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Crystal structure of bis(cyclohexylammonium) diphenyldioxalatostannate(IV)

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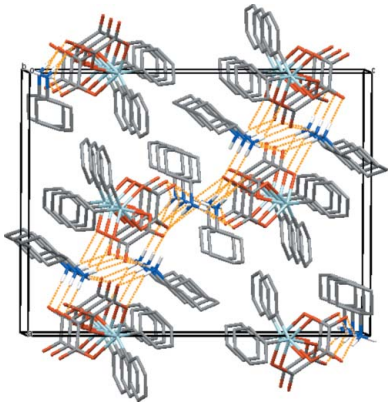
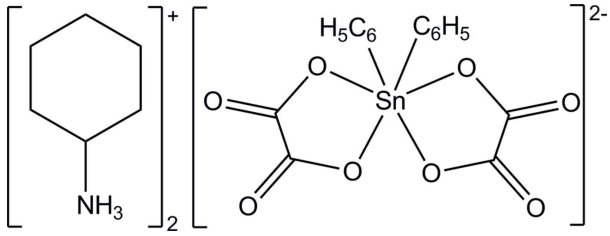
Reaction of oxalic acid and diphenyltin dichloride in the presence of cyclohexylamine led to the formation of the title salt, $(C_6H_{14}N)_2[Sn(C_6H_5)_2(C_2O_4)_2]$. The dianion is made up from an $Sn(C_6H_5)_2$ moiety *cis*-coordinated by two chelating oxalate anions, leading to an overall distorted octahedral coordination geometry of the Sn^{IV} atom. The negative charges are compensated by two surrounding cyclohexylammonium cations adopting chair conformations each. In the crystal, anions and cations are linked *via* a network of N—H···O hydrogen bonds into a layered arrangement parallel to (101).

1. Chemical context

Organotin(IV) complexes are particularly investigated for their catalytic applications as well as for their potential biocidal properties (Davies *et al.*, 2008). Thus, numerous studies have been carried out in order to determine the biological properties of organotin(IV) compounds against bacteria, fungi or cancer cell lines (Gielen, 2002). In this context, and in the course of our ongoing studies on organotin(IV) chemistry (Gueye *et al.*, 1993; Kane *et al.*, 2009; Fall, Okio *et al.*, 2010; Fall, Sow *et al.*, 2010), we have isolated the title stannate as colourless crystals from the reaction of oxalic acid and diphenyltin dichloride in the presence of cyclohexylamine. To date, several organotin(IV) oxalates have been characterized by X-ray crystallographic analysis showing *cis*- and *trans*-coordination of the oxalate anion, depending on the nature of the σ-bonded carbon ligand that is linked to Sn^{IV} (Ng, 1996, 1999; Ng *et al.*, 1992; Ng & Hook, 1999; Ng & Rae, 2000; Xu *et al.*, 2003*a*,*b*; Gueye *et al.*, 2010, 2012; Reichelt & Reuter, 2014).





2. Structural comment

In the title salt, $2(C_6H_{14}N)^+[Sn(C_6H_5)_2(C_2O_4)_2]^{2-}$ or $2(CyNH_3)^+[Sn(Ph_2)(C_2O_4)_2]^{2-}$ (Cy is cyclohexyl; Ph is phenyl), the $SnPh_2$ moiety is chelated by two oxalate anions,

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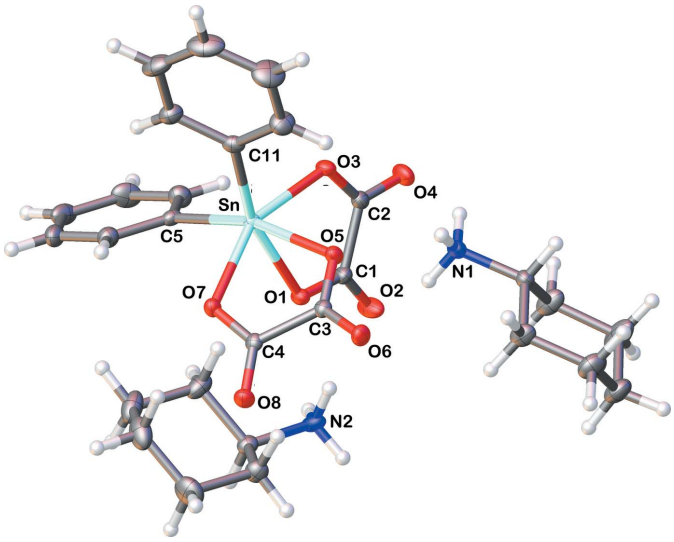

Figure 1
The molecular components of the title salt, showing the atom labelling and with displacement ellipsoids drawn at the 30% probability level. Colour code: Sn = light blue, O = red, N = blue, C = grey and H = white.

leading to a *cis* arrangement within the distorted octahedral coordination sphere of the Sn^{IV} atom. The Sn—C distances and angles of the $SnPh_2$ moiety [Sn—C5 = 2.1388 (15) Å, Sn—C11 = 2.1486 (15) Å with a C5—Sn—C11 angle of 106.94 (6)°] are similar to those previously reported for analogous diphenyltin(IV) derivatives (Xu *et al.*, 2003*a*,*b*; Ng & Rae, 2000).

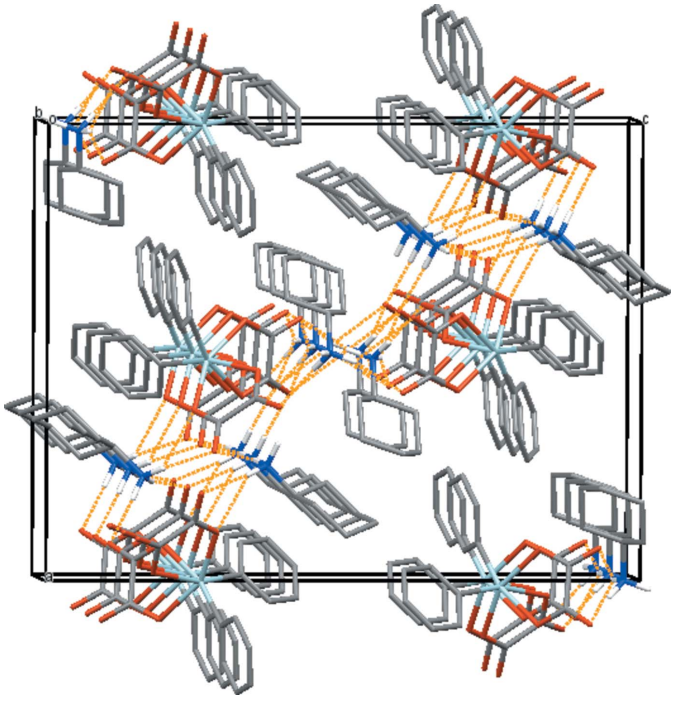

Figure 2
Crystal packing of the title compound, viewed approximately along the *b* axis, showing the layer-like arrangement parallel (101) *via* hydrogen-bonding interactions (dashed orange lines). H atoms not involved in hydrogen bonding have been omitted for clarity. Colour code: Sn = light blue, C = dark grey, H = white, N = dark blue and O = red.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2	0.91	1.90	2.7851 (18)	163
N2—H2*B*···O6^{i}	0.91	2.20	2.8885 (17)	132
N2—H2*B*···O8^{i}	0.91	2.23	3.0583 (18)	151
N2—H2*C*···O6^{ii}	0.91	2.68	3.2403 (18)	121
N2—H2*C*···O8^{ii}	0.91	2.01	2.8970 (18)	164
N1—H1*A*···O6^{i}	0.91	1.98	2.8842 (17)	177
N1—H1*B*···O3^{iii}	0.91	2.31	2.9393 (16)	126
N1—H1*B*···O4^{iii}	0.91	2.35	3.2550 (18)	177
N1—H1*C*···O4	0.91	2.13	3.0076 (18)	163

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

The chelation of both oxalate anions is relatively symmetrical [Sn—O1 = 2.2005 (10) Å and Sn—O3 2.1267 (10) Å; Sn—O5 2.1883 (10) Å and Sn—O7 2.1396 (10) Å]. However, the oxalate anions are slightly distorted with O1—C1—C2—O3 and O5—C3—C4—O7 torsion angles of −4.0 (2) and −9.98 (19)°, respectively. They form a dihedral angle of 77.40 (8)° between their least-squares planes. The molecular structure of the title compound, showing the atom-numbering scheme, is depicted in Fig. 1.

3. Supramolecular features

From a supramolecular point of view, anions and cations of the title salt exhibit intermolecular interactions through N—H···O hydrogen-bonding contacts. Both coordinating and non-coordinating oxygen atoms of both oxalate anions are involved in these interactions (Table 1). Compared to the related structures of bis(diisopropylammonium) [diphenyldioxalatostannates(IV)] (Xu *et al.*, 2003*a*,*b*) where the supramolecular arrangement defines infinite zigzag chains, the cyclohexylammonium cations in the title structure lead to a layer-like arrangement parallel to (101) (Fig. 2).

4. Synthesis and crystallization

Chemicals were purchased from Sigma–Aldrich, and used without further purification. The title compound was obtained by reacting $[(CyNH_3)_2C_2O_4]\cdot 1.5H_2O$ – obtained previously in crystalline form by mixing $CyNH_2$ with oxalic acid ($C_2O_4H_2$) in a 2:1 molar ratio in water and evaporation at 333 K – with $SnPh_2Cl_2$ in methanol (molar ratio 2:1). Colourless single crystals suitable for X-ray diffraction analysis were obtained by slow solvent evaporation at room temperature.

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atoms bonded to C or N atoms were placed at calculated positions using a riding model with C—H = 0.95 (aromatic), 0.99 (methylene) or N—H = 0.91 Å (amine) and with $U_{iso}(H) = 1.2U_{eq}$(C or N).

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Table 2
Experimental details.

Crystal data	
Chemical formula	$(C_6H_{14}N)_2[Sn(C_6H_5)_2(C_2O_2)_2]$
M_r	649.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	115
a, b, c (Å)	16.0084 (6), 8.9010 (3), 20.8060 (8)
β (°)	90.288 (1)
V (Å^3)	2964.63 (19)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.91
Crystal size (mm)	0.50 × 0.30 × 0.23
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.652, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	30318, 6831, 6077
R_{int}	0.025
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.652
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.020, 0.048, 1.05
No. of reflections	6831
No. of parameters	354
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.37, −0.38

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008).

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supporting information

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Crystal structure of bis(cyclohexylammonium) diphenyldioxalatostannate(IV)

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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).

Bis(cyclohexylammonium) diphenyldioxalatostannate(IV)

Crystal data

$(C_6H_{14}N)_2[Sn(C_6H_5)_2(C_2O_2)_2]$
M_r = 649.29
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 16.0084 (6) Å
b = 8.9010 (3) Å
c = 20.8060 (8) Å
β = 90.288 (1)°
V = 2964.63 (19) Å^3
Z = 4
$F(000)$ = 1336
D_x = 1.455 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9926 reflections
θ = 2.5–27.6°
μ = 0.91 mm^{-1}
T = 115 K
Prism, colourless
0.50 × 0.30 × 0.23 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2014)
T_{min} = 0.652, T_{max} = 0.746
30318 measured reflections
6831 independent reflections
6077 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 27.6°, θ_{min} = 2.6°
h = −19→20
k = −11→11
l = −27→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.020
$wR(F^2)$ = 0.048
S = 1.05
6831 reflections
354 parameters
0 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0188P)^2 + 1.6859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.37 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn	0.51059 (2)	0.63627 (2)	0.26048 (2)	0.01224 (3)
O1	0.53271 (6)	0.48705 (12)	0.34316 (5)	0.0161 (2)
O2	0.60914 (8)	0.28994 (15)	0.37435 (6)	0.0298 (3)
O3	0.62046 (6)	0.51474 (12)	0.23644 (5)	0.0167 (2)
O4	0.70720 (7)	0.33267 (14)	0.26676 (6)	0.0253 (3)
O5	0.59259 (6)	0.77093 (12)	0.32213 (5)	0.0168 (2)
O6	0.58885 (7)	0.92654 (13)	0.40624 (5)	0.0194 (2)
O7	0.42652 (6)	0.74042 (12)	0.32654 (5)	0.0154 (2)
O8	0.42376 (7)	0.85828 (12)	0.42139 (5)	0.0198 (2)
C1	0.59203 (9)	0.39309 (18)	0.33711 (8)	0.0178 (3)
C2	0.64560 (9)	0.41207 (18)	0.27566 (7)	0.0171 (3)
C3	0.55591 (9)	0.83851 (16)	0.36756 (7)	0.0140 (3)
C4	0.46009 (9)	0.81040 (16)	0.37349 (7)	0.0136 (3)
C5	0.41711 (9)	0.48308 (17)	0.22695 (7)	0.0152 (3)
C6	0.43554 (11)	0.33624 (18)	0.20842 (8)	0.0228 (3)
H6	0.4916	0.3013	0.2105	0.027*
C7	0.37264 (12)	0.2402 (2)	0.18690 (9)	0.0296 (4)
H7	0.3859	0.1402	0.1747	0.035*
C8	0.29096 (11)	0.2901 (2)	0.18317 (8)	0.0281 (4)
H8	0.2483	0.2247	0.1680	0.034*
C9	0.27154 (10)	0.4346 (2)	0.20153 (8)	0.0256 (4)
H9	0.2154	0.4688	0.1993	0.031*
C10	0.33417 (10)	0.53031 (19)	0.22323 (8)	0.0200 (3)
H10	0.3202	0.6298	0.2358	0.024*
C11	0.52458 (10)	0.80526 (17)	0.18759 (8)	0.0169 (3)
C12	0.46483 (11)	0.81749 (19)	0.13879 (8)	0.0229 (3)
H12	0.4193	0.7491	0.1375	0.027*
C13	0.47103 (13)	0.9286 (2)	0.09192 (9)	0.0319 (4)
H13	0.4294	0.9365	0.0594	0.038*
C14	0.53748 (14)	1.0273 (2)	0.09269 (10)	0.0371 (5)
H14	0.5415	1.1035	0.0609	0.045*
C15	0.59799 (13)	1.0150 (2)	0.13979 (10)	0.0375 (5)
H15	0.6443	1.0817	0.1398	0.045*
C16	0.59177 (11)	0.9056 (2)	0.18728 (9)	0.0268 (4)
H16	0.6335	0.8991	0.2198	0.032*
N2	0.48965 (9)	0.17026 (15)	0.45662 (6)	0.0198 (3)
H2A	0.5239	0.2274	0.4318	0.024*
H2B	0.4893	0.0742	0.4416	0.024*
H2C	0.5085	0.1712	0.4979	0.024*

C23	0.40312 (10)	0.23265 (17)	0.45409 (8)	0.0176 (3)
H23	0.3656	0.1662	0.4798	0.021*
C24	0.40273 (10)	0.38860 (18)	0.48363 (8)	0.0226 (3)
H24A	0.4429	0.4536	0.4607	0.027*
H24B	0.4204	0.3824	0.5292	0.027*
C25	0.31532 (12)	0.4573 (2)	0.47938 (10)	0.0357 (5)
H25A	0.2763	0.3981	0.5061	0.043*
H25B	0.3167	0.5612	0.4963	0.043*
C26	0.28439 (11)	0.4592 (2)	0.41009 (11)	0.0357 (5)
H26A	0.2268	0.4995	0.4087	0.043*
H26B	0.3204	0.5265	0.3844	0.043*
C27	0.28533 (12)	0.3030 (2)	0.38087 (10)	0.0345 (5)
H27A	0.2675	0.3087	0.3353	0.041*
H27B	0.2453	0.2380	0.4040	0.041*
C28	0.37231 (11)	0.23443 (19)	0.38491 (8)	0.0257 (4)
H28A	0.3708	0.1305	0.3680	0.031*
H28B	0.4113	0.2936	0.3582	0.031*
N1	0.73487 (8)	0.05755 (15)	0.34805 (6)	0.0182 (3)
H1A	0.6877	0.0187	0.3657	0.022*
H1B	0.7531	−0.0044	0.3163	0.022*
H1C	0.7236	0.1499	0.3313	0.022*
C17	0.80130 (9)	0.07153 (18)	0.39886 (7)	0.0171 (3)
H17	0.8533	0.1107	0.3783	0.021*
C18	0.81959 (12)	−0.0828 (2)	0.42605 (9)	0.0288 (4)
H18A	0.8401	−0.1493	0.3914	0.035*
H18B	0.7676	−0.1269	0.4434	0.035*
C19	0.88557 (14)	−0.0728 (2)	0.47965 (10)	0.0412 (5)
H19A	0.8935	−0.1733	0.4991	0.049*
H19B	0.9395	−0.0409	0.4610	0.049*
C20	0.85982 (12)	0.0381 (2)	0.53148 (9)	0.0319 (4)
H20A	0.8093	0.0005	0.5535	0.038*
H20B	0.9051	0.0470	0.5638	0.038*
C21	0.84186 (12)	0.1913 (2)	0.50270 (9)	0.0309 (4)
H21A	0.8937	0.2327	0.4840	0.037*
H21B	0.8231	0.2604	0.5370	0.037*
C22	0.77453 (11)	0.18142 (19)	0.45050 (8)	0.0241 (4)
H22A	0.7213	0.1477	0.4697	0.029*
H22B	0.7655	0.2818	0.4312	0.029*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.01278 (5)	0.01303 (5)	0.01090 (5)	−0.00039 (4)	0.00020 (3)	−0.00061 (4)
O1	0.0153 (5)	0.0196 (5)	0.0135 (5)	0.0037 (4)	0.0023 (4)	0.0018 (4)
O2	0.0287 (6)	0.0363 (7)	0.0244 (7)	0.0157 (5)	0.0075 (5)	0.0145 (6)
O3	0.0166 (5)	0.0200 (5)	0.0136 (5)	0.0018 (4)	0.0040 (4)	0.0023 (4)
O4	0.0175 (6)	0.0329 (7)	0.0256 (7)	0.0097 (5)	0.0053 (5)	0.0033 (5)
O5	0.0138 (5)	0.0205 (6)	0.0161 (6)	−0.0015 (4)	0.0009 (4)	−0.0040 (4)

O6	0.0173 (5)	0.0221 (6)	0.0189 (6)	−0.0023 (4)	−0.0023 (4)	−0.0056 (5)
O7	0.0132 (5)	0.0170 (5)	0.0160 (5)	0.0004 (4)	−0.0002 (4)	−0.0035 (4)
O8	0.0180 (5)	0.0244 (6)	0.0170 (6)	0.0019 (4)	0.0022 (4)	−0.0050 (5)
C1	0.0152 (7)	0.0237 (8)	0.0145 (7)	0.0021 (6)	−0.0001 (6)	0.0022 (6)
C2	0.0140 (7)	0.0216 (8)	0.0157 (7)	−0.0006 (6)	0.0005 (6)	−0.0009 (6)
C3	0.0153 (7)	0.0124 (7)	0.0141 (7)	0.0005 (5)	−0.0010 (6)	0.0022 (6)
C4	0.0146 (7)	0.0113 (6)	0.0149 (7)	0.0014 (5)	−0.0010 (6)	0.0019 (6)
C5	0.0189 (7)	0.0160 (7)	0.0107 (7)	−0.0021 (6)	−0.0001 (6)	0.0001 (6)
C6	0.0234 (8)	0.0214 (8)	0.0237 (9)	0.0003 (6)	0.0018 (7)	−0.0039 (7)
C7	0.0395 (10)	0.0205 (8)	0.0289 (10)	−0.0076 (7)	0.0048 (8)	−0.0095 (7)
C8	0.0300 (9)	0.0341 (10)	0.0201 (9)	−0.0173 (8)	0.0009 (7)	−0.0047 (7)
C9	0.0185 (8)	0.0368 (10)	0.0214 (9)	−0.0059 (7)	−0.0022 (6)	0.0000 (8)
C10	0.0212 (8)	0.0197 (8)	0.0191 (8)	−0.0007 (6)	−0.0005 (6)	−0.0009 (6)
C11	0.0212 (8)	0.0139 (7)	0.0157 (8)	0.0027 (6)	0.0044 (6)	−0.0002 (6)
C12	0.0270 (9)	0.0234 (8)	0.0182 (8)	0.0011 (7)	0.0006 (7)	0.0012 (7)
C13	0.0446 (11)	0.0328 (10)	0.0183 (9)	0.0123 (9)	0.0001 (8)	0.0063 (8)
C14	0.0603 (13)	0.0227 (9)	0.0285 (10)	0.0055 (9)	0.0130 (9)	0.0110 (8)
C15	0.0461 (12)	0.0260 (10)	0.0404 (12)	−0.0105 (9)	0.0076 (9)	0.0091 (9)
C16	0.0290 (9)	0.0237 (8)	0.0276 (9)	−0.0059 (7)	0.0011 (7)	0.0037 (7)
N2	0.0283 (7)	0.0188 (7)	0.0122 (6)	0.0068 (5)	0.0016 (5)	0.0004 (5)
C23	0.0204 (8)	0.0162 (7)	0.0163 (8)	−0.0004 (6)	0.0000 (6)	0.0020 (6)
C24	0.0250 (8)	0.0205 (8)	0.0223 (8)	0.0034 (6)	0.0003 (7)	−0.0032 (7)
C25	0.0312 (10)	0.0303 (10)	0.0456 (12)	0.0117 (8)	0.0072 (9)	−0.0008 (9)
C26	0.0232 (9)	0.0321 (10)	0.0516 (13)	0.0037 (8)	−0.0037 (9)	0.0154 (9)
C27	0.0308 (10)	0.0331 (10)	0.0394 (12)	−0.0095 (8)	−0.0151 (8)	0.0140 (9)
C28	0.0357 (10)	0.0220 (8)	0.0192 (8)	−0.0032 (7)	−0.0070 (7)	0.0023 (7)
N1	0.0158 (6)	0.0220 (7)	0.0167 (7)	0.0046 (5)	0.0022 (5)	0.0002 (5)
C17	0.0149 (7)	0.0204 (8)	0.0160 (8)	0.0006 (6)	0.0012 (6)	0.0006 (6)
C18	0.0408 (10)	0.0214 (8)	0.0243 (9)	0.0120 (8)	−0.0058 (8)	−0.0023 (7)
C19	0.0523 (13)	0.0412 (12)	0.0299 (11)	0.0266 (10)	−0.0150 (9)	−0.0054 (9)
C20	0.0395 (11)	0.0367 (10)	0.0195 (9)	0.0080 (8)	−0.0060 (8)	−0.0013 (8)
C21	0.0413 (11)	0.0280 (9)	0.0234 (9)	−0.0007 (8)	−0.0047 (8)	−0.0050 (8)
C22	0.0314 (9)	0.0192 (8)	0.0216 (9)	0.0076 (7)	−0.0003 (7)	−0.0029 (7)

Geometric parameters (Å, º)

Sn—O1	2.2005 (10)	N2—H2C	0.9100
Sn—O3	2.1267 (10)	N2—C23	1.493 (2)
Sn—O5	2.1883 (10)	C23—H23	1.0000
Sn—O7	2.1396 (10)	C23—C24	1.518 (2)
Sn—C5	2.1388 (15)	C23—C28	1.519 (2)
Sn—C11	2.1486 (15)	C24—H24A	0.9900
O1—C1	1.2721 (18)	C24—H24B	0.9900
O2—C1	1.2312 (19)	C24—C25	1.529 (2)
O3—C2	1.2883 (19)	C25—H25A	0.9900
O4—C2	1.2280 (19)	C25—H25B	0.9900
O5—C3	1.2672 (18)	C25—C26	1.522 (3)
O6—C3	1.2391 (18)	C26—H26A	0.9900

O7—C4	1.2751 (18)	C26—H26B	0.9900
O8—C4	1.2326 (18)	C26—C27	1.517 (3)
C1—C2	1.552 (2)	C27—H27A	0.9900
C3—C4	1.560 (2)	C27—H27B	0.9900
C5—C6	1.395 (2)	C27—C28	1.522 (3)
C5—C10	1.394 (2)	C28—H28A	0.9900
C6—H6	0.9500	C28—H28B	0.9900
C6—C7	1.393 (2)	N1—H1A	0.9100
C7—H7	0.9500	N1—H1B	0.9100
C7—C8	1.383 (3)	N1—H1C	0.9100
C8—H8	0.9500	N1—C17	1.5009 (19)
C8—C9	1.378 (3)	C17—H17	1.0000
C9—H9	0.9500	C17—C18	1.514 (2)
C9—C10	1.389 (2)	C17—C22	1.516 (2)
C10—H10	0.9500	C18—H18A	0.9900
C11—C12	1.396 (2)	C18—H18B	0.9900
C11—C16	1.398 (2)	C18—C19	1.535 (3)
C12—H12	0.9500	C19—H19A	0.9900
C12—C13	1.393 (2)	C19—H19B	0.9900
C13—H13	0.9500	C19—C20	1.521 (3)
C13—C14	1.380 (3)	C20—H20A	0.9900
C14—H14	0.9500	C20—H20B	0.9900
C14—C15	1.379 (3)	C20—C21	1.516 (3)
C15—H15	0.9500	C21—H21A	0.9900
C15—C16	1.391 (3)	C21—H21B	0.9900
C16—H16	0.9500	C21—C22	1.529 (2)
N2—H2A	0.9100	C22—H22A	0.9900
N2—H2B	0.9100	C22—H22B	0.9900

O3—Sn—O1	75.33 (4)	C24—C23—H23	108.7
O3—Sn—O5	85.53 (4)	C24—C23—C28	111.84 (13)
O3—Sn—O7	153.52 (4)	C28—C23—H23	108.7
O3—Sn—C5	100.20 (5)	C23—C24—H24A	109.6
O3—Sn—C11	95.78 (5)	C23—C24—H24B	109.6
O5—Sn—O1	77.21 (4)	C23—C24—C25	110.36 (14)
O7—Sn—O1	81.88 (4)	H24A—C24—H24B	108.1
O7—Sn—O5	76.33 (4)	C25—C24—H24A	109.6
O7—Sn—C11	102.60 (5)	C25—C24—H24B	109.6
C5—Sn—O1	88.84 (5)	C24—C25—H25A	109.5
C5—Sn—O5	163.15 (5)	C24—C25—H25B	109.5
C5—Sn—O7	92.55 (5)	H25A—C25—H25B	108.1
C5—Sn—C11	106.94 (6)	C26—C25—C24	110.63 (16)
C11—Sn—O1	163.22 (5)	C26—C25—H25A	109.5
C11—Sn—O5	88.05 (5)	C26—C25—H25B	109.5
C1—O1—Sn	115.90 (9)	C25—C26—H26A	109.3
C2—O3—Sn	117.90 (9)	C25—C26—H26B	109.3
C3—O5—Sn	114.73 (9)	H26A—C26—H26B	108.0
C4—O7—Sn	116.08 (9)	C27—C26—C25	111.46 (16)

O1—C1—C2	115.19 (13)	C27—C26—H26A	109.3
O2—C1—O1	126.29 (15)	C27—C26—H26B	109.3
O2—C1—C2	118.51 (14)	C26—C27—H27A	109.5
O3—C2—C1	115.26 (13)	C26—C27—H27B	109.5
O4—C2—O3	124.14 (14)	C26—C27—C28	110.87 (15)
O4—C2—C1	120.59 (14)	H27A—C27—H27B	108.1
O5—C3—C4	116.26 (13)	C28—C27—H27A	109.5
O6—C3—O5	125.96 (14)	C28—C27—H27B	109.5
O6—C3—C4	117.75 (13)	C23—C28—C27	110.43 (15)
O7—C4—C3	115.39 (13)	C23—C28—H28A	109.6
O8—C4—O7	126.13 (14)	C23—C28—H28B	109.6
O8—C4—C3	118.47 (13)	C27—C28—H28A	109.6
C6—C5—Sn	122.61 (12)	C27—C28—H28B	109.6
C10—C5—Sn	119.36 (11)	H28A—C28—H28B	108.1
C10—C5—C6	118.02 (14)	H1A—N1—H1B	109.5
C5—C6—H6	119.7	H1A—N1—H1C	109.5
C7—C6—C5	120.68 (16)	H1B—N1—H1C	109.5
C7—C6—H6	119.7	C17—N1—H1A	109.5
C6—C7—H7	119.9	C17—N1—H1B	109.5
C8—C7—C6	120.20 (16)	C17—N1—H1C	109.5
C8—C7—H7	119.9	N1—C17—H17	108.4
C7—C8—H8	120.0	N1—C17—C18	108.84 (13)
C9—C8—C7	119.91 (16)	N1—C17—C22	110.54 (12)
C9—C8—H8	120.0	C18—C17—H17	108.4
C8—C9—H9	120.0	C18—C17—C22	112.06 (14)
C8—C9—C10	119.93 (16)	C22—C17—H17	108.4
C10—C9—H9	120.0	C17—C18—H18A	109.6
C5—C10—H10	119.4	C17—C18—H18B	109.6
C9—C10—C5	121.24 (15)	C17—C18—C19	110.48 (16)
C9—C10—H10	119.4	H18A—C18—H18B	108.1
C12—C11—Sn	119.65 (11)	C19—C18—H18A	109.6
C12—C11—C16	118.11 (15)	C19—C18—H18B	109.6
C16—C11—Sn	122.24 (12)	C18—C19—H19A	109.3
C11—C12—H12	119.5	C18—C19—H19B	109.3
C13—C12—C11	120.91 (17)	H19A—C19—H19B	108.0
C13—C12—H12	119.5	C20—C19—C18	111.41 (15)
C12—C13—H13	119.9	C20—C19—H19A	109.3
C14—C13—C12	120.11 (18)	C20—C19—H19B	109.3
C14—C13—H13	119.9	C19—C20—H20A	109.5
C13—C14—H14	120.1	C19—C20—H20B	109.5
C15—C14—C13	119.77 (17)	H20A—C20—H20B	108.1
C15—C14—H14	120.1	C21—C20—C19	110.81 (16)
C14—C15—H15	119.7	C21—C20—H20A	109.5
C14—C15—C16	120.53 (18)	C21—C20—H20B	109.5
C16—C15—H15	119.7	C20—C21—H21A	109.4
C11—C16—H16	119.7	C20—C21—H21B	109.4
C15—C16—C11	120.54 (18)	C20—C21—C22	111.15 (15)
C15—C16—H16	119.7	H21A—C21—H21B	108.0

H2A—N2—H2B	109.5	C22—C21—H21A	109.4
H2A—N2—H2C	109.5	C22—C21—H21B	109.4
H2B—N2—H2C	109.5	C17—C22—C21	109.86 (14)
C23—N2—H2A	109.5	C17—C22—H22A	109.7
C23—N2—H2B	109.5	C17—C22—H22B	109.7
C23—N2—H2C	109.5	C21—C22—H22A	109.7
N2—C23—H23	108.7	C21—C22—H22B	109.7
N2—C23—C24	109.37 (13)	H22A—C22—H22B	108.2
N2—C23—C28	109.51 (13)		

Sn—O1—C1—O2	−171.88 (14)	C8—C9—C10—C5	0.0 (3)
Sn—O1—C1—C2	6.94 (17)	C10—C5—C6—C7	0.0 (2)
Sn—O3—C2—O4	178.78 (12)	C11—C12—C13—C14	0.9 (3)
Sn—O3—C2—C1	−1.22 (17)	C12—C11—C16—C15	0.5 (3)
Sn—O5—C3—O6	−176.13 (12)	C12—C13—C14—C15	0.4 (3)
Sn—O5—C3—C4	2.10 (16)	C13—C14—C15—C16	−1.2 (3)
Sn—O7—C4—O8	−168.51 (12)	C14—C15—C16—C11	0.8 (3)
Sn—O7—C4—C3	12.63 (16)	C16—C11—C12—C13	−1.4 (2)
Sn—C5—C6—C7	179.96 (13)	N2—C23—C24—C25	177.93 (14)
Sn—C5—C10—C9	179.79 (12)	N2—C23—C28—C27	−177.92 (13)
Sn—C11—C12—C13	178.20 (13)	C23—C24—C25—C26	−55.7 (2)
Sn—C11—C16—C15	−179.04 (14)	C24—C23—C28—C27	−56.52 (18)
O1—C1—C2—O3	−4.0 (2)	C24—C25—C26—C27	56.3 (2)
O1—C1—C2—O4	176.02 (15)	C25—C26—C27—C28	−56.5 (2)
O2—C1—C2—O3	174.93 (15)	C26—C27—C28—C23	55.9 (2)
O2—C1—C2—O4	−5.1 (2)	C28—C23—C24—C25	56.44 (19)
O5—C3—C4—O7	−9.98 (19)	N1—C17—C18—C19	−178.38 (14)
O5—C3—C4—O8	171.06 (13)	N1—C17—C22—C21	178.56 (14)
O6—C3—C4—O7	168.40 (13)	C17—C18—C19—C20	54.6 (2)
O6—C3—C4—O8	−10.6 (2)	C18—C17—C22—C21	56.96 (19)
C5—C6—C7—C8	0.5 (3)	C18—C19—C20—C21	−55.5 (2)
C6—C5—C10—C9	−0.2 (2)	C19—C20—C21—C22	56.9 (2)
C6—C7—C8—C9	−0.8 (3)	C20—C21—C22—C17	−57.1 (2)
C7—C8—C9—C10	0.5 (3)	C22—C17—C18—C19	−55.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2	0.91	1.90	2.7851 (18)	163
N2—H2*B*···O6^{i}	0.91	2.20	2.8885 (17)	132
N2—H2*B*···O8^{i}	0.91	2.23	3.0583 (18)	151
N2—H2*C*···O6^{ii}	0.91	2.68	3.2403 (18)	121
N2—H2*C*···O8^{ii}	0.91	2.01	2.8970 (18)	164
N1—H1*A*···O6^{i}	0.91	1.98	2.8842 (17)	177
N1—H1*B*···O3^{iii}	0.91	2.31	2.9393 (16)	126

N1—H1*B*···O4^{iii}	0.91	2.35	3.2550 (18)	177
N1—H1*C*···O4	0.91	2.13	3.0076 (18)	163

Symmetry codes: (i) x, $y-1$, z; (ii) $-x+1$, $-y+1$, $-z+1$; (iii) $-x+3/2$, $y-1/2$, $-z+1/2$.