two-domain reflection file for twin refinement (Sheldrick, 2015b). All non-hydrogen atoms were assigned anisotropic displacement parameters. H atoms attached to C were calculated in standard geometry and treated as riding [C-H =

0.95–0.99 Å; *U*<sub>iso</sub>(H) = 1.2*U*<sub>iso</sub>(C) or 1.5*U*<sub>iso</sub>(C-methyl)]. H atoms attached to N were located as local maxima in a difference-Fourier map and refined with a distance restraint N–H = 0.9 Å and an isotropic displacement parameter *U*<sub>iso</sub>(H) = 1.2*U*<sub>iso</sub>(N).

## Acknowledgements

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## supporting information

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## A new organic–inorganic compound, ethylenediammonium hexachloridostannate(IV) *p*-anisaldehyde disolvate

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### Computing details

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2009); data reduction: *SAINTE* (Bruker, 2009); program(s) used to solve structure: *SHELXT* (Sheldrick 2015a); program(s) used to refine structure: *SHELXL2018/3* (Sheldrick, 2015b); molecular graphics: *PLATON* (Spek, 2020); software used to prepare material for publication: *SHELXL2018/3* (Sheldrick, 2015b).

### Ethane-1,2-diaminium hexachloridostannate(IV)–4-methoxybenzaldehyde (1/2)

#### Crystal data

(C<sub>2</sub>H<sub>10</sub>N<sub>2</sub>)[SnCl<sub>6</sub>]·2C<sub>8</sub>H<sub>8</sub>O<sub>2</sub>

*M<sub>r</sub>* = 665.80

Monoclinic, *P*2<sub>1</sub>/*n*

*a* = 6.9762 (12) Å

*b* = 22.806 (4) Å

*c* = 8.0394 (13) Å

$\beta$  = 90.948 (4)°

*V* = 1278.9 (4) Å<sup>3</sup>

*Z* = 2

*F*(000) = 664

*D<sub>x</sub>* = 1.729 Mg m<sup>-3</sup>

Mo *K* $\alpha$  radiation,  $\lambda$  = 0.71073 Å

Cell parameters from 4273 reflections

$\theta$  = 2.7–27.3°

$\mu$  = 1.65 mm<sup>-1</sup>

*T* = 100 K

Block, light yellow

0.17 × 0.17 × 0.13 mm

#### Data collection

Bruker D8 goniometer with APEX CCD detector diffractometer

Radiation source: Incoatec microsource

Multilayer optics monochromator

$\omega$  scans

Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)

3929 measured reflections

3929 independent reflections

3182 reflections with *I* > 2 $\sigma$ (*I*)

*R*<sub>int</sub> = 0.112

$\theta_{\max}$  = 30.9°,  $\theta_{\min}$  = 1.8°

*h* = –9→9

*k* = –32→32

*l* = –11→11

#### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2 $\sigma$ (*F*<sup>2</sup>)] = 0.062

*wR*(*F*<sup>2</sup>) = 0.164

*S* = 1.07

3929 reflections

154 parameters

3 restraints

Primary atom site location: dual

Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement

*w* = 1/[ $\sigma^2(F_o^2) + (0.090P)^2 + 3.P$ ]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

( $\Delta/\sigma$ )<sub>max</sub> < 0.001

$\Delta\rho_{\max}$  = 2.91 e Å<sup>-3</sup>

$$\Delta\rho_{\min} = -2.69 \text{ e } \text{\AA}^{-3}$$

Extinction correction: SHELXL-2018/3  
(Sheldrick 2015b),  
 $F_c^* = kF_c [1 + 0.001x F_c^2 \lambda^3 / \sin(2\theta)]^{-1/4}$   
Extinction coefficient: 0.0073 (13)

### Special details

**Geometry.** All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

**Refinement.** Refined as a two-component twin.

### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.0054 (6)	0.20471 (16)	0.5640 (5)	0.0297 (8)
O2	0.0223 (7)	0.35799 (17)	-0.0922 (5)	0.0346 (9)
C1	0.0073 (7)	0.2253 (2)	0.4064 (6)	0.0216 (9)
C2	0.0110 (8)	0.1905 (2)	0.2647 (6)	0.0271 (11)
H2	0.011776	0.148942	0.273751	0.032*
C3	0.0134 (8)	0.2171 (2)	0.1100 (6)	0.0261 (10)
H3	0.014641	0.193476	0.012738	0.031*
C4	0.0141 (8)	0.2776 (2)	0.0945 (6)	0.0224 (9)
C5	0.0197 (8)	0.3047 (2)	-0.0684 (7)	0.0289 (11)
H5	0.021414	0.279678	-0.162937	0.035*
C6	0.0097 (8)	0.3121 (2)	0.2377 (6)	0.0262 (10)
H6	0.008962	0.353603	0.227991	0.031*
C7	0.0063 (9)	0.2865 (2)	0.3939 (7)	0.0281 (11)
H7	0.003288	0.310129	0.491121	0.034*
C8	0.0077 (9)	0.1422 (2)	0.5874 (7)	0.0299 (11)
H8A	-0.104360	0.124858	0.531118	0.045*
H8B	0.003967	0.133301	0.706506	0.045*
H8C	0.124940	0.125913	0.540404	0.045*
Sn1	0.000000	0.000000	0.000000	0.01522 (16)
Cl1	-0.23806 (17)	0.07591 (5)	-0.03230 (15)	0.0231 (3)
Cl2	0.02718 (18)	0.02031 (5)	0.29645 (13)	0.0225 (3)
Cl3	0.25385 (17)	0.06982 (5)	-0.05138 (14)	0.0207 (3)
N1	0.5008 (6)	0.02942 (18)	0.2818 (5)	0.0209 (8)
H1A	0.533 (8)	0.0662 (13)	0.313 (8)	0.025*
H1B	0.544 (9)	0.015 (3)	0.183 (5)	0.025*
H1C	0.372 (4)	0.029 (3)	0.255 (8)	0.025*
C9	0.5429 (9)	-0.0111 (2)	0.4218 (6)	0.0259 (11)
H9A	0.683408	-0.014942	0.437370	0.031*
H9B	0.490162	-0.050389	0.395586	0.031*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.049 (2)	0.0189 (17)	0.0210 (17)	0.0022 (16)	-0.0011 (16)	0.0025 (13)

O2	0.052 (3)	0.0207 (18)	0.031 (2)	-0.0010 (17)	0.0017 (18)	0.0066 (15)
C1	0.030 (2)	0.016 (2)	0.019 (2)	0.0003 (18)	-0.0028 (18)	0.0013 (16)
C2	0.043 (3)	0.014 (2)	0.025 (2)	0.001 (2)	-0.001 (2)	-0.0011 (17)
C3	0.041 (3)	0.015 (2)	0.022 (2)	-0.001 (2)	0.001 (2)	-0.0024 (16)
C4	0.030 (2)	0.017 (2)	0.020 (2)	-0.0004 (18)	-0.0019 (18)	0.0007 (16)
C5	0.040 (3)	0.022 (2)	0.024 (2)	0.000 (2)	-0.001 (2)	0.0026 (19)
C6	0.042 (3)	0.014 (2)	0.023 (2)	0.000 (2)	-0.001 (2)	-0.0024 (17)
C7	0.044 (3)	0.016 (2)	0.024 (2)	0.000 (2)	0.000 (2)	-0.0026 (17)
C8	0.043 (3)	0.018 (2)	0.029 (3)	0.003 (2)	-0.002 (2)	0.0067 (18)
Sn1	0.0197 (3)	0.0131 (2)	0.0128 (2)	-0.00059 (15)	-0.00159 (15)	0.00193 (13)
Cl1	0.0246 (6)	0.0173 (5)	0.0275 (6)	0.0032 (4)	0.0004 (4)	0.0059 (4)
Cl2	0.0294 (6)	0.0242 (6)	0.0138 (5)	-0.0038 (5)	-0.0010 (4)	-0.0003 (4)
Cl3	0.0240 (6)	0.0181 (5)	0.0199 (5)	-0.0040 (4)	-0.0016 (4)	0.0032 (4)
N1	0.028 (2)	0.0205 (19)	0.0145 (17)	-0.0016 (16)	-0.0025 (15)	0.0007 (14)
C9	0.035 (3)	0.026 (2)	0.017 (2)	0.007 (2)	0.003 (2)	0.0041 (18)

*Geometric parameters (Å, °)*

O1—C1	1.351 (6)	C8—H8B	0.9800
O1—C8	1.438 (6)	C8—H8C	0.9800
O2—C5	1.231 (6)	Sn1—Cl1 <sup>i</sup>	2.4100 (12)
C1—C2	1.390 (7)	Sn1—Cl1	2.4100 (12)
C1—C7	1.399 (7)	Sn1—Cl3 <sup>i</sup>	2.4220 (11)
C2—C3	1.384 (7)	Sn1—Cl3	2.4220 (11)
C2—H2	0.9500	Sn1—Cl2 <sup>i</sup>	2.4322 (11)
C3—C4	1.385 (6)	Sn1—Cl2	2.4322 (11)
C3—H3	0.9500	N1—C9	1.482 (6)
C4—C6	1.395 (7)	N1—H1A	0.902 (19)
C4—C5	1.449 (7)	N1—H1B	0.92 (2)
C5—H5	0.9500	N1—H1C	0.925 (19)
C6—C7	1.386 (7)	C9—C9 <sup>ii</sup>	1.490 (10)
C6—H6	0.9500	C9—H9A	0.9900
C7—H7	0.9500	C9—H9B	0.9900
C8—H8A	0.9800		
C1—O1—C8	117.8 (4)	Cl1 <sup>i</sup> —Sn1—Cl1	180.0
O1—C1—C2	124.8 (4)	Cl1 <sup>i</sup> —Sn1—Cl3 <sup>i</sup>	90.80 (4)
O1—C1—C7	114.4 (4)	Cl1—Sn1—Cl3 <sup>i</sup>	89.21 (4)
C2—C1—C7	120.7 (5)	Cl1 <sup>i</sup> —Sn1—Cl3	89.20 (4)
C3—C2—C1	119.1 (4)	Cl1—Sn1—Cl3	90.79 (4)
C3—C2—H2	120.4	Cl3 <sup>i</sup> —Sn1—Cl3	180.0
C1—C2—H2	120.4	Cl1 <sup>i</sup> —Sn1—Cl2 <sup>i</sup>	90.64 (4)
C2—C3—C4	121.2 (5)	Cl1—Sn1—Cl2 <sup>i</sup>	89.36 (4)
C2—C3—H3	119.4	Cl3 <sup>i</sup> —Sn1—Cl2 <sup>i</sup>	89.80 (4)
C4—C3—H3	119.4	Cl3—Sn1—Cl2 <sup>i</sup>	90.20 (4)
C3—C4—C6	119.1 (5)	Cl1 <sup>i</sup> —Sn1—Cl2	89.36 (4)
C3—C4—C5	120.4 (5)	Cl1—Sn1—Cl2	90.64 (4)
C6—C4—C5	120.5 (5)	Cl3 <sup>i</sup> —Sn1—Cl2	90.20 (4)

O2—C5—C4	124.2 (5)	Cl3—Sn1—Cl2	89.80 (4)
O2—C5—H5	117.9	Cl2 <sup>i</sup> —Sn1—Cl2	180.0
C4—C5—H5	117.9	C9—N1—H1A	109 (4)
C7—C6—C4	120.8 (4)	C9—N1—H1B	111 (4)
C7—C6—H6	119.6	H1A—N1—H1B	120 (6)
C4—C6—H6	119.6	C9—N1—H1C	110 (4)
C6—C7—C1	119.0 (5)	H1A—N1—H1C	109 (6)
C6—C7—H7	120.5	H1B—N1—H1C	97 (6)
C1—C7—H7	120.5	N1—C9—C9 <sup>ii</sup>	110.6 (5)
O1—C8—H8A	109.5	N1—C9—H9A	109.5
O1—C8—H8B	109.5	C9 <sup>ii</sup> —C9—H9A	109.5
H8A—C8—H8B	109.5	N1—C9—H9B	109.5
O1—C8—H8C	109.5	C9 <sup>ii</sup> —C9—H9B	109.5
H8A—C8—H8C	109.5	H9A—C9—H9B	108.1
H8B—C8—H8C	109.5		
C8—O1—C1—C2	0.1 (8)	C3—C4—C5—O2	-179.3 (6)
C8—O1—C1—C7	-179.6 (5)	C6—C4—C5—O2	0.6 (9)
O1—C1—C2—C3	-179.7 (5)	C3—C4—C6—C7	0.6 (9)
C7—C1—C2—C3	-0.1 (9)	C5—C4—C6—C7	-179.4 (5)
C1—C2—C3—C4	0.6 (9)	C4—C6—C7—C1	0.0 (9)
C2—C3—C4—C6	-0.9 (9)	O1—C1—C7—C6	179.5 (5)
C2—C3—C4—C5	179.1 (5)	C2—C1—C7—C6	-0.2 (9)

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6 $\cdots$ Cl1 <sup>iii</sup>	0.95	3.05	3.596 (5)	118
N1—H1A $\cdots$ O2 <sup>iii</sup>	0.90 (2)	1.89 (3)	2.763 (6)	162 (6)
N1—H1B $\cdots$ Cl1 <sup>iv</sup>	0.92 (2)	2.71 (5)	3.312 (4)	124 (5)
N1—H1B $\cdots$ Cl3 <sup>v</sup>	0.92 (2)	2.62 (4)	3.404 (4)	144 (5)
N1—H1C $\cdots$ Cl2	0.92 (2)	2.44 (3)	3.315 (5)	158 (6)
N1—H1C $\cdots$ Cl3	0.92 (2)	2.75 (6)	3.292 (4)	119 (5)
C9—H9B $\cdots$ O2 <sup>vi</sup>	0.99	2.62	3.319 (7)	128

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