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

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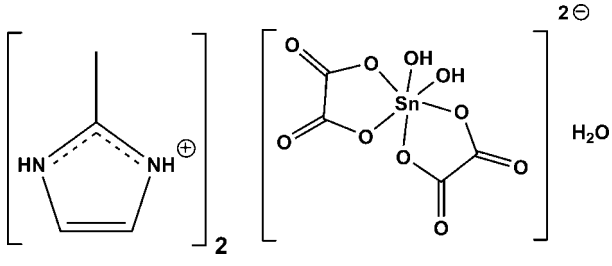
In the structure of the hydrated title salt, $(C_4H_7N_2)_2[Sn(C_2O_4)_2(OH)_2]\cdot H_2O$, the asymmetric unit comprises one stannate(IV) dianion, two organic cations and one water molecule of crystallization. The $[Sn(C_2O_4)_2(OH)_2]^{2-}$ dianion consists of an Sn^{IV} atom chelated by two oxalate anions and coordinated by two OH^- ligands in a *cis* octahedral arrangement. Neighbouring anions are connected through O—H···O hydrogen bonds between hydroxide groups and non-coordinating oxalate O atoms into layers expanding parallel to (100). In addition, cations and anions are linked through N—H···O hydrogen bonds, and the water molecule bridges two anions with two O—H···O hydrogen bonds and is also the acceptor of an N—H···O hydrogen bond with one of the cations. Weak C—H···O hydrogen bonds are also observed. The intricate hydrogen bonding leads to the formation of a three-dimensional network.

1. Chemical context

Organotin(IV) compounds are a class of compounds studied for their numerous applications in various fields involving biological activities (Sirajuddin *et al.*, 2014), biocidal properties (Davies *et al.*, 2008) or catalysis applications (Meneghetti & Meneghetti, 2015). Interested in tin(IV) chemistry, our group has so far synthesized and structurally characterized several compounds of this family, see, for example: Sarr *et al.* (2015); Diop *et al.* (2015); Gueye *et al.* (2014). In the course of designing new oxalatostannate(IV) complexes, we report here the result of the reaction between bis(methyl-2-imidazolium) oxalate and $SnCl_2\cdot 2H_2O$ that yielded the title compound $(C_4H_7N_2)_2[Sn(C_2O_4)_2(OH)_2]\cdot H_2O$ with tin in oxidation state +IV. A similar oxidation of Sn^{II} to Sn^{IV} has been reported recently (Diop *et al.*, 2015).



2. Structural commentary

The Sn^{IV} atom is chelated by two oxalate anions and is coordinated by two OH groups in a *cis* arrangement, leading to a

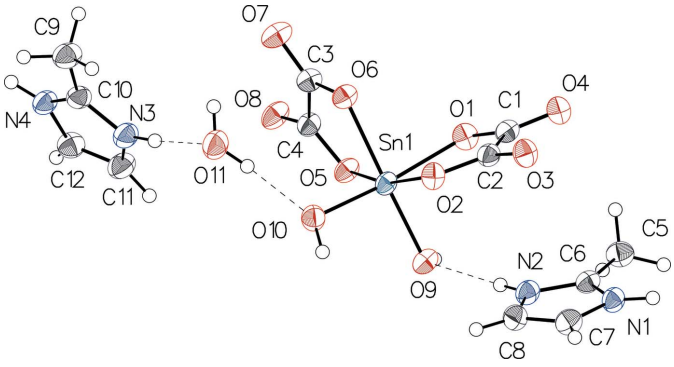


Figure 1
The structure of the molecular components in the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radius and hydrogen bonds are shown as dashed lines.

distorted octahedral environment (Fig. 1). The Sn—O distances involving the oxalate anions [2.103 (2) (O1), 2.077 (2) (O2), 2.074 (2) (O5) and 2.114 (2) Å (O6)] are in the typical range reported for oxalatostannate(IV) anions (Sarr *et al.*, 2015; Gueye *et al.*, 2014). The Sn—O distances involving the OH groups [2.001 (2) (O9) and 1.973 (2) Å (O10)] are shorter by *ca* 0.1 Å. The distortion from the ideal octahedron is reflected by the *trans* angle O1—Sn—O10 of 169.11 (9)° involving one of the hydroxyl groups and the oxalate O1 atom. Within the oxalate ligands, the distances [C1—O1 1.296 (4), C2—O2 1.300 (4), C3—O6 1.290 (4), C4—O5 1.299 (4) Å] and [C2—O3 1.215 (4), C1—O4 1.223 (4), O7—C3 1.220 (4), O8—C4 1.212 (4) Å] are compatible with single C—O and double C═O bonds, respectively. Bond lengths and angles within the two bis(2-methyl-1*H*-imidazol-3-ium) cations are in normal ranges.

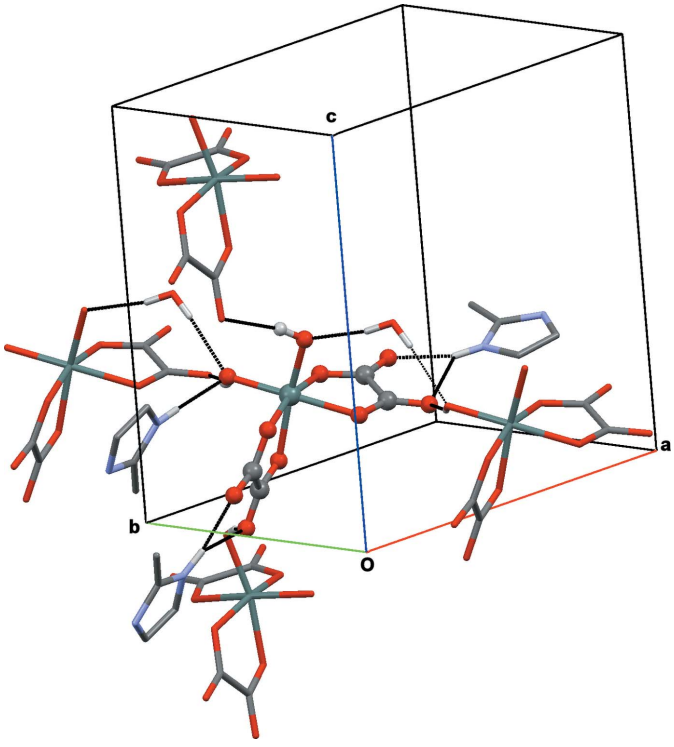


Figure 2
A view of a central stannate dianion (ball-and-stick representation) surrounded by its hydrogen-bonded neighbours (stick representation), *viz* three cations, two water molecules and four other stannate anions. Hydrogen bonds are displayed as black dotted lines and H atoms not involved in hydrogen bonding have been omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9···O7^{i}	0.86	2.00	2.835 (3)	163
O10—H10···O4^{ii}	0.87	2.06	2.909 (3)	167
O11—H11*A*···O10	0.83 (2)	1.95 (2)	2.766 (4)	169 (5)
O11—H11*B*···O9^{iii}	0.83 (2)	2.10 (2)	2.914 (4)	170 (7)
N1—H1···O3^{iv}	0.88	1.97	2.793 (4)	156
N1—H1···O4^{iv}	0.88	2.50	3.131 (3)	129
N2—H2···O9	0.88	1.90	2.742 (3)	160
N3—H3···O11	0.88	1.84	2.713 (4)	175
N4—H4···O8^{v}	0.88	1.94	2.787 (4)	161
C5—H5*A*···O4	0.98	2.55	3.460 (4)	155
C7—H7···O2^{vi}	0.95	2.39	3.327 (4)	169
C8—H8···O4^{ii}	0.95	2.58	3.444 (4)	152
C12—H12···O5^{vii}	0.95	2.33	3.232 (4)	159

Symmetry codes: (i) $x, y+1, z$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $x, y-1, z$; (iv) $-x, -y+2, -z$; (v) $-x+1, -y, -z+1$; (vi) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (vii) $-x+1, -y+1, -z+1$.

3. Supramolecular features

Each stannate dianion $[Sn(C_2O_4)_2(OH)_2]^{2-}$ is linked to two neighbouring anions through hydroxyl(OH)···O hydrogen bonds involving the non-coordinating oxalate O atoms as acceptor groups. These interactions lead to the formation of layers extending parallel to (100). The cations interact with the anions *via* N—H···O hydrogen bonds (one bifurcated) whereby the non-coordinating oxalate O atoms again are the acceptor groups with the exception of one hydroxyl O atom (O9) as an acceptor (Table 1). The two hydroxyl groups are also acceptor groups of two (water)OH···O interactions, giving a total of nine hydrogen-bonding interactions per stannate dianion (Fig. 2). In addition to the dominant classical O—H···O and N—H···O interactions, weak C—H···O hydrogen bonds are also present in the structure (Table 1).

4. Synthesis and crystallization

The title compound was obtained by reacting in methanol in a 2:1 ratio $SnCl_2{\cdot}2H_2O$ with bis(methyl-2-imidazolium) oxalate. The latter was previously prepared in aqueous solution by mixing in a 2:1 ratio methyl-2-imidazole with oxalic acid and allowing the water to evaporate at 333 K. Slow solvent evaporation at room temperature afforded colourless crystals suitable for X-ray diffraction analysis.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The coordinates of H atoms of the water molecules and hydroxy groups were obtained from a

Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_4H_7N_2)_2[Sn(C_2O_4)_2(H_2O)_2]\cdot H_2O$
M_r	512.99
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	110
a, b, c (Å)	20.1391 (13), 7.0651 (5), 13.4942 (9)
β (°)	106.582 (2)
V (Å^3)	1840.2 (2)
Z	4
Radiation type	Ga $K\alpha$, λ = 1.34139 Å
μ (mm^{-1})	7.83
Crystal size (mm)	0.19 × 0.11 × 0.09
Data collection	
Diffractometer	Bruker Venture Metaljet
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.509, 0.752
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	42907, 4235, 4110
R_{int}	0.058
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.651
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.101, 1.07
No. of reflections	4235
No. of parameters	265
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.87, −0.81

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

difference map and were refined using SADI and DFIX restraints (Sheldrick, 2015*b*). All other H atoms were positioned geometrically (C—H = 0.95, 0.98 Å, 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 other H atoms.

Acknowledgements

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

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

Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: SHELXT (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); 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 *publCIF* (Westrip, 2010).

Bis(2-methyl-1*H*-imidazol-3-ium) dihydroxidobis(oxalato-κ^2O^1,O^2)stannate(IV) monohydrate

Crystal data

$(C_4H_7N_2)_2[Sn(C_2O_4)_2(H_2O)_2]\cdot H_2O$
M_r = 512.99
Monoclinic, $P2_1/c$
a = 20.1391 (13) Å
b = 7.0651 (5) Å
c = 13.4942 (9) Å
β = 106.582 (2)°
V = 1840.2 (2) Å^3
Z = 4
$F(000)$ = 1024
D_x = 1.852 Mg m^{-3}
Ga $K\alpha$ radiation, λ = 1.34139 Å
Cell parameters from 9589 reflections
θ = 4.2–60.8°
μ = 7.83 mm^{-1}
T = 110 K
Block, clear light colourless
0.19 × 0.11 × 0.09 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} = 0.509, T_{max} = 0.752
42907 measured reflections
4235 independent reflections
4110 reflections with $I > 2\sigma(I)$
R_{int} = 0.058
θ_{max} = 60.9°, θ_{min} = 2.0°
h = −26→26
k = −8→9
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.101
S = 1.07
4235 reflections
265 parameters
4 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0612P)^2 + 2.7674P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001

$\Delta\rho_{max}$ = 1.87 e Å^{-3} $\Delta\rho_{min}$ = −0.81 e Å^{-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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.24060 (2)	0.62119 (3)	0.27535 (2)	0.02481 (10)
O1	0.22492 (11)	0.6762 (3)	0.11720 (17)	0.0312 (4)
O2	0.13386 (12)	0.5897 (3)	0.21916 (18)	0.0293 (5)
O3	0.04507 (12)	0.6473 (3)	0.07971 (18)	0.0330 (5)
O4	0.13911 (12)	0.7325 (3)	−0.02786 (17)	0.0347 (5)
O5	0.34706 (12)	0.6212 (3)	0.29967 (19)	0.0278 (5)
O6	0.25904 (10)	0.3368 (3)	0.24215 (18)	0.0280 (4)
O7	0.34600 (13)	0.1302 (3)	0.2613 (2)	0.0368 (6)
O8	0.43752 (11)	0.4264 (3)	0.3297 (2)	0.0347 (5)
O9	0.24047 (12)	0.9006 (3)	0.2994 (2)	0.0306 (5)
H9	0.2722	0.9540	0.2777	0.046*
O10	0.24113 (12)	0.5339 (3)	0.41448 (17)	0.0321 (5)
H10	0.2163	0.6085	0.4403	0.048*
C1	0.16053 (15)	0.6868 (4)	0.0632 (2)	0.0274 (6)
C2	0.10678 (17)	0.6380 (4)	0.1231 (2)	0.0273 (6)
C3	0.32352 (15)	0.2896 (4)	0.2648 (2)	0.0280 (6)
C4	0.37567 (15)	0.4559 (4)	0.3017 (2)	0.0275 (6)
N1	0.01942 (13)	1.1771 (4)	0.1086 (2)	0.0289 (5)
H1	−0.0115	1.2288	0.0559	0.043*
N2	0.11571 (14)	1.0703 (4)	0.2068 (2)	0.0299 (5)
H2	0.1597	1.0387	0.2303	0.045*
C5	0.12035 (18)	1.2002 (5)	0.0351 (3)	0.0343 (7)
H5A	0.1243	1.0864	−0.0043	0.051*
H5B	0.1667	1.2509	0.0683	0.051*
H5C	0.0928	1.2956	−0.0116	0.051*
C6	0.08607 (16)	1.1515 (4)	0.1151 (2)	0.0271 (6)
C7	0.00616 (19)	1.1103 (4)	0.1971 (3)	0.0332 (7)
H7	−0.0372	1.1110	0.2118	0.040*
C8	0.06634 (17)	1.0440 (5)	0.2585 (2)	0.0334 (6)
H8	0.0736	0.9893	0.3250	0.040*
N3	0.40483 (15)	0.0861 (4)	0.5690 (2)	0.0342 (6)
H3	0.3611	0.1160	0.5404	0.051*
N4	0.49720 (14)	−0.0750 (4)	0.6344 (2)	0.0306 (5)
H4	0.5252	−0.1712	0.6567	0.046*

C9	0.38714 (19)	−0.2637 (5)	0.5737 (3)	0.0390 (7)
H9A	0.4017	−0.3457	0.6346	0.059*
H9B	0.3941	−0.3298	0.5136	0.059*
H9C	0.3380	−0.2320	0.5604	0.059*
C10	0.42895 (17)	−0.0874 (5)	0.5925 (2)	0.0298 (6)
C11	0.45913 (19)	0.2124 (5)	0.5965 (3)	0.0380 (7)
H11	0.4562	0.3460	0.5881	0.046*
C12	0.5171 (2)	0.1116 (4)	0.6374 (3)	0.0347 (7)
H12	0.5628	0.1599	0.6633	0.042*
O11	0.26942 (14)	0.1609 (4)	0.4740 (2)	0.0406 (6)
H11A	0.258 (3)	0.267 (3)	0.449 (4)	0.074 (18)*
H11B	0.259 (4)	0.079 (6)	0.428 (4)	0.10 (2)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01935 (13)	0.02397 (14)	0.02993 (14)	0.00241 (6)	0.00517 (9)	0.00129 (6)
O1	0.0245 (10)	0.0368 (11)	0.0333 (11)	−0.0011 (9)	0.0097 (8)	0.0009 (9)
O2	0.0236 (10)	0.0338 (11)	0.0311 (11)	0.0006 (9)	0.0088 (9)	0.0052 (9)
O3	0.0233 (11)	0.0407 (12)	0.0327 (11)	−0.0004 (9)	0.0043 (9)	0.0021 (9)
O4	0.0353 (12)	0.0380 (12)	0.0295 (11)	0.0011 (9)	0.0073 (9)	0.0035 (9)
O5	0.0205 (10)	0.0245 (11)	0.0389 (12)	0.0019 (7)	0.0092 (9)	0.0008 (8)
O6	0.0216 (10)	0.0263 (10)	0.0357 (11)	−0.0001 (8)	0.0075 (8)	−0.0016 (9)
O7	0.0286 (12)	0.0265 (12)	0.0561 (16)	0.0006 (8)	0.0136 (11)	−0.0043 (9)
O8	0.0218 (10)	0.0284 (10)	0.0524 (14)	0.0023 (9)	0.0080 (10)	0.0003 (10)
O9	0.0266 (12)	0.0241 (10)	0.0408 (12)	0.0015 (8)	0.0090 (9)	0.0010 (9)
O10	0.0329 (11)	0.0344 (12)	0.0297 (10)	0.0044 (9)	0.0100 (9)	0.0037 (9)
C1	0.0257 (14)	0.0237 (14)	0.0321 (14)	0.0011 (11)	0.0070 (11)	−0.0011 (11)
C2	0.0263 (15)	0.0241 (14)	0.0295 (14)	−0.0003 (10)	0.0046 (12)	−0.0011 (10)
C3	0.0250 (14)	0.0259 (14)	0.0335 (14)	−0.0011 (11)	0.0089 (11)	−0.0020 (11)
C4	0.0253 (14)	0.0256 (14)	0.0311 (14)	0.0012 (11)	0.0071 (11)	0.0005 (11)
N1	0.0238 (12)	0.0302 (13)	0.0311 (12)	0.0037 (10)	0.0055 (10)	0.0016 (10)
N2	0.0241 (12)	0.0287 (12)	0.0342 (13)	0.0026 (10)	0.0039 (10)	−0.0011 (11)
C5	0.0340 (16)	0.0342 (17)	0.0375 (16)	−0.0007 (13)	0.0146 (13)	−0.0016 (13)
C6	0.0242 (14)	0.0246 (13)	0.0324 (15)	0.0008 (11)	0.0077 (12)	−0.0019 (11)
C7	0.0300 (17)	0.0335 (17)	0.0377 (17)	0.0005 (12)	0.0122 (14)	−0.0001 (12)
C8	0.0378 (17)	0.0298 (16)	0.0319 (15)	−0.0003 (13)	0.0086 (13)	0.0019 (12)
N3	0.0305 (14)	0.0313 (13)	0.0377 (14)	0.0056 (11)	0.0048 (11)	−0.0020 (11)
N4	0.0262 (13)	0.0274 (12)	0.0360 (14)	0.0032 (11)	0.0052 (11)	−0.0020 (11)
C9	0.0348 (17)	0.0329 (17)	0.0463 (18)	−0.0007 (14)	0.0067 (14)	−0.0071 (14)
C10	0.0266 (15)	0.0309 (14)	0.0313 (15)	0.0035 (12)	0.0071 (12)	−0.0041 (12)
C11	0.0416 (18)	0.0270 (15)	0.0443 (18)	0.0000 (13)	0.0106 (15)	−0.0007 (13)
C12	0.0328 (17)	0.0324 (17)	0.0384 (17)	−0.0040 (12)	0.0092 (14)	−0.0029 (12)
O11	0.0375 (13)	0.0423 (13)	0.0409 (13)	0.0100 (11)	0.0095 (11)	0.0049 (12)

Geometric parameters (Å, º)

Sn1—O1	2.103 (2)	N2—C8	1.380 (4)
Sn1—O2	2.077 (2)	C5—H5A	0.9800
Sn1—O5	2.074 (2)	C5—H5B	0.9800
Sn1—O6	2.114 (2)	C5—H5C	0.9800
Sn1—O9	2.001 (2)	C5—C6	1.478 (4)
Sn1—O10	1.973 (2)	C7—H7	0.9500
O1—C1	1.296 (4)	C7—C8	1.342 (5)
O2—C2	1.300 (4)	C8—H8	0.9500
O3—C2	1.215 (4)	N3—H3	0.8800
O4—C1	1.223 (4)	N3—C10	1.324 (4)
O5—C4	1.299 (4)	N3—C11	1.378 (5)
O6—C3	1.290 (4)	N4—H4	0.8800
O7—C3	1.220 (4)	N4—C10	1.332 (4)
O8—C4	1.212 (4)	N4—C12	1.375 (4)
O9—H9	0.8616	C9—H9A	0.9800
O10—H10	0.8653	C9—H9B	0.9800
C1—C2	1.563 (4)	C9—H9C	0.9800
C3—C4	1.560 (4)	C9—C10	1.484 (5)
N1—H1	0.8800	C11—H11	0.9500
N1—C6	1.332 (4)	C11—C12	1.344 (5)
N1—C7	1.379 (4)	C12—H12	0.9500
N2—H2	0.8800	O11—H11A	0.831 (15)
N2—C6	1.339 (4)	O11—H11B	0.827 (16)
O1—Sn1—O6	86.86 (9)	C8—N2—H2	125.4
O2—Sn1—O1	79.01 (9)	H5A—C5—H5B	109.5
O2—Sn1—O6	92.69 (8)	H5A—C5—H5C	109.5
O5—Sn1—O1	90.55 (9)	H5B—C5—H5C	109.5
O5—Sn1—O2	166.65 (9)	C6—C5—H5A	109.5
O5—Sn1—O6	78.32 (8)	C6—C5—H5B	109.5
O9—Sn1—O1	88.58 (10)	C6—C5—H5C	109.5
O9—Sn1—O2	96.65 (9)	N1—C6—N2	107.1 (3)
O9—Sn1—O5	91.33 (8)	N1—C6—C5	126.3 (3)
O9—Sn1—O6	168.64 (9)	N2—C6—C5	126.6 (3)
O10—Sn1—O1	169.11 (9)	N1—C7—H7	126.6
O10—Sn1—O2	92.17 (9)	C8—C7—N1	106.8 (3)
O10—Sn1—O5	97.17 (9)	C8—C7—H7	126.6
O10—Sn1—O6	87.19 (9)	N2—C8—H8	126.4
O10—Sn1—O9	98.87 (10)	C7—C8—N2	107.2 (3)
C1—O1—Sn1	114.71 (19)	C7—C8—H8	126.4
C2—O2—Sn1	115.6 (2)	C10—N3—H3	125.5
C4—O5—Sn1	115.80 (18)	C10—N3—C11	109.1 (3)
C3—O6—Sn1	114.93 (19)	C11—N3—H3	125.5
Sn1—O9—H9	110.0	C10—N4—H4	125.3
Sn1—O10—H10	110.2	C10—N4—C12	109.4 (3)
O1—C1—C2	115.2 (3)	C12—N4—H4	125.3

O4—C1—O1	126.1 (3)	H9A—C9—H9B	109.5
O4—C1—C2	118.7 (3)	H9A—C9—H9C	109.5
O2—C2—C1	114.7 (3)	H9B—C9—H9C	109.5
O3—C2—O2	125.1 (3)	C10—C9—H9A	109.5
O3—C2—C1	120.2 (3)	C10—C9—H9B	109.5
O6—C3—C4	114.9 (3)	C10—C9—H9C	109.5
O7—C3—O6	126.1 (3)	N3—C10—N4	107.7 (3)
O7—C3—C4	119.0 (3)	N3—C10—C9	125.8 (3)
O5—C4—C3	114.6 (2)	N4—C10—C9	126.5 (3)
O8—C4—O5	124.8 (3)	N3—C11—H11	126.4
O8—C4—C3	120.6 (3)	C12—C11—N3	107.3 (3)
C6—N1—H1	125.2	C12—C11—H11	126.4
C6—N1—C7	109.7 (3)	N4—C12—H12	126.7
C7—N1—H1	125.2	C11—C12—N4	106.6 (3)
C6—N2—H2	125.4	C11—C12—H12	126.7
C6—N2—C8	109.2 (3)	H11A—O11—H11B	110 (3)

Sn1—O1—C1—O4	173.7 (3)	O7—C3—C4—O8	−2.5 (5)
Sn1—O1—C1—C2	−5.5 (3)	N1—C7—C8—N2	−0.2 (4)
Sn1—O2—C2—O3	−172.4 (2)	C6—N1—C7—C8	0.4 (4)
Sn1—O2—C2—C1	7.4 (3)	C6—N2—C8—C7	0.0 (4)
Sn1—O5—C4—O8	−168.6 (3)	C7—N1—C6—N2	−0.4 (4)
Sn1—O5—C4—C3	11.0 (3)	C7—N1—C6—C5	178.5 (3)
Sn1—O6—C3—O7	172.8 (3)	C8—N2—C6—N1	0.2 (4)
Sn1—O6—C3—C4	−6.1 (3)	C8—N2—C6—C5	−178.7 (3)
O1—C1—C2—O2	−1.2 (4)	N3—C11—C12—N4	−0.1 (4)
O1—C1—C2—O3	178.6 (3)	C10—N3—C11—C12	0.0 (4)
O4—C1—C2—O2	179.6 (3)	C10—N4—C12—C11	0.2 (4)
O4—C1—C2—O3	−0.7 (4)	C11—N3—C10—N4	0.1 (4)
O6—C3—C4—O5	−3.2 (4)	C11—N3—C10—C9	−179.0 (3)
O6—C3—C4—O8	176.5 (3)	C12—N4—C10—N3	−0.2 (4)
O7—C3—C4—O5	177.8 (3)	C12—N4—C10—C9	179.0 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O9—H9···O7^{i}	0.86	2.00	2.835 (3)	163
O10—H10···O4^{ii}	0.87	2.06	2.909 (3)	167
O11—H11*A*···O10	0.83 (2)	1.95 (2)	2.766 (4)	169 (5)
O11—H11*B*···O9^{iii}	0.83 (2)	2.10 (2)	2.914 (4)	170 (7)
N1—H1···O3^{iv}	0.88	1.97	2.793 (4)	156
N1—H1···O4^{iv}	0.88	2.50	3.131 (3)	129
N2—H2···O9	0.88	1.90	2.742 (3)	160
N3—H3···O11	0.88	1.84	2.713 (4)	175
N4—H4···O8^{v}	0.88	1.94	2.787 (4)	161
C5—H5*A*···O4	0.98	2.55	3.460 (4)	155
C7—H7···O2^{vi}	0.95	2.39	3.327 (4)	169

C8—H8···O4^{ii}	0.95	2.58	3.444 (4)	152
C12—H12···O5^{vii}	0.95	2.33	3.232 (4)	159

Symmetry codes: (i) x, y+1, z; (ii) x, −y+3/2, z+1/2; (iii) x, y−1, z; (iv) −x, −y+2, −z; (v) −x+1, −y, −z+1; (vi) −x, y+1/2, −z+1/2; (vii) −x+1, −y+1, −z+1.