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Crystal structure of 2-methyl-1*H*-imidazol-3-ium aquatrichlorido(oxalato- κ^2 O,O')stannate(IV)

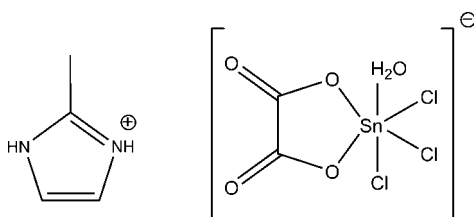
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The tin(IV) atom in the complex anion of the title salt, $(C_4H_7N_2)[Sn(C_2O_4)Cl_3(H_2O)]$, is in a distorted octahedral coordination environment defined by three chlorido ligands, an oxygen atom from a water molecule and two oxygen atoms from a chelating oxalate anion. The organic cation is linked through a bifurcated $N-H \cdots O$ hydrogen bond to the free oxygen atoms of the oxalate ligand of the complex $[Sn(H_2O)Cl_3(C_2O_4)]^-$ anion. Neighbouring stannate(IV) anions are linked through $O-H \cdots O$ hydrogen bonds involving the water molecule and the two non-coordinating oxalate oxygen atoms. In combination with additional $N-H \cdots Cl$ hydrogen bonds between cations and anions, a three-dimensional network is spanned.

1. Chemical Context

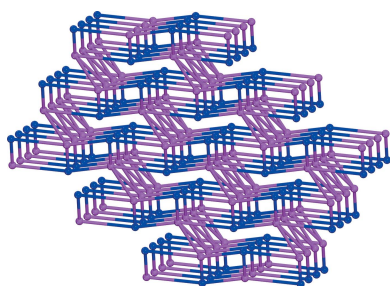
With many applications found in catalysis (see, for example: Meneghetti & Meneghetti, 2015) or as a result of their biological activities (Sirajuddin *et al.*, 2014), organotin(IV) complexes are still a widely studied class of compounds. For more than two decades, the Senegalese group has focused research on attempts to obtain new halo- and organotin(IV) compounds, especially compounds with oxalato ligands (Gueye *et al.*, 2010, 2012, 2014; Sarr *et al.*, 2015; Sow *et al.*, 2012, 2013).



In this communication we report on the interaction between methyl-2-imidazolium hydrogenoxalate dihydrate and $SnCl_2 \cdot 2H_2O$ in methanolic solution, which yielded the title compound, $(C_4H_7N_2)[Sn(C_2O_4)Cl_3(H_2O)]$.

2. Structural commentary

The oxalate anion chelates the $[SnCl_3(H_2O)]^+$ moiety and completes a distorted octahedral environment around the tin(IV) atom in the anion (Fig. 1). The Sn–Cl distances [2.359 (2)–2.378 (3) Å] and the Sn–O distances [2.097 (6) Å and 2.111 (6) Å] are similar to those reported for the same anion in $((H_3C)_4N)[Sn(H_2O)Cl_3(C_2O_4)]$ (Sow *et al.*, 2013). The pairwise distribution of C–O bond lengths with two shorter [1.235 (12)/1.243 (12) Å for O3/O4] and two longer bonds



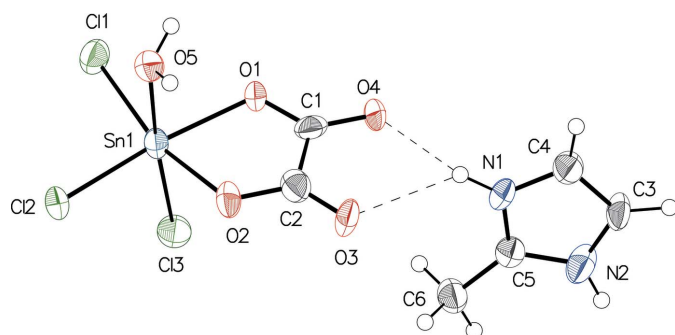


Figure 1
The molecular components of the title compound, with atom labels and 50% displacement ellipsoids at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radius.

[1.277 (11)/1.282 (12) Å for O1/O2] is attributed to additional bonding to the Sn^{IV} atom for the longer bonds. The water molecule is *trans* to one of the Cl atoms and the Sn—O5 bond linking the water molecule to the tin(IV) atom [2.124 (7) Å] is slightly longer than the Sn—O bonds involving the oxalate O atoms. The angles in the [Sn(H₂O)Cl₃(C₂O₄)][−] anion and in the organic cation have typical values.

3. Supramolecular features

Each complex [Sn(H₂O)Cl₃(C₂O₄)][−] anion is linked with two other anions through O—H...O hydrogen bonds between the

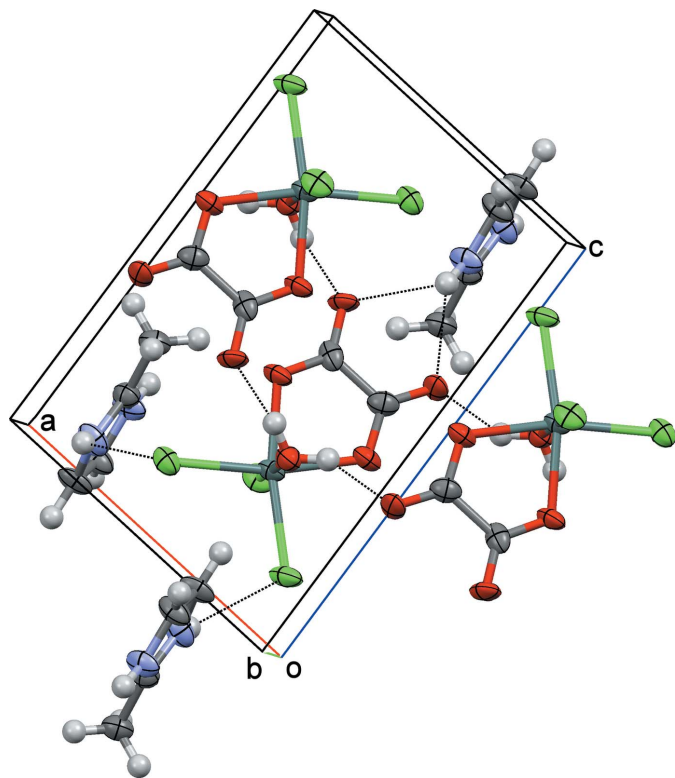


Figure 2
View approximately around the *b* axis showing a central complex anion acting as a hydrogen-bond donor toward two other anions and as a hydrogen-bond acceptor of three methyl-2-imidazolium cations.

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

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O4 ⁱ	0.87	1.76	2.618 (9)	170
O5—H5B...O3 ⁱⁱ	0.87	1.83	2.602 (9)	146
N1—H1...O3	0.88	2.32	3.010 (11)	136
N1—H1...O4	0.88	2.31	2.974 (10)	132
N2—H2...Cl2 ⁱⁱⁱ	0.88	2.70	3.354 (8)	132
N2—H2...Cl1 ^{iv}	0.88	2.84	3.435 (10)	126

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

water molecules as donor and non-coordinating oxalate O atoms as acceptor groups (Table 1). The cations are connected to the anions through a bifurcated N—H...O hydrogen bond. Additional N—H...Cl hydrogen bonding between cations and anions stabilizes this three-dimensional arrangement (Table 1, Fig. 2). Topological analysis according to *TOPOS* (Alexandrov *et al.*, 2011) reveals a net with 3,5T1 topological type (Fig. 3).

4. Database Survey

A search of the Cambridge Structural Database (Version 5.36 with one update, Groom & Allen, 2014) returned about 50 different structures with bidentate oxalate anions linked to a Sn^{IV} atom, from which 23 have their oxalate anions acting as bridging ligands, while 20 have the same configuration as in the title compound with a pairwise distribution of C—O bond lengths. Four structures include both configurations, see, for example: Gueye *et al.* (2010) or Ng *et al.* (1992).

5. Synthesis and crystallization

Crystals of methyl-2-imidazolium hydrogenoxalate dihydrate (*L*) were obtained by mixing methyl-2-imidazole with oxalic acid in a 1:1 ratio in water and evaporation of the solvent at

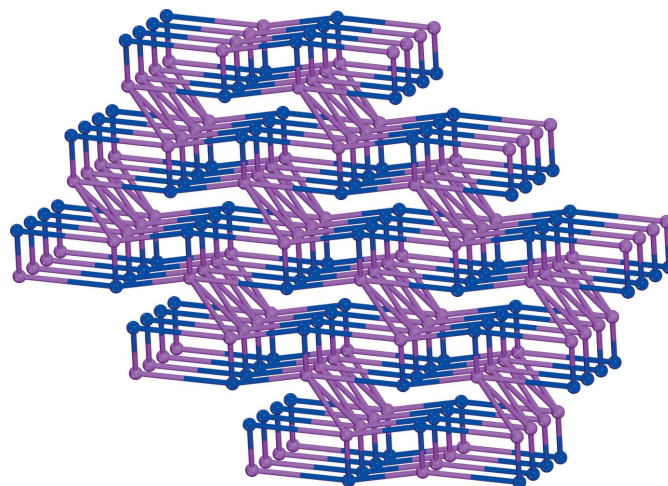


Figure 3
The 3,5T1 topological network in the structure of the title compound. The purple nodes correspond to the Sn^{IV} atoms while the blue nodes are the centres of the organic cations.

Table 2
Experimental details.

Crystal data	
Chemical formula	(C ₄ H ₇ N ₂)[Sn(C ₂ O ₄)Cl ₃ (H ₂ O)]
<i>M</i> _r	414.19
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	120
<i>a</i> , <i>b</i> , <i>c</i> (Å)	7.4757 (9), 8.0857 (10), 11.2846 (14)
α , β , γ (°)	80.856 (8), 83.946 (9), 86.587 (8)
<i>V</i> (Å ³)	669.05 (14)
<i>Z</i>	2
Radiation type	Ga <i>K</i> α , λ = 1.34139 Å
μ (mm ⁻¹)	13.92
Crystal size (mm)	0.05 × 0.04 × 0.04
Data collection	
Diffractometer	Bruker Venture Metaljet
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.133, 0.255
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	5497, 2520, 1604
<i>R</i> _{int}	0.112
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.619
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.062, 0.150, 1.07
No. of reflections	2520
No. of parameters	156
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	2.10, -1.23

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXT* (Sheldrick, 2015a), *SHELXL2014* (Sheldrick, 2015b), *OLEX2* (Dolomanov *et al.*, 2009), *Mercury* (Macrae *et al.*, 2008) and *publCIF* (Westrip, 2010).

333 K. On allowing (*L*) to react with SnCl₂·2H₂O in a 1:2 ratio in methanol, crystals of (C₄H₇N₂)⁺[Sn(H₂O)Cl₃(C₂O₄)⁻] were obtained after slow solvent evaporation at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms of the water molecules were obtained from a difference map and were refined with an O—H distance of 0.87 Å and *U*_{iso}(H) = 1.5*U*_{eq}(O). The other H atoms were positioned geometrically (C—H = 0.95 for aromatic and 0.98 Å for methyl groups; N—H = 0.88 Å) and

refined as riding with *U*_{iso}(H) = *xU*_{eq}(C,N) with *x* = 1.5 for methyl and *x* = 1.2 for all other H atoms.

Acknowledgements

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Acta Cryst. (2015). E71, 520-522 [doi:10.1107/S2056989015005988]

Crystal structure of 2-methyl-1*H*-imidazol-3-ium aquatrichlorido(oxalato- κ^2 O,*O'*)stannate(IV)

Mouhamadou Birame Diop, Libasse Diop, Laurent Plasseraud and Thierry Maris

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINTE* (Bruker, 2014); data reduction: *SAINTE* (Bruker, 2014); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009) and *pubCIF* (Westrip, 2010).

2-Methyl-1*H*-imidazol-3-ium aquatrichlorido(oxalato- κ^2 O,*O'*)stannate(IV)

Crystal data

(C₄H₇N₂)[Sn(C₂O₄)Cl₃(H₂O)]

$M_r = 414.19$

Triclinic, $P\bar{1}$

$a = 7.4757$ (9) Å

$b = 8.0857$ (10) Å

$c = 11.2846$ (14) Å

$\alpha = 80.856$ (8)°

$\beta = 83.946$ (9)°

$\gamma = 86.587$ (8)°

$V = 669.05$ (14) Å³

$Z = 2$

$F(000) = 400$

$D_x = 2.056$ Mg m⁻³

Ga $K\alpha$ radiation, $\lambda = 1.34139$ Å

Cell parameters from 2537 reflections

$\theta = 3.5$ – 53.3 °

$\mu = 13.92$ mm⁻¹

$T = 120$ K

Block, clear light colourless

$0.05 \times 0.04 \times 0.04$ mm

Data collection

Bruker Venture Metaljet
diffractometer

Radiation source: Metal Jet, Gallium Liquid
Metal Jet Source

Helios MX Mirror Optics monochromator

Detector resolution: 10.24 pixels mm⁻¹

ω and ϕ scans

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

$T_{\min} = 0.133$, $T_{\max} = 0.255$

5497 measured reflections

2520 independent reflections

1604 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.112$

$\theta_{\max} = 56.1$ °, $\theta_{\min} = 4.8$ °

$h = -8 \rightarrow 9$

$k = -9 \rightarrow 9$

$l = -12 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.062$

$wR(F^2) = 0.150$

$S = 1.07$

2520 reflections

156 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Hydrogen site location: mixed

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 1.7851P]$

where $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} < 0.001$$

$$\Delta\rho_{\max} = 2.10 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -1.23 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. X-ray crystallographic data for I were collected from a single-crystal sample, which was mounted on a loop fiber. Data were collected using a Bruker Venture diffractometer equipped with a Photon 100 CMOS Detector, a Helios MX optics and a Kappa goniometer. The crystal-to-detector distance was 4.0 cm, and the data collection was carried out in 1024 x 1024 pixel mode.

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.

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.29887 (9)	0.93269 (8)	0.27360 (5)	0.0317 (2)
Cl2	0.0743 (4)	1.0116 (3)	0.1403 (2)	0.0435 (6)
Cl3	0.3305 (4)	0.6485 (3)	0.2412 (2)	0.0440 (6)
Cl1	0.5565 (3)	1.0303 (3)	0.1490 (2)	0.0408 (6)
O1	0.4545 (9)	0.8696 (8)	0.4197 (5)	0.0350 (16)
O5	0.2658 (9)	1.1790 (8)	0.3182 (6)	0.0353 (16)
H5A	0.3590	1.2042	0.3507	0.053*
H5B	0.1714	1.1866	0.3693	0.053*
O3	0.0676 (9)	0.7477 (9)	0.6101 (6)	0.0382 (16)
O2	0.0984 (9)	0.8685 (8)	0.4173 (5)	0.0346 (15)
O4	0.4338 (9)	0.7392 (9)	0.6108 (6)	0.0384 (17)
N1	0.2275 (12)	0.5715 (10)	0.8327 (7)	0.042 (2)
H1	0.2288	0.6585	0.7749	0.050*
C1	0.3663 (13)	0.8049 (12)	0.5176 (9)	0.035 (2)
C5	0.2088 (13)	0.4176 (12)	0.8164 (9)	0.034 (2)
C2	0.1599 (14)	0.8079 (13)	0.5178 (9)	0.038 (2)
N2	0.2132 (12)	0.3254 (11)	0.9248 (7)	0.046 (2)
H2	0.2019	0.2162	0.9399	0.055*
C3	0.2380 (15)	0.4238 (12)	1.0101 (9)	0.041 (3)
H3	0.2481	0.3874	1.0935	0.050*
C4	0.2450 (16)	0.5808 (14)	0.9517 (9)	0.044 (3)
H4	0.2592	0.6791	0.9854	0.053*
C6	0.1870 (14)	0.3569 (13)	0.7014 (9)	0.040 (2)
H6A	0.0680	0.3939	0.6757	0.060*
H6B	0.1982	0.2342	0.7134	0.060*
H6C	0.2804	0.4026	0.6393	0.060*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0409 (4)	0.0320 (4)	0.0223 (4)	-0.0033 (3)	-0.0078 (2)	-0.0003 (3)
Cl2	0.0552 (15)	0.0464 (15)	0.0291 (13)	-0.0117 (12)	-0.0202 (11)	0.0076 (12)
Cl3	0.0584 (15)	0.0350 (14)	0.0407 (14)	-0.0062 (12)	-0.0077 (12)	-0.0090 (12)

C11	0.0482 (13)	0.0417 (14)	0.0302 (12)	-0.0063 (11)	0.0016 (11)	-0.0003 (11)
O1	0.049 (4)	0.037 (4)	0.020 (3)	-0.012 (3)	-0.010 (3)	0.004 (3)
O5	0.038 (4)	0.039 (4)	0.029 (4)	-0.006 (3)	-0.003 (3)	-0.005 (3)
O3	0.037 (4)	0.042 (4)	0.029 (4)	0.002 (3)	-0.001 (3)	0.014 (3)
O2	0.049 (4)	0.034 (4)	0.021 (3)	0.005 (3)	-0.005 (3)	-0.004 (3)
O4	0.041 (4)	0.042 (4)	0.031 (4)	-0.007 (3)	-0.020 (3)	0.012 (3)
N1	0.061 (6)	0.029 (5)	0.033 (5)	-0.013 (4)	-0.011 (4)	0.010 (4)
C1	0.046 (6)	0.030 (5)	0.033 (6)	-0.018 (5)	0.005 (5)	-0.010 (5)
C5	0.038 (5)	0.033 (5)	0.032 (5)	-0.003 (4)	-0.005 (4)	-0.003 (5)
C2	0.048 (6)	0.031 (6)	0.037 (6)	0.002 (5)	-0.012 (5)	-0.005 (5)
N2	0.066 (6)	0.032 (5)	0.035 (5)	0.000 (4)	0.002 (4)	0.003 (4)
C3	0.072 (7)	0.025 (5)	0.026 (5)	0.004 (5)	-0.012 (5)	0.003 (5)
C4	0.068 (7)	0.035 (6)	0.031 (6)	-0.011 (5)	-0.005 (5)	-0.007 (5)
C6	0.049 (6)	0.038 (6)	0.035 (6)	0.001 (5)	-0.012 (5)	-0.004 (5)

Geometric parameters (Å, °)

Sn1—C12	2.364 (3)	N1—C5	1.304 (13)
Sn1—C13	2.378 (3)	N1—C4	1.377 (12)
Sn1—C11	2.359 (2)	C1—C2	1.542 (14)
Sn1—O1	2.097 (6)	C5—N2	1.330 (12)
Sn1—O5	2.124 (7)	C5—C6	1.486 (13)
Sn1—O2	2.111 (6)	N2—H2	0.8800
O1—C1	1.277 (11)	N2—C3	1.375 (12)
O5—H5A	0.8700	C3—H3	0.9500
O5—H5B	0.8691	C3—C4	1.336 (14)
O3—C2	1.235 (12)	C4—H4	0.9500
O2—C2	1.282 (12)	C6—H6A	0.9800
O4—C1	1.243 (12)	C6—H6B	0.9800
N1—H1	0.8800	C6—H6C	0.9800
C12—Sn1—C13	95.47 (10)	O4—C1—O1	125.3 (9)
C11—Sn1—C12	100.40 (9)	O4—C1—C2	118.3 (8)
C11—Sn1—C13	97.56 (9)	N1—C5—N2	105.5 (8)
O1—Sn1—C12	168.07 (19)	N1—C5—C6	127.6 (9)
O1—Sn1—C13	88.82 (19)	N2—C5—C6	126.9 (9)
O1—Sn1—C11	90.03 (18)	O3—C2—O2	125.0 (10)
O1—Sn1—O5	87.8 (3)	O3—C2—C1	119.3 (9)
O1—Sn1—O2	78.6 (3)	O2—C2—C1	115.6 (9)
O5—Sn1—C12	87.18 (19)	C5—N2—H2	124.6
O5—Sn1—C13	175.21 (18)	C5—N2—C3	110.9 (8)
O5—Sn1—C11	85.86 (18)	C3—N2—H2	124.6
O2—Sn1—C12	90.23 (19)	N2—C3—H3	127.0
O2—Sn1—C13	90.25 (19)	C4—C3—N2	106.0 (9)
O2—Sn1—C11	166.09 (18)	C4—C3—H3	127.0
O2—Sn1—O5	85.7 (2)	N1—C4—H4	126.9
C1—O1—Sn1	114.2 (6)	C3—C4—N1	106.1 (10)
Sn1—O5—H5A	110.8	C3—C4—H4	126.9

Sn1—O5—H5B	110.3	C5—C6—H6A	109.5
H5A—O5—H5B	108.2	C5—C6—H6B	109.5
C2—O2—Sn1	114.3 (6)	C5—C6—H6C	109.5
C5—N1—H1	124.2	H6A—C6—H6B	109.5
C5—N1—C4	111.5 (9)	H6A—C6—H6C	109.5
C4—N1—H1	124.2	H6B—C6—H6C	109.5
O1—C1—C2	116.5 (9)		
Sn1—O1—C1—O4	170.5 (8)	N1—C5—N2—C3	-0.9 (12)
Sn1—O1—C1—C2	-8.7 (10)	C5—N1—C4—C3	0.6 (13)
Sn1—O2—C2—O3	-172.8 (8)	C5—N2—C3—C4	1.3 (13)
Sn1—O2—C2—C1	4.3 (10)	N2—C3—C4—N1	-1.1 (13)
O1—C1—C2—O3	-179.7 (8)	C4—N1—C5—N2	0.2 (12)
O1—C1—C2—O2	3.0 (13)	C4—N1—C5—C6	-179.8 (10)
O4—C1—C2—O3	1.1 (14)	C6—C5—N2—C3	179.1 (10)
O4—C1—C2—O2	-176.2 (8)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O5—H5A...O4 ⁱ	0.87	1.76	2.618 (9)	170
O5—H5B...O3 ⁱⁱ	0.87	1.83	2.602 (9)	146
N1—H1...O3	0.88	2.32	3.010 (11)	136
N1—H1...O4	0.88	2.31	2.974 (10)	132
N2—H2...C12 ⁱⁱⁱ	0.88	2.70	3.354 (8)	132
N2—H2...C11 ^{iv}	0.88	2.84	3.435 (10)	126

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