Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Di-μ_3-oxido-bis(μ_2-quinaldato-κ^2O:O)-bis(quinaldato-κ^2N,O)tetrakis[di-*n*-butyltin(IV)]

Hongyun Wang and Handong Yin*

College of Chemistry and Chemical Engineering, Liaocheng University, Shandong 252059, People's Republic of China
Correspondence e-mail: handongyin@163.com

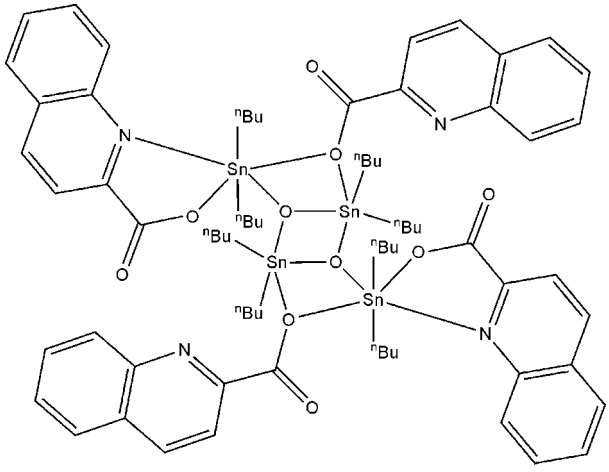
Received 20 November 2007; accepted 10 December 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.011 Å; disorder in main residue; R factor = 0.039; wR factor = 0.127; data-to-parameter ratio = 15.7.

The title tetranuclear Sn^{IV} complex, $[Sn_4(C_4H_9)_8(C_{10}H_6NO_2)_4O_2]$, is a cluster built up by inversion symmetry around the central Sn_2O_2 ring. The coordination geometries of the Sn atoms involved can be classified into two types: the five-coordinate Sn atoms of the central Sn_2O_2 core have a trigonal–bipyramidal geometry, with axial positions occupied by a μ_3-O atom and a μ_2-O atom belonging to the nonchelating quinaldate ligand. The peripheral Sn atoms are six-coordinate, with a distorted octahedral geometry. The methyl group of an *n*-butyl ligand is disordered over two sites, with occupancies of 0.643 (12) and 0.357 (12).

Related literature

For related tin complexes, see: Ma *et al.* (2004); Tian *et al.* (2005).



Experimental

Crystal data

$[Sn_4(C_4H_9)_8(C_{10}H_6NO_2)_4O_2]$
M_r = 1652.29
Monoclinic, $P2_1/n$
a = 13.096 (5) Å
b = 12.551 (5) Å
c = 22.278 (9) Å
β = 93.971 (5)°
V = 3653 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.41 mm^{-1}
T = 298 (2) K
0.52 × 0.31 × 0.24 mm

Data collection

Bruker SMART diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.517, T_{max} = 0.714
18614 measured reflections
6437 independent reflections
4499 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.127
S = 1.00
6437 reflections
410 parameters
169 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O5	2.042 (4)	Sn2—O5	2.049 (4)
Sn1—O5^{i}	2.141 (4)	Sn2—O3	2.111 (4)
Sn1—O1	2.304 (4)	Sn2—O1	2.488 (4)
Sn1—N1	3.184 (5)	Sn2—N2	2.539 (5)
O5—Sn1—C25	110.7 (2)	O5—Sn2—O3	80.36 (15)
O5—Sn1—C21	113.6 (2)	O5—Sn2—C29	105.4 (2)
C25—Sn1—C21	135.5 (3)	O3—Sn2—C29	103.7 (2)
O5—Sn1—O5^{i}	74.10 (15)	O5—Sn2—C33	102.6 (2)
C25—Sn1—O5^{i}	98.0 (2)	O3—Sn2—C33	105.7 (2)
C21—Sn1—O5^{i}	97.2 (2)	C29—Sn2—C33	142.1 (3)
O5—Sn1—O1	72.85 (14)	O5—Sn2—O1	68.81 (14)
C25—Sn1—O1	94.3 (2)	O3—Sn2—O1	149.11 (14)
C21—Sn1—O1	95.2 (2)	C29—Sn2—O1	83.4 (2)
O5^{i}—Sn1—O1	146.94 (14)	C33—Sn2—O1	83.5 (2)
O5—Sn1—N1	129.19 (14)	O5—Sn2—N2	149.32 (15)
C25—Sn1—N1	70.85 (19)	O3—Sn2—N2	69.24 (16)
C21—Sn1—N1	78.7 (2)	C29—Sn2—N2	86.3 (2)
O5^{i}—Sn1—N1	156.19 (13)	C33—Sn2—N2	82.4 (2)
O1—Sn1—N1	56.67 (14)	O1—Sn2—N2	141.64 (14)

Symmetry code: (i) $-x+1, -y+2, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXTL*.

We thank the National Natural Science Foundation of China (20771053) and the Natural Science Foundation of Shandong Province (2005ZX09) for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2155).

 doi:10.1107/S1600536807066378

References

Ma, C. L., Jiang, Q., Zhang, R. F. & Wang, D. Q. (2004). *J. Chem. Soc. Dalton Trans.* pp. 1832–1840.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Siemens (1996). *SMART* (Version 4.0), *SAINT* (Version 4.0) and *SHELXTL* (Version 5.1). Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Tian, G.-R., Zhang, R.-F., Ma, C.-L. & Ng, S. W. (2005). *Acta Cryst.* E**61**, m2528–m2530.

supporting information

Acta Cryst. (2008). E**64**, m197–m198 [https://doi.org/10.1107/S1600536807066378]

Di-μ_3-oxido-bis(μ_2-quinaldato-κ^2O:O)bis(quinaldato-κ^2N,O)tetrakis[di-*n*-butyltin(IV)]

Hongyun Wang and Handong Yin

S1. Comment

The title compound, (I), is a cluster containing four Sn atoms (Fig. 1). The whole molecule lies on an inversion center, with a central Sn_2O_2 core. The structure is similar to that previously characterized with 3-hydroxypyridine-2-carboxylate as main ligand (Tian *et al.*, 2005). The three-coordinated μ_3 atom O5 in the Sn_2O_2 ring is bonded to a Bu_2SnO_2N unit. Moreover, the C1 carboxylate group coordinates to each independent Sn atom in a bridging mode (Fig. 2). The geometry of the Sn1 atom in the Sn_2O_2 ring is distorted trigonal-bipyramidal with atoms O1 and O5^i [symmetry code (*i*): -*x* + 1, -*y* + 2, -*z*] in axial positions, while two *n*-butyl groups and atom O5 form the equatorial plane. For the Sn2 atoms, six primary bonds are formed: three to the O atoms, two to the C atom of *n*-butyl groups, and one to the chelating quinoline N atom. Thus, the Sn2 centers display a distorted octahedral coordinated geometry. The Sn—O and Sn—N bond lengths (Table 1) are similar to those observed in related organotin carboxylates (Ma *et al.*, 2004).

S2. Experimental

The reaction was carried out under a nitrogen atmosphere. Quinaldic acid (1 mmol) and sodium ethoxide (1.2 mmol) were dissolved in ethanol (30 ml) in a Schlenk flask and stirred for 0.5 h. Dibutyltin dichloride (1 mmol) was then added and the reaction mixture was stirred for 12 h at 313 K. The resulting clear solution was evaporated under vacuum. The product was crystallized from a mixture of dichloromethane/methanol (1:1). Yield: 83%; m.p. 426 K. Analysis: calculated for $C_{72}H_{96}N_4O_{10}Sn_4$: C 52.33, H 5.86, N 3.39%. found: C 52.27, H 5.95, N 3.47%.

S3. Refinement

Atoms C24 was found to be disordered over two positions (C24 and C24′). Site occupation factors were refined and converged to 0.643 (12) and 0.357 (12) for C24 and C24′, respectively. All C—C bonds lengths in *n*-butyl groups were restrained to 1.53 (2) Å. In *n*-butyl groups, C atoms closer than 1.7 Å were restrained, with deviation of 0.04 Å^2, to have the same U_{ij} components. H atoms were positioned geometrically, with C—H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, and constrained to ride on their parent C atoms, with U_{iso}(H) = xU_{eq}(carrier C) where x = 1.5 for methyl groups and x = 1.2 otherwise.

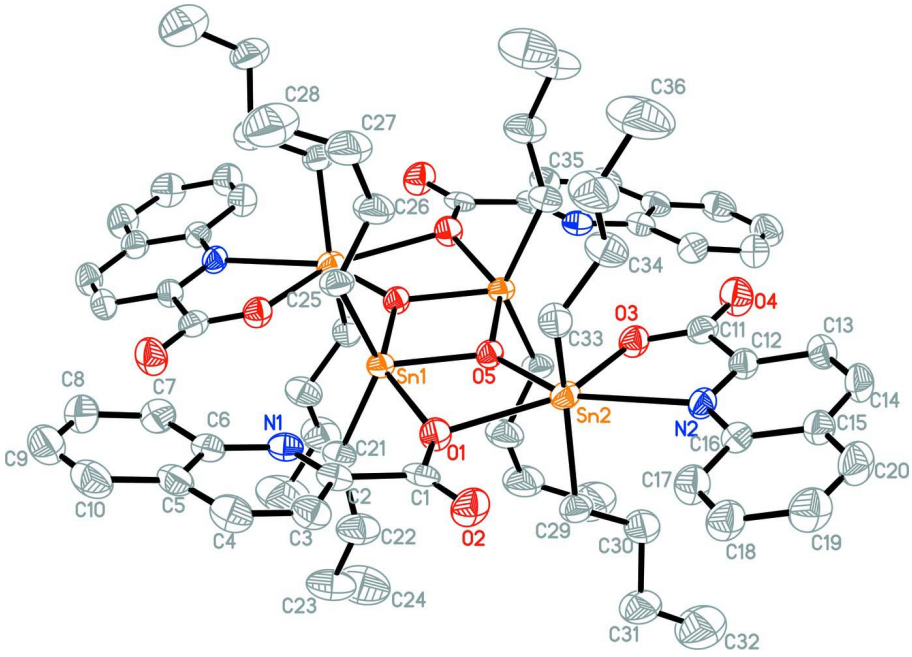


Figure 1

The molecular structure of (I), with 30% probability displacement ellipsoids (H atoms have been omitted for clarity). The ′A′ labeled atoms are generated by the symmetry operation -*x* + 1, -*y* + 2, -*z*.

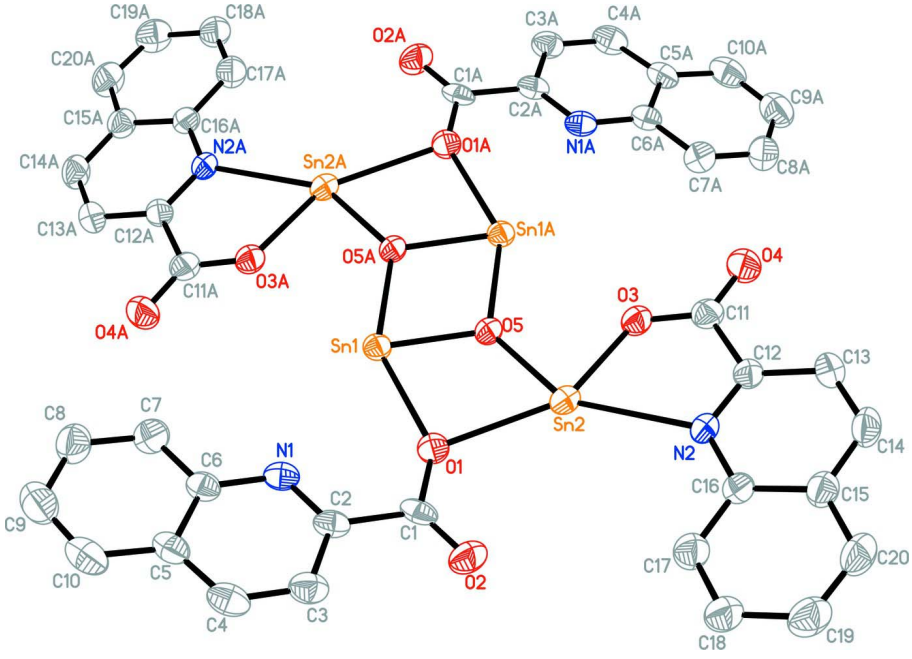


Figure 2

In this view the *n*-butyl groups have been omitted for clarity. Atoms with the suffix ′A′ are generated by the symmetry operation -*x* + 1, -*y* + 2, -*z*.

Di-μ_3-oxido-bis(μ_2-quinaldato-κ^2O:O)bis(quinaldato- κ^2N,O)tetrakis[di-*n*-butyltin(IV)]

Crystal data

$[Sn_4(C_4H_9)_8(C_{10}H_6NO_2)_4O_2]$
M_r = 1652.29
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 13.096 (5) Å
b = 12.551 (5) Å
c = 22.278 (9) Å
β = 93.971 (5)°
V = 3653 (3) Å^3
Z = 2
$F(000)$ = 1672
D_x = 1.502 Mg m^{-3}
Melting point: 426 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5520 reflections
θ = 2.4–22.8°
μ = 1.41 mm^{-1}
T = 298 K
Block, colourless
0.52 × 0.31 × 0.24 mm

Data collection

Bruker SMART diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.517, T_{max} = 0.714
18614 measured reflections
6437 independent reflections
4499 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 25.0°, θ_{min} = 1.8°
h = −15→15
k = −14→13
l = −26→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.127
S = 1.00
6437 reflections
410 parameters
169 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 1.6257P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.58177 (3)	0.91100 (3)	0.031663 (18)	0.04351 (14)	
Sn2	0.40982 (3)	1.01477 (3)	0.134696 (18)	0.04798 (15)	
N1	0.7010 (4)	0.7402 (4)	0.1158 (2)	0.0499 (12)	
N2	0.2731 (4)	1.0753 (4)	0.2026 (2)	0.0496 (12)	
O1	0.5611 (3)	0.8952 (3)	0.13314 (18)	0.0552 (11)	
O2	0.5595 (4)	0.8522 (4)	0.2299 (2)	0.0719 (14)	
O3	0.3094 (3)	1.1246 (3)	0.08965 (17)	0.0552 (11)	
O4	0.1692 (4)	1.2240 (4)	0.0797 (2)	0.0786 (15)	
O5	0.4664 (3)	1.0120 (3)	0.05126 (16)	0.0447 (9)	
C1	0.5892 (4)	0.8379 (5)	0.1812 (3)	0.0508 (16)	
C2	0.6629 (4)	0.7465 (5)	0.1691 (3)	0.0502 (15)	
C3	0.6865 (5)	0.6729 (6)	0.2153 (3)	0.0622 (18)	
H3	0.6594	0.6808	0.2526	0.075*	

C4	0.7488 (6)	0.5906 (6)	0.2050 (3)	0.069 (2)	
H4	0.7640	0.5412	0.2355	0.083*	
C5	0.7915 (5)	0.5774 (5)	0.1495 (3)	0.0598 (17)	
C6	0.7649 (4)	0.6572 (5)	0.1053 (3)	0.0526 (15)	
C7	0.8052 (5)	0.6484 (6)	0.0482 (3)	0.0696 (19)	
H7	0.7904	0.6999	0.0189	0.083*	
C8	0.8655 (6)	0.5647 (7)	0.0368 (4)	0.079 (2)	
H8	0.8904	0.5582	−0.0011	0.095*	
C9	0.8916 (6)	0.4870 (7)	0.0806 (4)	0.085 (2)	
H9	0.9333	0.4301	0.0714	0.102*	
C10	0.8567 (6)	0.4944 (6)	0.1359 (4)	0.081 (2)	
H10	0.8762	0.4440	0.1650	0.097*	
C11	0.2277 (5)	1.1646 (5)	0.1088 (3)	0.0571 (16)	
C12	0.2061 (5)	1.1373 (5)	0.1730 (3)	0.0500 (15)	
C13	0.1163 (5)	1.1745 (5)	0.1979 (3)	0.0602 (17)	
H13	0.0703	1.2185	0.1760	0.072*	
C14	0.0994 (5)	1.1438 (6)	0.2547 (3)	0.0667 (19)	
H14	0.0406	1.1670	0.2720	0.080*	
C15	0.1684 (5)	1.0780 (6)	0.2880 (3)	0.0601 (17)	
C16	0.2572 (5)	1.0449 (5)	0.2604 (3)	0.0518 (15)	
C17	0.3286 (6)	0.9802 (6)	0.2931 (3)	0.0681 (19)	
H17	0.3881	0.9598	0.2757	0.082*	
C18	0.3127 (6)	0.9473 (6)	0.3487 (3)	0.074 (2)	
H18	0.3609	0.9040	0.3694	0.089*	
C19	0.2245 (7)	0.9772 (7)	0.3759 (4)	0.083 (2)	
H19	0.2139	0.9532	0.4145	0.099*	
C20	0.1536 (6)	1.0415 (7)	0.3465 (3)	0.077 (2)	
H20	0.0951	1.0613	0.3652	0.093*	
C21	0.7297 (5)	0.9809 (5)	0.0427 (3)	0.0567 (16)	
H21A	0.7774	0.9317	0.0261	0.068*	
H21B	0.7288	1.0446	0.0180	0.068*	
C22	0.7727 (6)	1.0111 (7)	0.1038 (3)	0.085 (2)	
H22A	0.7805	0.9471	0.1280	0.102*	
H22B	0.7237	1.0566	0.1222	0.102*	
C23	0.8746 (7)	1.0681 (8)	0.1058 (4)	0.103 (3)	
H23A	0.9024	1.0704	0.1473	0.124*	0.643 (12)
H23B	0.9212	1.0263	0.0834	0.124*	0.643 (12)
H23C	0.8602	1.1432	0.0992	0.124*	0.357 (12)
H23D	0.9063	1.0618	0.1463	0.124*	0.357 (12)
C24	0.8726 (12)	1.1728 (12)	0.0829 (8)	0.131 (5)	0.643 (12)
H24A	0.9407	1.1940	0.0747	0.196*	0.643 (12)
H24B	0.8465	1.2203	0.1119	0.196*	0.643 (12)
H24C	0.8293	1.1753	0.0464	0.196*	0.643 (12)
C24′	0.9529 (19)	1.033 (2)	0.0654 (12)	0.131 (5)	0.357 (12)
H24D	0.9294	0.9707	0.0440	0.196*	0.357 (12)
H24E	1.0154	1.0176	0.0888	0.196*	0.357 (12)
H24F	0.9648	1.0892	0.0373	0.196*	0.357 (12)
C25	0.5233 (5)	0.7567 (5)	0.0104 (3)	0.0580 (16)	

H25A	0.5715	0.7200	−0.0135	0.070*
H25B	0.5193	0.7171	0.0475	0.070*
C26	0.4205 (5)	0.7548 (6)	−0.0231 (4)	0.086 (2)
H26A	0.4267	0.7831	−0.0632	0.103*
H26B	0.3747	0.8011	−0.0028	0.103*
C27	0.3720 (7)	0.6405 (7)	−0.0285 (5)	0.114 (3)
H27A	0.3720	0.6090	0.0113	0.136*
H27B	0.3014	0.6465	−0.0444	0.136*
C28	0.4260 (9)	0.5720 (9)	−0.0665 (6)	0.153 (5)
H28A	0.4157	0.5958	−0.1074	0.230*
H28B	0.4009	0.5005	−0.0634	0.230*
H28C	0.4977	0.5737	−0.0543	0.230*
C29	0.5124 (5)	1.1132 (5)	0.1885 (3)	0.0577 (16)
H29A	0.5268	1.0781	0.2269	0.069*
H29B	0.5764	1.1173	0.1691	0.069*
C30	0.4775 (6)	1.2250 (6)	0.2003 (4)	0.084 (2)
H30A	0.4157	1.2227	0.2219	0.101*
H30B	0.4614	1.2611	0.1623	0.101*
C31	0.5616 (7)	1.2885 (7)	0.2378 (4)	0.100 (3)
H31A	0.5800	1.2495	0.2745	0.119*
H31B	0.6220	1.2927	0.2151	0.119*
C32	0.5318 (10)	1.3937 (9)	0.2531 (6)	0.159 (5)
H32A	0.5133	1.4331	0.2170	0.238*
H32B	0.5878	1.4286	0.2752	0.238*
H32C	0.4742	1.3904	0.2774	0.238*
C33	0.3270 (5)	0.8681 (5)	0.1364 (3)	0.0619 (17)
H33A	0.3613	0.8166	0.1123	0.074*
H33B	0.3317	0.8420	0.1775	0.074*
C34	0.2147 (5)	0.8700 (6)	0.1144 (4)	0.078 (2)
H34A	0.1785	0.9167	0.1404	0.094*
H34B	0.2087	0.9002	0.0742	0.094*
C35	0.1644 (6)	0.7645 (7)	0.1129 (5)	0.108 (3)
H35A	0.1667	0.7366	0.1535	0.130*
H35B	0.2036	0.7166	0.0892	0.130*
C36	0.0566 (8)	0.7635 (10)	0.0878 (6)	0.174 (5)
H36A	0.0230	0.8275	0.0994	0.262*
H36B	0.0221	0.7028	0.1031	0.262*
H36C	0.0548	0.7595	0.0447	0.262*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0420 (2)	0.0421 (3)	0.0458 (2)	−0.00321 (18)	−0.00117 (17)	−0.00413 (18)
Sn2	0.0527 (3)	0.0511 (3)	0.0405 (2)	−0.0060 (2)	0.00546 (18)	−0.00393 (18)
N1	0.053 (3)	0.050 (3)	0.046 (3)	−0.009 (3)	−0.005 (2)	0.007 (2)
N2	0.054 (3)	0.056 (3)	0.040 (3)	0.005 (3)	0.007 (2)	−0.005 (2)
O1	0.058 (3)	0.062 (3)	0.046 (2)	0.007 (2)	0.005 (2)	0.005 (2)
O2	0.089 (4)	0.086 (4)	0.041 (3)	0.006 (3)	0.011 (2)	0.004 (2)

O3	0.063 (3)	0.062 (3)	0.042 (2)	0.006 (2)	0.007 (2)	0.002 (2)
O4	0.082 (3)	0.094 (4)	0.059 (3)	0.030 (3)	0.001 (3)	0.012 (3)
O5	0.048 (2)	0.050 (2)	0.036 (2)	0.0018 (18)	0.0065 (17)	0.0003 (17)
C1	0.045 (3)	0.045 (4)	0.059 (4)	−0.009 (3)	−0.024 (3)	0.005 (3)
C2	0.044 (3)	0.060 (4)	0.045 (4)	−0.012 (3)	−0.006 (3)	0.009 (3)
C3	0.060 (4)	0.077 (5)	0.049 (4)	−0.005 (4)	0.000 (3)	0.012 (3)
C4	0.074 (5)	0.069 (5)	0.062 (5)	0.000 (4)	−0.008 (4)	0.025 (4)
C5	0.052 (4)	0.059 (4)	0.066 (4)	0.001 (3)	−0.014 (3)	0.006 (3)
C6	0.046 (3)	0.056 (4)	0.055 (4)	−0.005 (3)	−0.007 (3)	0.001 (3)
C7	0.068 (5)	0.077 (5)	0.063 (5)	0.001 (4)	0.003 (4)	−0.006 (4)
C8	0.068 (5)	0.089 (6)	0.082 (6)	0.006 (4)	0.010 (4)	−0.015 (5)
C9	0.071 (5)	0.076 (6)	0.107 (7)	0.011 (4)	−0.009 (5)	−0.003 (5)
C10	0.073 (5)	0.077 (6)	0.090 (6)	0.008 (4)	−0.020 (5)	0.016 (5)
C11	0.061 (4)	0.053 (4)	0.056 (4)	−0.002 (3)	−0.004 (3)	−0.010 (3)
C12	0.052 (4)	0.053 (4)	0.045 (3)	0.004 (3)	0.004 (3)	0.002 (3)
C13	0.053 (4)	0.061 (4)	0.067 (4)	0.011 (3)	0.005 (3)	−0.001 (3)
C14	0.055 (4)	0.078 (5)	0.069 (5)	0.004 (4)	0.022 (3)	−0.006 (4)
C15	0.056 (4)	0.067 (5)	0.058 (4)	−0.003 (3)	0.011 (3)	−0.007 (3)
C16	0.053 (4)	0.056 (4)	0.046 (3)	0.000 (3)	0.004 (3)	−0.005 (3)
C17	0.077 (5)	0.070 (5)	0.059 (4)	0.011 (4)	0.009 (4)	0.006 (4)
C18	0.088 (5)	0.083 (5)	0.053 (4)	0.014 (4)	0.005 (4)	0.005 (4)
C19	0.096 (6)	0.097 (6)	0.057 (5)	−0.006 (5)	0.017 (4)	0.012 (4)
C20	0.079 (5)	0.094 (6)	0.062 (5)	−0.002 (5)	0.029 (4)	0.001 (4)
C21	0.049 (4)	0.058 (4)	0.061 (4)	−0.011 (3)	−0.005 (3)	0.003 (3)
C22	0.073 (5)	0.106 (6)	0.075 (5)	−0.034 (4)	−0.001 (4)	−0.002 (4)
C23	0.091 (6)	0.116 (7)	0.099 (6)	−0.042 (5)	−0.022 (5)	0.004 (5)
C24	0.121 (9)	0.125 (10)	0.143 (10)	−0.044 (8)	−0.022 (8)	0.028 (9)
C24′	0.121 (9)	0.125 (10)	0.143 (10)	−0.044 (8)	−0.022 (8)	0.028 (9)
C25	0.061 (4)	0.045 (4)	0.065 (4)	−0.003 (3)	−0.015 (3)	−0.005 (3)
C26	0.069 (5)	0.066 (5)	0.118 (6)	−0.011 (4)	−0.024 (4)	−0.011 (4)
C27	0.096 (6)	0.093 (6)	0.146 (8)	−0.014 (5)	−0.030 (6)	−0.031 (6)
C28	0.160 (11)	0.131 (10)	0.165 (11)	−0.028 (8)	−0.016 (9)	−0.038 (8)
C29	0.058 (4)	0.057 (4)	0.058 (4)	−0.009 (3)	−0.001 (3)	−0.009 (3)
C30	0.068 (4)	0.075 (5)	0.109 (6)	−0.008 (4)	−0.002 (4)	−0.027 (5)
C31	0.105 (6)	0.070 (5)	0.119 (6)	−0.003 (5)	−0.024 (5)	−0.031 (5)
C32	0.164 (11)	0.130 (10)	0.177 (12)	−0.007 (9)	−0.023 (9)	−0.050 (9)
C33	0.057 (4)	0.053 (4)	0.077 (4)	−0.006 (3)	0.010 (3)	−0.002 (3)
C34	0.063 (4)	0.077 (5)	0.094 (5)	−0.021 (4)	−0.002 (4)	0.009 (4)
C35	0.085 (6)	0.085 (6)	0.153 (8)	−0.028 (5)	0.000 (6)	−0.004 (6)
C36	0.120 (9)	0.159 (11)	0.238 (14)	−0.064 (8)	−0.038 (9)	−0.009 (10)

Geometric parameters (Å, º)

Sn1—O5	2.042 (4)	C21—H21A	0.9700
Sn1—C25	2.124 (6)	C21—H21B	0.9700
Sn1—C21	2.126 (6)	C22—C23	1.512 (9)
Sn1—O5^{i}	2.141 (4)	C22—H22A	0.9700
Sn1—O1	2.304 (4)	C22—H22B	0.9700

Sn1—N1	3.184 (5)	C23—C24	1.409 (13)
Sn2—O5	2.049 (4)	C23—C24′	1.476 (18)
Sn2—O3	2.111 (4)	C23—H23A	0.9700
Sn2—C29	2.131 (6)	C23—H23B	0.9700
Sn2—C33	2.138 (6)	C23—H23C	0.9700
Sn2—O1	2.488 (4)	C23—H23D	0.9700
Sn2—N2	2.539 (5)	C24—H23C	0.5516
N1—C2	1.322 (7)	C24—H24A	0.9600
N1—C6	1.367 (8)	C24—H24B	0.9600
N2—C12	1.315 (7)	C24—H24C	0.9600
N2—C16	1.373 (8)	C24′—H24D	0.9600
O1—C1	1.321 (7)	C24′—H24E	0.9600
O2—C1	1.191 (7)	C24′—H24F	0.9600
O3—C11	1.281 (8)	C25—C26	1.493 (8)
O4—C11	1.223 (7)	C25—H25A	0.9700
O5—Sn1^{i}	2.141 (4)	C25—H25B	0.9700
C1—C2	1.535 (9)	C26—C27	1.570 (10)
C2—C3	1.402 (8)	C26—H26A	0.9700
C3—C4	1.346 (9)	C26—H26B	0.9700
C3—H3	0.9300	C27—C28	1.428 (12)
C4—C5	1.402 (10)	C27—H27A	0.9700
C4—H4	0.9300	C27—H27B	0.9700
C5—C10	1.395 (10)	C28—H28A	0.9600
C5—C6	1.429 (9)	C28—H28B	0.9600
C6—C7	1.415 (9)	C28—H28C	0.9600
C7—C8	1.348 (10)	C29—C30	1.506 (8)
C7—H7	0.9300	C29—H29A	0.9700
C8—C9	1.406 (11)	C29—H29B	0.9700
C8—H8	0.9300	C30—C31	1.555 (9)
C9—C10	1.345 (12)	C30—H30A	0.9700
C9—H9	0.9300	C30—H30B	0.9700
C10—H10	0.9300	C31—C32	1.426 (11)
C11—C12	1.517 (9)	C31—H31A	0.9700
C12—C13	1.413 (8)	C31—H31B	0.9700
C13—C14	1.356 (9)	C32—H32A	0.9600
C13—H13	0.9300	C32—H32B	0.9600
C14—C15	1.398 (9)	C32—H32C	0.9600
C14—H14	0.9300	C33—C34	1.518 (8)
C15—C20	1.408 (9)	C33—H33A	0.9700
C15—C16	1.416 (9)	C33—H33B	0.9700
C16—C17	1.403 (9)	C34—C35	1.479 (9)
C17—C18	1.335 (9)	C34—H34A	0.9700
C17—H17	0.9300	C34—H34B	0.9700
C18—C19	1.394 (11)	C35—C36	1.482 (11)
C18—H18	0.9300	C35—H35A	0.9700
C19—C20	1.363 (11)	C35—H35B	0.9700
C19—H19	0.9300	C36—H36A	0.9600
C20—H20	0.9300	C36—H36B	0.9600

C21—C22	1.486 (8)	C36—H36C	0.9600
O5—Sn1—C25	110.7 (2)	C21—C22—H22A	108.5
O5—Sn1—C21	113.6 (2)	C23—C22—H22A	108.5
C25—Sn1—C21	135.5 (3)	C21—C22—H22B	108.5
O5—Sn1—O5^{i}	74.10 (15)	C23—C22—H22B	108.5
C25—Sn1—O5^{i}	98.0 (2)	H22A—C22—H22B	107.5
C21—Sn1—O5^{i}	97.2 (2)	C24—C23—C24′	92.9 (15)
O5—Sn1—O1	72.85 (14)	C24—C23—C22	115.9 (10)
C25—Sn1—O1	94.3 (2)	C24′—C23—C22	119.4 (14)
C21—Sn1—O1	95.2 (2)	C24—C23—H23A	108.3
O5^{i}—Sn1—O1	146.94 (14)	C24′—C23—H23A	111.0
O5—Sn1—N1	129.19 (14)	C22—C23—H23A	108.3
C25—Sn1—N1	70.85 (19)	C24—C23—H23B	108.3
C21—Sn1—N1	78.7 (2)	C22—C23—H23B	108.3
O5^{i}—Sn1—N1	156.19 (13)	H23A—C23—H23B	107.4
O1—Sn1—N1	56.67 (14)	C24′—C23—H23C	109.2
O5—Sn2—O3	80.36 (15)	C22—C23—H23C	107.0
O5—Sn2—C29	105.4 (2)	H23A—C23—H23C	100.0
O3—Sn2—C29	103.7 (2)	H23B—C23—H23C	124.7
O5—Sn2—C33	102.6 (2)	C24—C23—H23D	114.2
O3—Sn2—C33	105.7 (2)	C24′—C23—H23D	105.8
C29—Sn2—C33	142.1 (3)	C22—C23—H23D	108.0
O5—Sn2—O1	68.81 (14)	H23B—C23—H23D	101.0
O3—Sn2—O1	149.11 (14)	H23C—C23—H23D	106.7
C29—Sn2—O1	83.4 (2)	C23—C24—H24A	109.5
C33—Sn2—O1	83.5 (2)	H23C—C24—H24A	129.2
O5—Sn2—N2	149.32 (15)	C23—C24—H24B	109.5
O3—Sn2—N2	69.24 (16)	H23C—C24—H24B	80.8
C29—Sn2—N2	86.3 (2)	H24A—C24—H24B	109.5
C33—Sn2—N2	82.4 (2)	C23—C24—H24C	109.5
O1—Sn2—N2	141.64 (14)	H23C—C24—H24C	113.3
C2—N1—C6	118.2 (5)	H24A—C24—H24C	109.5
C2—N1—Sn1	106.8 (4)	H24B—C24—H24C	109.5
C6—N1—Sn1	134.0 (4)	C23—C24′—H24D	109.5
C12—N2—C16	119.7 (5)	C23—C24′—H24E	109.5
C12—N2—Sn2	110.7 (4)	H24D—C24′—H24E	109.5
C16—N2—Sn2	129.4 (4)	C23—C24′—H24F	109.5
C1—O1—Sn1	142.9 (4)	H24D—C24′—H24F	109.5
C1—O1—Sn2	119.6 (4)	H24E—C24′—H24F	109.5
Sn1—O1—Sn2	96.27 (14)	C26—C25—Sn1	115.1 (5)
C11—O3—Sn2	127.2 (4)	C26—C25—H25A	108.5
Sn1—O5—Sn2	121.61 (18)	Sn1—C25—H25A	108.5
Sn1—O5—Sn1^{i}	105.90 (15)	C26—C25—H25B	108.5
Sn2—O5—Sn1^{i}	132.19 (19)	Sn1—C25—H25B	108.5
O2—C1—O1	124.5 (6)	H25A—C25—H25B	107.5
O2—C1—C2	121.5 (5)	C25—C26—C27	113.5 (7)
O1—C1—C2	114.0 (6)	C25—C26—H26A	108.9

N1—C2—C3	122.9 (6)	C27—C26—H26A	108.9
N1—C2—C1	118.9 (5)	C25—C26—H26B	108.9
C3—C2—C1	118.2 (6)	C27—C26—H26B	108.9
C4—C3—C2	119.1 (6)	H26A—C26—H26B	107.7
C4—C3—H3	120.5	C28—C27—C26	112.4 (9)
C2—C3—H3	120.5	C28—C27—H27A	109.1
C3—C4—C5	121.6 (6)	C26—C27—H27A	109.1
C3—C4—H4	119.2	C28—C27—H27B	109.1
C5—C4—H4	119.2	C26—C27—H27B	109.1
C10—C5—C4	124.6 (7)	H27A—C27—H27B	107.9
C10—C5—C6	119.8 (7)	C27—C28—H28A	109.5
C4—C5—C6	115.6 (6)	C27—C28—H28B	109.5
N1—C6—C7	118.9 (6)	H28A—C28—H28B	109.5
N1—C6—C5	122.6 (6)	C27—C28—H28C	109.5
C7—C6—C5	118.5 (6)	H28A—C28—H28C	109.5
C8—C7—C6	119.3 (7)	H28B—C28—H28C	109.5
C8—C7—H7	120.4	C30—C29—Sn2	116.8 (5)
C6—C7—H7	120.4	C30—C29—H29A	108.1
C7—C8—C9	121.8 (8)	Sn2—C29—H29A	108.1
C7—C8—H8	119.1	C30—C29—H29B	108.1
C9—C8—H8	119.1	Sn2—C29—H29B	108.1
C10—C9—C8	120.4 (8)	H29A—C29—H29B	107.3
C10—C9—H9	119.8	C29—C30—C31	111.0 (6)
C8—C9—H9	119.8	C29—C30—H30A	109.4
C9—C10—C5	120.2 (7)	C31—C30—H30A	109.4
C9—C10—H10	119.9	C29—C30—H30B	109.4
C5—C10—H10	119.9	C31—C30—H30B	109.4
O4—C11—O3	124.7 (6)	H30A—C30—H30B	108.0
O4—C11—C12	119.1 (6)	C32—C31—C30	114.1 (8)
O3—C11—C12	116.2 (6)	C32—C31—H31A	108.7
N2—C12—C13	123.0 (6)	C30—C31—H31A	108.7
N2—C12—C11	116.3 (5)	C32—C31—H31B	108.7
C13—C12—C11	120.7 (6)	C30—C31—H31B	108.7
C14—C13—C12	117.8 (6)	H31A—C31—H31B	107.6
C14—C13—H13	121.1	C31—C32—H32A	109.5
C12—C13—H13	121.1	C31—C32—H32B	109.5
C13—C14—C15	121.4 (6)	H32A—C32—H32B	109.5
C13—C14—H14	119.3	C31—C32—H32C	109.5
C15—C14—H14	119.3	H32A—C32—H32C	109.5
C14—C15—C20	123.9 (7)	H32B—C32—H32C	109.5
C14—C15—C16	117.6 (6)	C34—C33—Sn2	117.5 (5)
C20—C15—C16	118.5 (7)	C34—C33—H33A	107.9
N2—C16—C17	120.7 (6)	Sn2—C33—H33A	107.9
N2—C16—C15	120.5 (6)	C34—C33—H33B	107.9
C17—C16—C15	118.8 (6)	Sn2—C33—H33B	107.9
C18—C17—C16	121.3 (7)	H33A—C33—H33B	107.2
C18—C17—H17	119.3	C35—C34—C33	114.4 (7)
C16—C17—H17	119.3	C35—C34—H34A	108.7

C17—C18—C19	120.5 (8)	C33—C34—H34A	108.7
C17—C18—H18	119.8	C35—C34—H34B	108.7
C19—C18—H18	119.8	C33—C34—H34B	108.7
C20—C19—C18	120.5 (7)	H34A—C34—H34B	107.6
C20—C19—H19	119.7	C34—C35—C36	115.3 (9)
C18—C19—H19	119.7	C34—C35—H35A	108.4
C19—C20—C15	120.3 (7)	C36—C35—H35A	108.4
C19—C20—H20	119.8	C34—C35—H35B	108.4
C15—C20—H20	119.8	C36—C35—H35B	108.4
C22—C21—Sn1	119.7 (5)	H35A—C35—H35B	107.5
C22—C21—H21A	107.4	C35—C36—H36A	109.5
Sn1—C21—H21A	107.4	C35—C36—H36B	109.5
C22—C21—H21B	107.4	H36A—C36—H36B	109.5
Sn1—C21—H21B	107.4	C35—C36—H36C	109.5
H21A—C21—H21B	106.9	H36A—C36—H36C	109.5
C21—C22—C23	115.2 (7)	H36B—C36—H36C	109.5

Symmetry code: (i) $-x+1, -y+2, -z$.