Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis(dicyclohexylammonium) μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$-bis[aqua(oxalato-$\kappa^2O^1,O^2$)diphenylstannate(IV)]

Ndongo Gueye,[a] Libasse Diop,[a]* K. C. Kieran Molloy[b] and Gabrielle Kociok-Köhn[b]

[a]Laboratoire de Chimie Minérale et Analytique, Département de Chimie, Faculté des Sciences et Techniques, Université Cheikh Anta Diop, Dakar, Senegal, and [b]Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, England
Correspondence e-mail: dlibasse@gmail.com

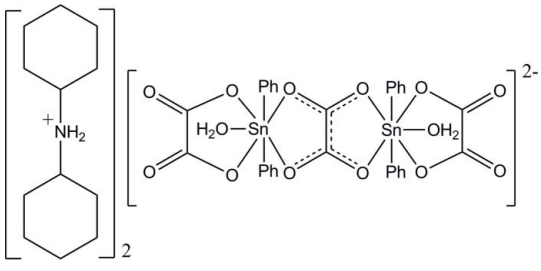
Received 2 September 2010; accepted 11 November 2010

Key indicators: single-crystal X-ray study; T = 150 K; mean σ(C–C) = 0.005 Å; R factor = 0.040; wR factor = 0.082; data-to-parameter ratio = 17.9.

The structure of the title compound, $(C_{12}H_{24}N)_2[Sn_2(C_6H_5)_4(C_2O_4)_3(H_2O)_2]$, consists of a bischelating oxalate ion, located on an inversion center, which is linked to two $SnPh_2$ groups. The coordination sphere of the Sn(IV) ion is completed by a monochelating oxalate anion and a water molecule. The Sn(IV) atoms are thus seven-coordinated. The discrete binuclear units are further connected by hydrogen bonds, leading to a supramolecular crystal structure. The asymmetric unit contains one half dianion and one $(Cy_2NH_2)^+$ cation.

Related literature

For background to organotin(IV) chemistry, see: Ballmann *et al.* (2009); Diallo *et al.* (2007); Diassé-Sarr *et al.* (1997); Ng *et al.* (1992); Singh *et al.* (2008); de Sousa *et al.* (2007); Wang *et al.* (2009); Xanthopoulou *et al.* (2007, 2008); Zia-ur-Rahman *et al.* (2007). For related Sn(IV) structures, see: Diop *et al.* (2002, 2003).



Experimental

Crystal data

$(C_{12}H_{24}N)_2[Sn_2(C_6H_5)_4(C_2O_4)_3(H_2O)_2]$
M_r = 1210.52
Monoclinic, $P2_1/n$
a = 13.1725 (4) Å
b = 14.6121 (4) Å
c = 14.1139 (4) Å
β = 100.869 (2)°
V = 2667.88 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.00 mm^{-1}
T = 150 K
0.2 × 0.2 × 0.2 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.825, T_{max} = 0.825
48411 measured reflections
6114 independent reflections
4069 reflections with $I > 2\sigma(I)$
R_{int} = 0.126

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.082
S = 1.01
6114 reflections
341 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.72 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7B···O4^{i}	0.90 (4)	1.77 (4)	2.663 (3)	175 (4)
N—H1A···O3^{ii}	0.84 (4)	2.12 (3)	2.910 (4)	155 (3)
N—H1A···O4^{ii}	0.84 (4)	2.37 (4)	2.986 (4)	130 (3)
N—H1B···O6^{iii}	0.91 (4)	2.08 (4)	2.960 (4)	164 (4)

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2310).

References

Altomare, A., Burla, M. C., Camalli, M., Cascarano, G. L., Giacovazzo, C., Guagliardi, A., Moliterni, A. G. G., Polidori, G. & Spagna, R. (1999). *J. Appl. Cryst.* **32**, 115–119.
Ballmann, J., Fuchs, M. G. G., Dechert, S., John, M. & Meyer, F. (2009). *Inorg. Chem.* **48**, 90–99.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Diallo, W., Diop, C. A. K., Diop, L., Mahon, M. F., Molloy, K. C., Russo, U., Biesemans, M. & Willem, R. (2007). *J. Organomet. Chem.* **692**, 2187–2192.
Diassé-Sarr, A., Diop, L., Mahon, M. F. & Molloy, K. C. (1997). *Main Group Met. Chem.* **20**, 223–229.
Diop, C. A. K., Diop, L. & Toscano, A. R. (2002). *Main Group Met. Chem.* **25**, 327–328.
Diop, L., Mahieu, B., Mahon, M. F., Molloy, K. C. & Okio, K. Y. A. (2003). *Appl. Organomet. Chem.* **17**, 881–882.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Ng, S. W., Das, V. G. K., Gielen, M. & Tiekink, E. R. T. (1992). *Appl. Organomet. Chem.* **6**, 19–25.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Singh, N., Kumar, A., Molloy, K. C. & Kociok-Köhn, G. (2008). *Acta Cryst.* E**64**, m115.
Sousa, G. F. de, Deflon, V. M., Manso, L. C. C., Ellena, J. E., Mascarenhas, Y. P., Lang, E. S., Gatto, C. C. & Mahieu, B. (2007). *Transition Met. Chem.* **32**, 649–655.
Wang, Z., Zhao, G. & Tian, L. (2009). *Acta Cryst.* E**65**, m528.
Xanthopoulou, M. N., Hadjikakou, S. K., Hadjiliadis, N., Kubicki, M., Skoulika, S., Bakas, T., baril, M. & Butler, I. S. (2007). *Inorg. Chem.* **46**, 1187–1195.
Xanthopoulou, M. N., Kourkoumelis, N., Hadjikakou, S. K., Hadjiliadis, N., Kubicki, M., Karkabounas, S. & Bakas, T. (2008). *Polyhedron*, **27**, 3318–3324.
Zia-ur-Rahman, Ali, S., Muhammed, N. & Meetsma, A. (2007). *Acta Cryst.* E**63**, m89–m90.

supporting information

Acta Cryst. (2010). E**66**, m1645–m1646 [https://doi.org/10.1107/S1600536810046738]

Bis(dicyclohexylammonium) μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$-bis[aqua(oxalato-$\kappa^2O^1,O^2$)diphenylstannate(IV)]

Ndongo Gueye, Libasse Diop, K. C. Kieran Molloy and Gabrielle Kociok-Köhn

S1. Comment

In the dynamic of our research work on organotin(IV) chemistry (Diallo *et al.*, 2007; Diassé-Sarr *et al.*, 1997) because of several applications found (Xanthopoulou *et al.*, 2007, 2008; Zia-ur-Rahman *et al.*, 2007; Singh *et al.*, 2008; Wang *et al.*, 2009; Ballmann *et al.*, 2009; de Sousa *et al.*, 2007) and our interest in the coordinating behaviour of oxyanions in this family of compounds, we had yet reported the crystal structures of $C_2O_4(SnPh_3)_2$ (Diop *et al.*, 2003) and $SO_4(SnPh_3)_2.H_2O$ (Diop *et al.*, 2002) and have initiated here the study of the interactions between $(Cy_2NH_2)_2C_2O_4.2H_2O$ and $C_2O_4(SnPh_3)_2$ which has yielded the studied compound.

The asymmetric unit consists of one half of the molecule, located about an inversion centre at the mid-point of the C3—C3^i bond (symmetry code i: -*x*, 1 - *y*, -*z*). In its units structure two $SnPh_2$ residues are linked by a central bichelating oxalate ion [O_5O_6:O_5O_6] and every $SnPh_2$ residue is then linked to another monochelating anion [O1, O2]. A water molecule completes the tin centre coordination to seven, which can be described as a distorted *trans*-C_2SnO_5 pentagonal bipyramidal geometry [C—Sn—C angle: 168.75 (13)°]. Within the bridging carboxylate all the C—O bonds are equal within experimental error, implying complete delocalization of double-bond character within this residue. The bond lengths C1—O1 and C2—O2, [1.273 (4) Å], and C2—O3, C1—O4 [1.225 (4) and 1.247 (4) Å] indicate respectively a single and double bond character; the bond length C1—O4 results from involvement of O4 in two distinct hydrogen bonds. Among the Sn—O bonds, Sn1—O6 is notably longer, O6 being the only oxygen of this kind involved in hydrogen bonding.

Every moiety is then connected to its neighbour by three types of hydrogen bonds: one O—H···O type involving an H atom of the water molecule and one O atom of monochelating oxalate [O7—H7B···O4], one N—H···O contact involving one O atom of the bichelating oxalate anion and the cation [N—H1B···O6] and a third bifurcated one also involving the cation [N—H1A···O3 and N—H1A···O4], giving a supramolecular crystal structure.

A similar structure, bearing butyl groups in place of phenyl, was previously reported (Ng *et al.*, 1992).

S2. Experimental

Crystals of the title compound were obtained by allowing $(Cy_2NH_2)_2C_2O_4.2H_2O$ (90 mmol in 15 ml e thanol) to react with $C_2O_4(SnPh_3)_2$ (45 mmol in 15 ml e thanol). The mixture was stirred during several hours and slow solvent evaporation afforded crystals suitable for X-rays studies.

S3. Refinement

All C–bonded H atoms were placed in idealized positions (C—H in the range 0.95 to 1.00 Å), while H atoms bonded to N and O atoms were considered as free atoms. Isotropic displacement parameters for H atoms were calculated from U_{eq} of their parent atoms.

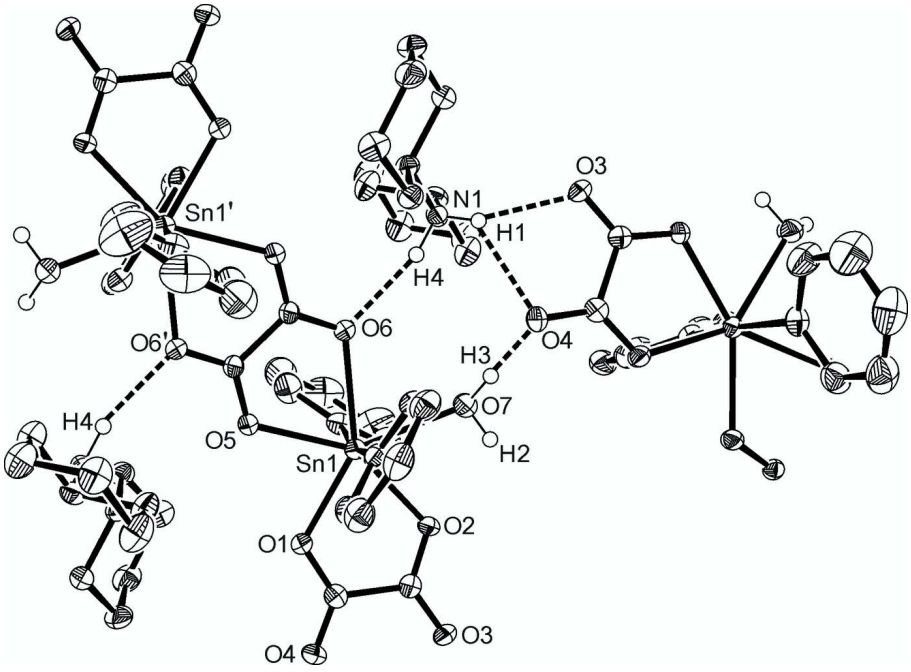


Figure 1

A part of the crystal structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Dashed bonds represent hydrogen bonds.

Bis(dicyclohexylammonium) μ-oxalato-$\kappa^4O^1,O^2:O^{1'},O^{2'}$- bis[aqua(oxalato-$\kappa^2O^1,O^2$)diphenylstannate(IV)]

Crystal data

$(C_{12}H_{24}N)_2[Sn_2(C_6H_5)_4(C_2O_4)_3(H_2O)_2]$
M_r = 1210.52
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.1725 (4) Å
b = 14.6121 (4) Å
c = 14.1139 (4) Å
β = 100.869 (2)°
V = 2667.88 (13) Å^3
Z = 2
$F(000)$ = 1244
D_x = 1.507 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 29450 reflections
θ = 2.9–27.5°
μ = 1.00 mm^{-1}
T = 150 K
Irregular, colourless
0.2 × 0.2 × 0.2 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
293 2.0 degree images with φ and ω scans
Absorption correction: multi-scan (*SORTAV*;Blessing, 1995)
T_{min} = 0.825, T_{max} = 0.825
48411 measured reflections
6114 independent reflections
4069 reflections with $I > 2\sigma(I)$
R_{int} = 0.126
θ_{max} = 27.5°, θ_{min} = 4.1°
h = −17→17
k = −18→18
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.082$
$S = 1.01$
6114 reflections
341 parameters
2 restraints
0 constraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0335P)^2 + 0.6086P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.54$ e Å^{-3}
$\Delta\rho_{min} = -0.72$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn	0.208644 (18)	0.515508 (15)	0.133115 (17)	0.02034 (8)
O1	0.27245 (18)	0.37817 (14)	0.16466 (16)	0.0235 (5)
O2	0.35282 (17)	0.53257 (14)	0.24319 (16)	0.0242 (5)
O3	0.47106 (18)	0.45574 (15)	0.34724 (17)	0.0285 (6)
O4	0.38762 (18)	0.29623 (15)	0.26721 (17)	0.0275 (6)
O5	0.09563 (17)	0.41884 (14)	0.04184 (16)	0.0230 (5)
O6	0.06436 (17)	0.60103 (14)	0.04207 (15)	0.0210 (5)
O7	0.2413 (2)	0.67274 (16)	0.18266 (19)	0.0292 (6)
H7A	0.292 (2)	0.669 (3)	0.233 (2)	0.052 (14)*
H7B	0.197 (3)	0.712 (3)	0.202 (3)	0.074 (16)*
N	−0.0015 (2)	0.2042 (2)	−0.0277 (2)	0.0214 (6)
H1A	−0.019 (3)	0.170 (2)	−0.076 (3)	0.027 (10)*
H1B	−0.027 (3)	0.261 (3)	−0.044 (3)	0.038 (11)*
C1	0.3500 (3)	0.3702 (2)	0.2332 (2)	0.0216 (8)
C2	0.3979 (3)	0.4602 (2)	0.2795 (2)	0.0211 (7)
C3	0.0088 (3)	0.4480 (2)	−0.0001 (2)	0.0196 (7)
C4	0.1110 (3)	0.5052 (2)	0.2372 (2)	0.0225 (7)
C5	0.0459 (3)	0.5767 (2)	0.2523 (3)	0.0277 (8)
H5	0.0467	0.6321	0.2172	0.033*
C6	−0.0202 (3)	0.5686 (3)	0.3177 (3)	0.0331 (9)
H6	−0.0632	0.6185	0.3277	0.040*
C7	−0.0237 (3)	0.4886 (3)	0.3681 (3)	0.0356 (9)
H7	−0.0690	0.4828	0.4127	0.043*
C8	0.0399 (3)	0.4162 (3)	0.3531 (3)	0.0359 (9)
H8	0.0380	0.3607	0.3880	0.043*
C9	0.1059 (3)	0.4239 (2)	0.2882 (3)	0.0295 (8)
H9	0.1482	0.3735	0.2781	0.035*
C10	0.2855 (3)	0.5464 (2)	0.0178 (3)	0.0276 (8)
C11	0.3816 (3)	0.5881 (3)	0.0352 (3)	0.0453 (11)
H11	0.4136	0.6027	0.0995	0.054*
C12	0.4320 (4)	0.6091 (4)	−0.0408 (4)	0.0664 (15)
H12	0.4979	0.6378	−0.0276	0.080*
C13	0.3872 (4)	0.5888 (3)	−0.1337 (3)	0.0533 (13)

H13	0.4220	0.6032	−0.1850	0.064*
C14	0.2922 (4)	0.5477 (3)	−0.1528 (3)	0.0485 (11)
H14	0.2609	0.5336	−0.2174	0.058*
C15	0.2416 (3)	0.5266 (3)	−0.0778 (3)	0.0377 (9)
H15	0.1756	0.4981	−0.0919	0.045*
C16	0.1143 (2)	0.2108 (2)	−0.0052 (2)	0.0218 (7)
H16	0.1344	0.2502	0.0533	0.026*
C17	0.1521 (3)	0.2565 (2)	−0.0890 (2)	0.0256 (8)
H17A	0.1338	0.2183	−0.1476	0.031*
H17B	0.1180	0.3168	−0.1024	0.031*
C18	0.2684 (3)	0.2693 (2)	−0.0643 (3)	0.0308 (9)
H18A	0.2863	0.3099	−0.0075	0.037*
H18B	0.2927	0.2986	−0.1192	0.037*
C19	0.3215 (3)	0.1774 (3)	−0.0425 (3)	0.0355 (9)
H19A	0.3969	0.1869	−0.0231	0.043*
H19B	0.3092	0.1392	−0.1015	0.043*
C20	0.2811 (3)	0.1276 (3)	0.0380 (3)	0.0327 (9)
H20A	0.3134	0.0663	0.0471	0.039*
H20B	0.3018	0.1621	0.0990	0.039*
C21	0.1647 (3)	0.1171 (2)	0.0165 (3)	0.0270 (8)
H21A	0.1413	0.0894	0.0727	0.032*
H21B	0.1439	0.0761	−0.0396	0.032*
C22	−0.0561 (3)	0.1646 (2)	0.0476 (2)	0.0234 (8)
H22	−0.0323	0.1001	0.0613	0.028*
C23	−0.1710 (3)	0.1642 (3)	0.0064 (3)	0.0332 (9)
H23A	−0.1847	0.1254	−0.0521	0.040*
H23B	−0.1942	0.2272	−0.0123	0.040*
C24	−0.2322 (3)	0.1273 (3)	0.0812 (3)	0.0368 (10)
H24A	−0.3071	0.1303	0.0542	0.044*
H24B	−0.2137	0.0623	0.0953	0.044*
C25	−0.2087 (3)	0.1823 (3)	0.1736 (3)	0.0371 (9)
H25A	−0.2462	0.1557	0.2216	0.045*
H25B	−0.2330	0.2461	0.1607	0.045*
C26	−0.0935 (3)	0.1823 (3)	0.2141 (3)	0.0402 (10)
H26A	−0.0706	0.1190	0.2321	0.048*
H26B	−0.0795	0.2203	0.2732	0.048*
C27	−0.0316 (3)	0.2196 (3)	0.1407 (2)	0.0324 (9)
H27A	−0.0494	0.2848	0.1271	0.039*
H27B	0.0433	0.2158	0.1678	0.039*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn	0.01965 (13)	0.01890 (12)	0.02124 (13)	0.00066 (11)	0.00070 (8)	0.00046 (11)
O1	0.0233 (14)	0.0203 (12)	0.0240 (13)	0.0026 (10)	−0.0033 (11)	−0.0020 (10)
O2	0.0238 (13)	0.0161 (13)	0.0292 (13)	0.0016 (9)	−0.0043 (10)	0.0021 (10)
O3	0.0284 (14)	0.0251 (13)	0.0266 (14)	−0.0012 (10)	−0.0089 (11)	0.0018 (10)
O4	0.0286 (14)	0.0193 (13)	0.0314 (14)	0.0034 (10)	−0.0025 (11)	0.0037 (10)

O5	0.0225 (13)	0.0177 (12)	0.0262 (13)	0.0014 (10)	−0.0020 (11)	−0.0027 (10)
O6	0.0217 (13)	0.0192 (12)	0.0201 (12)	0.0006 (10)	−0.0009 (10)	−0.0002 (10)
O7	0.0260 (16)	0.0237 (14)	0.0353 (16)	0.0013 (11)	−0.0007 (13)	−0.0018 (12)
N	0.0246 (17)	0.0186 (17)	0.0208 (17)	−0.0001 (12)	0.0042 (14)	−0.0004 (14)
C1	0.021 (2)	0.0227 (19)	0.0225 (19)	0.0008 (14)	0.0082 (16)	−0.0007 (15)
C2	0.0206 (19)	0.0233 (19)	0.0203 (18)	−0.0011 (14)	0.0060 (15)	−0.0010 (14)
C3	0.023 (2)	0.0193 (17)	0.0166 (16)	0.0008 (14)	0.0031 (14)	−0.0021 (13)
C4	0.0218 (17)	0.027 (2)	0.0175 (17)	−0.0008 (14)	−0.0009 (13)	−0.0022 (14)
C5	0.024 (2)	0.029 (2)	0.028 (2)	0.0001 (15)	−0.0010 (16)	0.0000 (15)
C6	0.021 (2)	0.045 (2)	0.033 (2)	−0.0008 (17)	0.0036 (17)	−0.0033 (18)
C7	0.029 (2)	0.048 (2)	0.032 (2)	−0.0127 (18)	0.0105 (17)	−0.0046 (19)
C8	0.036 (2)	0.038 (2)	0.034 (2)	−0.0119 (18)	0.0066 (19)	0.0024 (18)
C9	0.031 (2)	0.027 (2)	0.031 (2)	−0.0032 (16)	0.0058 (17)	−0.0017 (16)
C10	0.029 (2)	0.0265 (19)	0.029 (2)	0.0055 (15)	0.0077 (16)	0.0054 (15)
C11	0.030 (2)	0.070 (3)	0.036 (2)	−0.007 (2)	0.0053 (19)	0.008 (2)
C12	0.033 (3)	0.105 (4)	0.065 (4)	−0.011 (3)	0.017 (3)	0.019 (3)
C13	0.050 (3)	0.072 (3)	0.045 (3)	0.015 (2)	0.028 (2)	0.016 (2)
C14	0.069 (3)	0.048 (3)	0.031 (2)	0.004 (2)	0.015 (2)	0.0013 (19)
C15	0.048 (3)	0.035 (2)	0.033 (2)	−0.0038 (18)	0.0124 (19)	−0.0001 (18)
C16	0.0198 (19)	0.0236 (18)	0.0212 (18)	0.0027 (14)	0.0020 (15)	0.0001 (14)
C17	0.029 (2)	0.0263 (19)	0.0211 (19)	0.0022 (15)	0.0042 (16)	0.0009 (15)
C18	0.026 (2)	0.040 (2)	0.028 (2)	0.0013 (16)	0.0100 (17)	0.0019 (17)
C19	0.024 (2)	0.045 (2)	0.036 (2)	0.0081 (17)	0.0031 (17)	−0.0076 (18)
C20	0.027 (2)	0.035 (2)	0.034 (2)	0.0090 (16)	−0.0025 (17)	−0.0011 (17)
C21	0.028 (2)	0.0224 (19)	0.029 (2)	0.0033 (15)	0.0002 (16)	−0.0016 (15)
C22	0.027 (2)	0.0194 (18)	0.0237 (19)	0.0025 (14)	0.0054 (16)	0.0037 (14)
C23	0.030 (2)	0.042 (2)	0.028 (2)	−0.0047 (17)	0.0056 (17)	−0.0043 (17)
C24	0.026 (2)	0.049 (2)	0.037 (2)	−0.0064 (18)	0.0085 (18)	−0.0029 (19)
C25	0.032 (2)	0.047 (2)	0.035 (2)	−0.0018 (18)	0.0132 (18)	−0.0056 (19)
C26	0.038 (3)	0.058 (3)	0.026 (2)	−0.010 (2)	0.0104 (18)	−0.0021 (19)
C27	0.030 (2)	0.043 (2)	0.023 (2)	−0.0064 (17)	0.0038 (17)	−0.0043 (17)

Geometric parameters (Å, º)

Sn—C10	2.121 (3)	C13—C14	1.368 (6)
Sn—C4	2.132 (3)	C13—H13	0.9500
Sn—O1	2.189 (2)	C14—C15	1.388 (5)
Sn—O2	2.229 (2)	C14—H14	0.9500
Sn—O5	2.269 (2)	C15—H15	0.9500
Sn—O7	2.416 (2)	C16—C17	1.522 (4)
Sn—O6	2.430 (2)	C16—C21	1.527 (4)
O1—C1	1.273 (4)	C16—H16	1.0000
O2—C2	1.273 (4)	C17—C18	1.517 (5)
O3—C2	1.225 (4)	C17—H17A	0.9900
O4—C1	1.247 (4)	C17—H17B	0.9900
O5—C3	1.259 (4)	C18—C19	1.518 (5)
O6—C3^{i}	1.256 (4)	C18—H18A	0.9900
O7—H7A	0.886 (19)	C18—H18B	0.9900

O7—H7B	0.896 (19)	C19—C20	1.527 (5)
N—C16	1.500 (4)	C19—H19A	0.9900
N—C22	1.507 (4)	C19—H19B	0.9900
N—H1A	0.85 (4)	C20—C21	1.514 (5)
N—H1B	0.91 (4)	C20—H20A	0.9900
C1—C2	1.548 (5)	C20—H20B	0.9900
C3—O6^{i}	1.256 (4)	C21—H21A	0.9900
C3—C3^{i}	1.537 (7)	C21—H21B	0.9900
C4—C5	1.394 (5)	C22—C23	1.516 (5)
C4—C9	1.397 (5)	C22—C27	1.522 (5)
C5—C6	1.389 (5)	C22—H22	1.0000
C5—H5	0.9500	C23—C24	1.540 (5)
C6—C7	1.373 (5)	C23—H23A	0.9900
C6—H6	0.9500	C23—H23B	0.9900
C7—C8	1.390 (5)	C24—C25	1.514 (5)
C7—H7	0.9500	C24—H24A	0.9900
C8—C9	1.382 (5)	C24—H24B	0.9900
C8—H8	0.9500	C25—C26	1.518 (5)
C9—H9	0.9500	C25—H25A	0.9900
C10—C11	1.385 (5)	C25—H25B	0.9900
C10—C15	1.394 (5)	C26—C27	1.534 (5)
C11—C12	1.398 (6)	C26—H26A	0.9900
C11—H11	0.9500	C26—H26B	0.9900
C12—C13	1.366 (7)	C27—H27A	0.9900
C12—H12	0.9500	C27—H27B	0.9900

C10—Sn—C4	168.75 (13)	C14—C15—C10	121.4 (4)
C10—Sn—O1	97.50 (11)	C14—C15—H15	119.3
C4—Sn—O1	93.06 (10)	C10—C15—H15	119.3
C10—Sn—O2	92.53 (12)	N—C16—C17	109.4 (3)
C4—Sn—O2	94.18 (11)	N—C16—C21	111.8 (3)
O1—Sn—O2	73.55 (8)	C17—C16—C21	110.9 (3)
C10—Sn—O5	93.06 (12)	N—C16—H16	108.2
C4—Sn—O5	86.04 (10)	C17—C16—H16	108.2
O1—Sn—O5	74.35 (8)	C21—C16—H16	108.2
O2—Sn—O5	147.87 (8)	C18—C17—C16	109.9 (3)
C10—Sn—O7	86.30 (11)	C18—C17—H17A	109.7
C4—Sn—O7	88.01 (10)	C16—C17—H17A	109.7
O1—Sn—O7	140.57 (9)	C18—C17—H17B	109.7
O2—Sn—O7	67.06 (8)	C16—C17—H17B	109.7
O5—Sn—O7	144.90 (8)	H17A—C17—H17B	108.2
C10—Sn—O6	85.62 (11)	C17—C18—C19	110.2 (3)
C4—Sn—O6	83.54 (10)	C17—C18—H18A	109.6
O1—Sn—O6	144.21 (8)	C19—C18—H18A	109.6
O2—Sn—O6	142.15 (7)	C17—C18—H18B	109.6
O5—Sn—O6	69.87 (8)	C19—C18—H18B	109.6
O7—Sn—O6	75.09 (8)	H18A—C18—H18B	108.1
C1—O1—Sn	117.4 (2)	C18—C19—C20	111.1 (3)

C2—O2—Sn	117.3 (2)	C18—C19—H19A	109.4
C3—O5—Sn	119.8 (2)	C20—C19—H19A	109.4
C3^{i}—O6—Sn	114.2 (2)	C18—C19—H19B	109.4
Sn—O7—H7A	104 (3)	C20—C19—H19B	109.4
Sn—O7—H7B	127 (3)	H19A—C19—H19B	108.0
H7A—O7—H7B	103 (4)	C21—C20—C19	112.4 (3)
C16—N—C22	118.5 (3)	C21—C20—H20A	109.1
C16—N—H1A	108 (2)	C19—C20—H20A	109.1
C22—N—H1A	105 (2)	C21—C20—H20B	109.1
C16—N—H1B	108 (2)	C19—C20—H20B	109.1
C22—N—H1B	109 (2)	H20A—C20—H20B	107.9
H1A—N—H1B	108 (3)	C20—C21—C16	109.6 (3)
O4—C1—O1	125.1 (3)	C20—C21—H21A	109.8
O4—C1—C2	118.2 (3)	C16—C21—H21A	109.8
O1—C1—C2	116.6 (3)	C20—C21—H21B	109.8
O3—C2—O2	126.6 (3)	C16—C21—H21B	109.8
O3—C2—C1	118.9 (3)	H21A—C21—H21B	108.2
O2—C2—C1	114.4 (3)	N—C22—C23	107.8 (3)
O6^{i}—C3—O5	125.2 (3)	N—C22—C27	110.8 (3)
O6^{i}—C3—C3^{i}	117.5 (4)	C23—C22—C27	111.5 (3)
O5—C3—C3^{i}	117.2 (4)	N—C22—H22	108.9
C5—C4—C9	117.9 (3)	C23—C22—H22	108.9
C5—C4—Sn	121.4 (2)	C27—C22—H22	108.9
C9—C4—Sn	120.6 (2)	C22—C23—C24	110.6 (3)
C6—C5—C4	121.3 (3)	C22—C23—H23A	109.5
C6—C5—H5	119.4	C24—C23—H23A	109.5
C4—C5—H5	119.4	C22—C23—H23B	109.5
C7—C6—C5	120.2 (3)	C24—C23—H23B	109.5
C7—C6—H6	119.9	H23A—C23—H23B	108.1
C5—C6—H6	119.9	C25—C24—C23	110.9 (3)
C6—C7—C8	119.4 (3)	C25—C24—H24A	109.5
C6—C7—H7	120.3	C23—C24—H24A	109.5
C8—C7—H7	120.3	C25—C24—H24B	109.5
C9—C8—C7	120.7 (3)	C23—C24—H24B	109.5
C9—C8—H8	119.7	H24A—C24—H24B	108.1
C7—C8—H8	119.7	C24—C25—C26	110.5 (3)
C8—C9—C4	120.6 (3)	C24—C25—H25A	109.5
C8—C9—H9	119.7	C26—C25—H25A	109.5
C4—C9—H9	119.7	C24—C25—H25B	109.5
C11—C10—C15	117.5 (3)	C26—C25—H25B	109.5
C11—C10—Sn	120.6 (3)	H25A—C25—H25B	108.1
C15—C10—Sn	121.9 (3)	C25—C26—C27	111.5 (3)
C10—C11—C12	120.7 (4)	C25—C26—H26A	109.3
C10—C11—H11	119.6	C27—C26—H26A	109.3
C12—C11—H11	119.6	C25—C26—H26B	109.3
C13—C12—C11	120.5 (4)	C27—C26—H26B	109.3
C13—C12—H12	119.7	H26A—C26—H26B	108.0
C11—C12—H12	119.7	C22—C27—C26	110.0 (3)

C12—C13—C14	119.8 (4)	C22—C27—H27A	109.7
C12—C13—H13	120.1	C26—C27—H27A	109.7
C14—C13—H13	120.1	C22—C27—H27B	109.7
C13—C14—C15	120.0 (4)	C26—C27—H27B	109.7
C13—C14—H14	120.0	H27A—C27—H27B	108.2
C15—C14—H14	120.0		

Symmetry code: (i) −*x*, −*y*+1, −*z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O7—H7*B*···O4^{ii}	0.90 (4)	1.77 (4)	2.663 (3)	175 (4)
N—H1*A*···O3^{iii}	0.84 (4)	2.12 (3)	2.910 (4)	155 (3)
N—H1*A*···O4^{iii}	0.84 (4)	2.37 (4)	2.986 (4)	130 (3)
N—H1*B*···O6^{i}	0.91 (4)	2.08 (4)	2.960 (4)	164 (4)

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1/2, *y*+1/2, −*z*+1/2; (iii) *x*−1/2, −*y*+1/2, *z*−1/2.