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ISSN 2414-3146

Bis(μ_2-4-nitrophenolato)bis(4-nitrophenolato)-di-μ_3-oxido-octaphenyltetratin chloroform sesquisolvate [+ solvate]: a tetranuclear stannoxane

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Received 26 July 2019
Accepted 30 July 2019

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

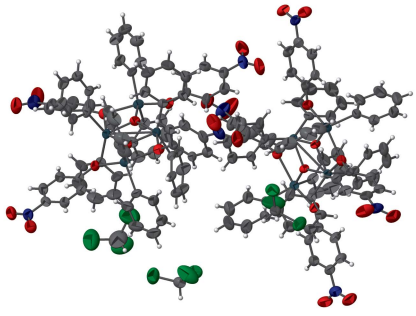
Keywords: crystal structure; tetranuclear stannoxane; oxo-tin core; Sn···O contacts; C—H···O hydrogen bonds.

CCDC reference: 1941837

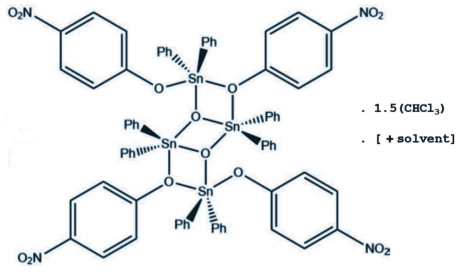
Structural data: full structural data are available from iucrdata.iucr.org

The title tetranuclear stannoxane, $[Sn_4(C_6H_5)_8(C_6H_4NO_3)_4O_2]\cdot 1.5CHCl_3\cdot$-solvent, crystallized with two independent complex molecules, *A* and *B*, in the asymmetric unit together with 1.5 molecules of chloroform. There is also a region of disordered electron density, which was corrected for using the SQUEEZE routine [Spek (2015). *Acta Cryst*. C**71**, 9–18]. The oxo-tin core of each complex is in a planar 'ladder' arrangement and each Sn atom is fivefold SnO_3C_2 coordinated, with one tin centre having an almost perfect square-pyramidal coordination geometry, while the other three Sn centres have distorted shapes. In the crystal, the complex molecules are arranged in layers, composed of *A* or *B* complexes, lying parallel to the *bc* plane. The complex molecules are linked by a number of C—H···O hydrogen bonds within the layers and between the layers, forming a supramolecular three-dimensional structure.

3D view



Chemical scheme



Structure description

Stannoxanes represent an intriguing class of tin complexes characterized by a polynuclear oxo-tin core. A large variety of stannoxanes have been described from simple dimers (Gross, 1989) to hexameric macrocycles (Prabusankar & Murugavel, 2004). In recent years, these versatile structures have gained considerable interest as anti-tumour cytotoxins (Gerasimchuk *et al.*, 2007; Sun *et al.*, 2011) and as supports for the development of nanomaterials (Strachota *et al.*, 2012; Chandrasekhar *et al.*, 2006). The preparation of stannoxanes typically involves hydrolysis of an organotin halide reagent with the halides often being displaced by the addition of carboxylate ligands (Basu Baul *et al.*, 2010). A number of tetranuclear stannoxanes have been reported containing

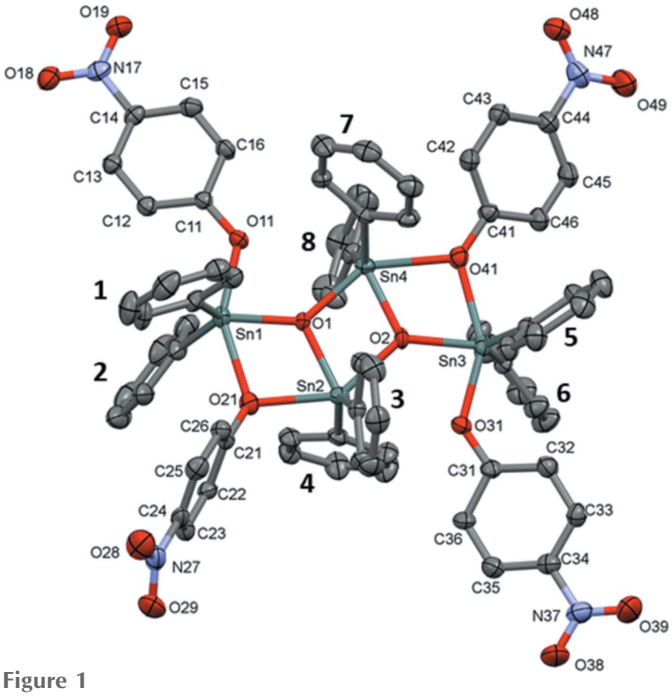


Figure 1
The molecular structure of complex *A*. Displacement ellipsoids are drawn at the 30% probability level. Phenyl ring 1 = C51–C56, 2 = C61–C66, 3 = C71–C76, 4 = C81–C86, 5 = C91–C96, 6 = C101–C106, 7 = C111–C116, 8 = C121–C126. For clarity, the hydrogen atoms have been omitted.

carboxylate ligands (Khoo & Hazell, 1999; Chandrasekhar *et al.*, 2002; Kumara Swamy *et al.*, 1988; Win *et al.*, 2008; Zhang *et al.*, 2005). However, as demonstrated previously (Devi *et al.*, 2015; Beckmann *et al.*, 2004; Wang *et al.*, 2005; Gómez *et al.*, 2010; Vatsa *et al.* 1991) and by the structure reported here, in the case of tetranuclear stannoxanes phenolate ligands are also amenable.

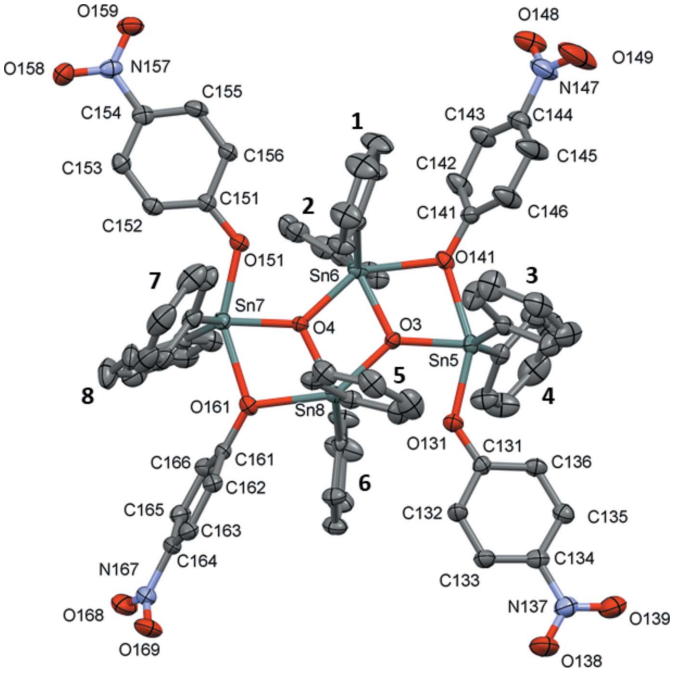


Figure 2
The molecular structure of complex *B*. Displacement ellipsoids are drawn at the 30% probability level. Phenyl ring 1 = C171–C176, 2 = C181–C186, 3 = C191–C196, 4 = C201–C206, 5 = C211–C216, 6 = C221–C226, 7 = C231–C236, 8 = C241–C246. For clarity, the hydrogen atoms have been omitted.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C82—H82···O31	0.93	2.35	3.144 (13)	143
C116—H116···O11	0.93	2.55	3.289 (11)	137
C182—H182···O151	0.93	2.52	3.259 (12)	137
C216—H216···O131	0.93	2.37	3.161 (13)	143
C3—H3···O148^{i}	0.98	2.44	3.27 (2)	143
C16—H16···O138^{ii}	0.93	2.60	3.301 (13)	133
C22—H22···O159^{i}	0.93	2.47	3.388 (11)	168
C84—H84···O39^{i}	0.93	2.55	3.264 (16)	134
C94—H94···O138^{iii}	0.93	2.57	3.470 (16)	162
C96—H96···O49^{iv}	0.93	2.53	3.305 (14)	142
C156—H156···O38	0.93	2.53	3.271 (13)	136
C162—H162···O19^{v}	0.93	2.43	3.343 (12)	168
C202—H202···O149^{vi}	0.93	2.53	3.293 (16)	139

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

The title stannoxane complex was prepared by reaction of Ph_2SnCl_2 with 4-nitrophenol. It was crystallized by vapour diffusion of a concentrated chloroform solution of the compound with hexane at ambient temperature. The asymmetric contains two independent complex molecules (*A* and *B*) of the stannoxane (Figs. 1 and 2), and 1.5 $CHCl_3$ solvent molecules, plus an unknown solvate. The oxo-tin core of each complex is in a planar 'ladder' arrangement. Each Sn atom is fivefold SnO_3C_2 coordinate with one tin centre having an almost perfect square-pyramidal coordination geometry, *viz*. atom Sn2 in complex *A* and atom Sn8 in complex *B*, with τ_5 factors of 0.04 and 0.09, respectively (τ_5 = 0 for a perfect square-pyramidal geometry and = 1 for a perfect trigonal–

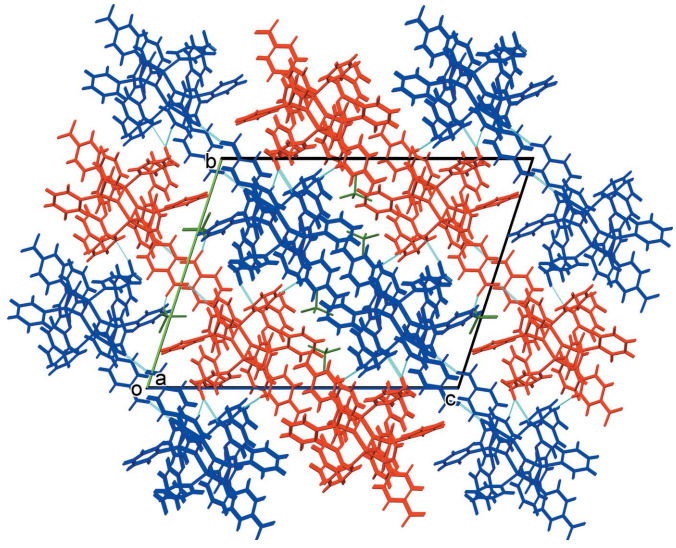


Figure 3
A view along the *a* axis of the crystal packing of the title compound. The C—H···O hydrogen bonds are shown as dashed lines (Table 1). Colour code: *A* complexes blue, *B* complexes red, $CHCl_3$ solvent molecules green.

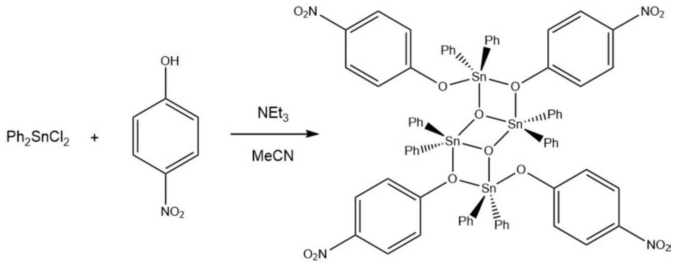


Figure 4
The reaction scheme for the synthesis of the title compound.

pyramidal geometry; Addison *et al.*, 1984). The other three Sn centres in each complex molecule have distorted shapes with τ_5 factors of 0.35 for Sn1, 0.27 for Sn3 and 0.15 for Sn4 in complex *A*, and 0.25 for Sn5, 0.15 for Sn6 and 0.38 for Sn7 in complex *B*.

One pair of opposing phenolate ligands are identified as bridging ligands with Sn—O bond lengths varying from 2.243 (5) to 2.305 (6) Å. For the monodentate phenolate ligands the Sn—O bond lengths are shorter, varying from 2.071 (5) Å to 2.095 (6) Å. The positioning of these ligands notably suggests additional long-distance Sn···O interactions, ranging from 3.082 (6) to 3.161 (6) Å, with the adjacent non-bonded tin centres.

In each complex there are two intramolecular C—H···O hydrogen bonds involving the monodentate phenol O atoms (O11 and O31 in complex *A*, and O131 and O151 in complex *B*) and neighbouring phenyl rings (Table 1).

In the crystal, there are further C—H···O hydrogen bonds present linking the complexes to form separate layers of *A* and *B* complex molecules parallel to the *bc* plane (Fig. 3, Table 1). The layers are also linked by C—H···O contacts, forming a supramolecular three-dimensional structure.

Synthesis and crystallization

The reaction scheme for the synthesis of the title compound is shown in Fig. 4. To a dry acetonitrile (18 ml) solution of 4-nitrophenol (100 mg, 0.72 mmol) was added triethylamine (0.053 ml, 0.72 mmol). The resulting orange solution was frozen with liquid nitrogen and diphenyltin dichloride (124 mg, 0.36 mmol) was added. While still frozen, the reaction flask was evacuated and back-filled with nitrogen (× 4) then allowed to warm to r.t. before being heated to reflux for 8 h. Thereafter, all volatiles were removed under reduced pressure and the crude product re-suspended in methanol (25 ml). After sonicating for 80 min, the title compound was isolated by filtration. Needle-like colourless crystals, suitable crystal X-ray diffraction analysis, were obtained by vapour diffusion of a concentrated chloroform solution of the compound with hexane at ambient temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. No sensible disordered model could be formulated for a region of disordered electron density related to an unknown solvate, most probably hexane. The SQUEEZE routine within *PLATON* (Spek, 2015) was used to account for the electron density in this region of the unit cell. The program identified solvent-accessible voids totalling *ca* 516 Å^3 and 118 electrons per unit cell were recovered. The formula weight, density *etc.* listed in Table 2 does not include any correction for the missing solvate. The largest residual electron density peaks and holes are near the tin atoms, for example, that of 3.49 e Å^{-3} is 0.88 Å from atom Sn2, while the most negative of −2.38 e Å^{-3} is 0.87 Å from atom Sn3.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[Sn_4(C_6H_5)_8(C_6H_4NO_3)_4O_2]$·1.5$CHCl_2$ + solvent
M_r	1855.02
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	150
a, *b*, *c* (Å)	12.8262 (2), 22.1075 (4), 28.9552 (5)
α, β, γ (°)	72.349 (2), 79.800 (2), 89.827 (1)
V (Å^3)	7689.0 (2)
Z	4
Radiation type	Cu *Kα*
μ (mm^{-1})	12.18
Crystal size (mm)	0.16 × 0.06 × 0.02
Data collection	
Diffractometer	Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, EosS2
Absorption correction	For a sphere (*CrysAlis PRO*; Rigaku OD, 2015)
T_{min}, T_{max}	0.584, 0.615
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	52013, 30192, 21951
R_{int}	0.040
(sin θ/λ)$_{max}$ (Å^{-1})	0.624
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.069, 0.197, 1.04
No. of reflections	30192
No. of parameters	1801
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	3.88, −2.32

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *SHELXT* (Sheldrick, 2015*a*), *SHELXL* (Sheldrick, 2015*b*), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury* (Macrae *et al.*, 2008.

Acknowledgements

The author thanks the Ward Group for their support in funding this work.

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full crystallographic data

IUCrData (2019). **4**, x191067 [https://doi.org/10.1107/S2414314619010678]

Bis(μ_2-4-nitrophenolato)bis(4-nitrophenolato)di-μ_3-oxido-octaphenyltetratin chloroform sesquisolvate [+ solvate]: a tetranuclear stannoxane

Patrick Butler

Bis(μ_2-4-nitrophenolato)bis(4-nitrophenolato)di-μ_3-oxido-octaphenyltetratin chloroform sesquisolvate [+ solvate]

Crystal data

$[Sn_4(C_6H_5)_8(C_6H_4NO_3)_4O_2]\cdot 1.5CHCl_3\cdot$solvent
M_r = 1855.02
Triclinic, $P\overline{1}$
a = 12.8262 (2) Å
b = 22.1075 (4) Å
c = 28.9552 (5) Å
α = 72.349 (2)°
β = 79.800 (2)°
γ = 89.827 (1)°
V = 7689.0 (2) Å^3
Z = 4
$F(000)$ = 3660
D_x = 1.602 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 18171 reflections
θ = 4.2–73.6°
μ = 12.18 mm^{-1}
T = 150 K
Plate, colourless
0.16 × 0.06 × 0.02 × 0.03 (radius) mm

Data collection

Rigaku Oxford Diffraction SuperNova, Dual, Cu at zero, EosS2 diffractometer
Radiation source: micro-focus sealed X-ray tube, SuperNova (Cu) X-ray Source
Mirror monochromator
Detector resolution: 8.1297 pixels mm^{-1}
ω scans
Absorption correction: for a sphere (CrysAlisPro; Rigaku OD, 2015)
T_{min} = 0.584, T_{max} = 0.615
52013 measured reflections
30192 independent reflections
21951 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 74.1°, θ_{min} = 4.0°
h = −15→15
k = −17→27
l = −32→35

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.197
S = 1.04
30192 reflections
1801 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0961P)^2 + 23.2885P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 3.88 e Å^{-3}
$\Delta\rho_{min}$ = −2.32 e Å^{-3}

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. The C-bound H hydrogen were fixed geometrically and allowed to ride on their parent atom: C—H = 0.93 - 0.98 Å with U_{iso}(H) = 1.2U_{eq}(*C*).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.53861 (4)	0.65920 (3)	0.34840 (2)	0.04212 (13)
Sn2	0.77097 (4)	0.62717 (2)	0.28055 (2)	0.03858 (12)
Sn3	0.92558 (4)	0.73917 (3)	0.16305 (2)	0.04266 (13)
Sn4	0.69375 (4)	0.77305 (2)	0.23106 (2)	0.03783 (12)
Sn5	0.85368 (4)	0.23602 (3)	0.16023 (2)	0.04028 (12)
Sn6	1.02791 (4)	0.27083 (2)	0.22917 (2)	0.03723 (12)
Sn7	1.08118 (4)	0.15952 (3)	0.34960 (2)	0.04118 (13)
Sn8	0.90618 (4)	0.12653 (2)	0.28113 (2)	0.03754 (12)
Cl1	0.5708 (3)	0.1827 (3)	0.47571 (14)	0.1293 (19)
Cl2	0.5721 (3)	0.17084 (18)	0.57722 (13)	0.0849 (9)
Cl3	0.4834 (3)	0.06952 (17)	0.55210 (16)	0.0983 (11)
Cl11	0.1342 (2)	0.33339 (18)	0.41801 (13)	0.0856 (9)
Cl12	0.0225 (3)	0.43345 (18)	0.44377 (18)	0.1093 (14)
Cl13	0.0551 (4)	0.3206 (3)	0.51985 (14)	0.134 (2)
Cl21	0.4673 (5)	0.6781 (4)	0.0325 (3)	0.172 (3)
Cl22	0.2931 (6)	0.7580 (3)	0.0183 (3)	0.176 (3)
Cl23	0.3618 (5)	0.6885 (3)	−0.04883 (16)	0.146 (2)
O1	0.6555 (4)	0.6888 (2)	0.29002 (17)	0.0336 (10)
O2	0.8112 (4)	0.7134 (3)	0.22283 (18)	0.0383 (12)
O3	0.9177 (4)	0.2106 (2)	0.22149 (18)	0.0354 (11)
O4	1.0151 (4)	0.1880 (2)	0.28904 (18)	0.0367 (11)
O11	0.4839 (5)	0.7456 (3)	0.3118 (2)	0.0414 (12)
O18	0.0402 (6)	0.8282 (4)	0.3929 (3)	0.0635 (18)
O19	0.0968 (6)	0.9116 (4)	0.3314 (3)	0.072 (2)
O21	0.6598 (5)	0.5822 (3)	0.3522 (2)	0.0458 (13)
O28	0.7848 (8)	0.4093 (5)	0.5472 (3)	0.092 (3)
O29	0.7736 (8)	0.3396 (4)	0.5099 (3)	0.086 (3)
O31	0.9699 (5)	0.6482 (3)	0.1991 (2)	0.0455 (13)
O38	1.3145 (8)	0.4500 (4)	0.1913 (4)	0.094 (3)
O39	1.3943 (7)	0.5314 (5)	0.1350 (4)	0.102 (3)
O41	0.8173 (5)	0.8209 (3)	0.1610 (2)	0.0472 (13)
O48	0.7535 (8)	1.0995 (4)	0.0345 (3)	0.085 (3)
O49	0.8620 (9)	1.0676 (4)	−0.0189 (3)	0.099 (3)
O131	0.7719 (5)	0.1478 (3)	0.1977 (2)	0.0453 (13)
O138	0.4221 (8)	−0.0444 (4)	0.1934 (4)	0.088 (3)
O139	0.3969 (7)	0.0350 (4)	0.1328 (4)	0.086 (3)
O141	0.9691 (5)	0.3169 (3)	0.15790 (18)	0.0422 (12)

O148	1.1389 (8)	0.5950 (4)	0.0333 (3)	0.087 (3)
O149	1.1724 (14)	0.5476 (6)	−0.0220 (4)	0.156 (7)
O151	1.1679 (5)	0.2449 (3)	0.3116 (2)	0.0453 (13)
O158	1.5434 (6)	0.3310 (4)	0.3925 (3)	0.0654 (19)
O159	1.5456 (6)	0.4092 (3)	0.3264 (3)	0.068 (2)
O161	0.9568 (5)	0.0830 (3)	0.35384 (19)	0.0413 (12)
O168	0.6702 (8)	−0.0895 (5)	0.5470 (3)	0.092 (3)
O169	0.7188 (7)	−0.1605 (4)	0.5107 (3)	0.085 (3)
N17	0.1083 (7)	0.8577 (4)	0.3577 (3)	0.0545 (19)
N27	0.7665 (7)	0.3949 (5)	0.5120 (3)	0.068 (3)
N37	1.3169 (8)	0.5057 (5)	0.1659 (4)	0.066 (2)
N47	0.8087 (9)	1.0597 (5)	0.0220 (4)	0.076 (3)
N137	0.4462 (7)	0.0093 (4)	0.1662 (3)	0.062 (2)
N147	1.1357 (10)	0.5480 (5)	0.0201 (4)	0.085 (3)
N157	1.5084 (6)	0.3579 (4)	0.3550 (3)	0.0484 (17)
N167	0.7204 (8)	−0.1052 (5)	0.5127 (3)	0.069 (3)
C1	0.5052 (8)	0.1525 (5)	0.5352 (4)	0.058 (2)
H1	0.4358	0.1712	0.5377	0.069*
C2	0.0343 (8)	0.3513 (5)	0.4602 (4)	0.060 (2)
H2	−0.0327	0.3319	0.4582	0.072*
C3	0.3508 (18)	0.6891 (10)	0.0104 (6)	0.125 (7)
H3	0.3018	0.6533	0.0308	0.150*
C11	0.3935 (6)	0.7707 (4)	0.3247 (3)	0.0385 (16)
C12	0.3172 (7)	0.7406 (4)	0.3660 (3)	0.0454 (18)
H12	0.3294	0.7007	0.3863	0.054*
C13	0.2241 (7)	0.7686 (4)	0.3775 (3)	0.0437 (18)
H13	0.1735	0.7480	0.4051	0.052*
C14	0.2076 (7)	0.8277 (4)	0.3472 (3)	0.0427 (18)
C15	0.2823 (8)	0.8602 (4)	0.3056 (3)	0.051 (2)
H15	0.2696	0.9005	0.2861	0.062*
C16	0.3747 (7)	0.8319 (4)	0.2941 (3)	0.0458 (19)
H16	0.4249	0.8527	0.2664	0.055*
C21	0.6856 (6)	0.5375 (4)	0.3918 (3)	0.0382 (16)
C22	0.6668 (6)	0.4729 (4)	0.3971 (3)	0.0433 (18)
H22	0.6355	0.4616	0.3740	0.052*
C23	0.6947 (7)	0.4256 (5)	0.4365 (4)	0.054 (2)
H23	0.6837	0.3828	0.4398	0.065*
C24	0.7394 (7)	0.4441 (5)	0.4707 (3)	0.052 (2)
C25	0.7578 (8)	0.5073 (5)	0.4671 (3)	0.055 (2)
H25	0.7865	0.5184	0.4909	0.066*
C26	0.7321 (7)	0.5535 (4)	0.4269 (3)	0.0449 (18)
H26	0.7462	0.5961	0.4232	0.054*
C31	1.0540 (7)	0.6162 (4)	0.1903 (3)	0.0448 (18)
C32	1.1464 (8)	0.6438 (5)	0.1564 (4)	0.053 (2)
H32	1.1502	0.6869	0.1390	0.064*
C33	1.2335 (7)	0.6067 (5)	0.1486 (4)	0.054 (2)
H33	1.2948	0.6251	0.1262	0.065*
C34	1.2265 (8)	0.5427 (5)	0.1748 (4)	0.052 (2)

C35	1.1377 (8)	0.5137 (5)	0.2089 (4)	0.056 (2)
H35	1.1361	0.4709	0.2268	0.067*
C36	1.0509 (8)	0.5496 (4)	0.2158 (3)	0.050 (2)
H36	0.9894	0.5300	0.2374	0.060*
C41	0.8185 (7)	0.8798 (4)	0.1277 (3)	0.0441 (18)
C42	0.7689 (8)	0.9298 (5)	0.1416 (3)	0.054 (2)
H42	0.7381	0.9235	0.1744	0.065*
C43	0.7653 (8)	0.9888 (5)	0.1067 (3)	0.056 (2)
H43	0.7306	1.0216	0.1158	0.067*
C44	0.8143 (9)	0.9979 (5)	0.0582 (4)	0.058 (2)
C45	0.8669 (9)	0.9493 (5)	0.0449 (4)	0.066 (3)
H45	0.9010	0.9562	0.0124	0.080*
C46	0.8693 (9)	0.8911 (5)	0.0789 (3)	0.059 (3)
H46	0.9051	0.8588	0.0695	0.071*
C51	0.5744 (7)	0.6762 (5)	0.4111 (3)	0.0471 (19)
C52	0.6548 (8)	0.7222 (5)	0.4052 (4)	0.054 (2)
H52	0.6869	0.7468	0.3737	0.064*
C53	0.6871 (9)	0.7315 (5)	0.4464 (4)	0.063 (3)
H53	0.7406	0.7621	0.4422	0.076*
C54	0.6399 (11)	0.6955 (7)	0.4928 (4)	0.081 (4)
H54	0.6617	0.7016	0.5202	0.097*
C55	0.5606 (10)	0.6503 (7)	0.4994 (4)	0.079 (4)
H55	0.5296	0.6260	0.5311	0.095*
C56	0.5261 (8)	0.6404 (6)	0.4592 (3)	0.064 (3)
H56	0.4714	0.6103	0.4641	0.077*
C61	0.4203 (7)	0.5961 (4)	0.3425 (4)	0.052 (2)
C62	0.4039 (8)	0.5342 (5)	0.3736 (5)	0.067 (3)
H62	0.4407	0.5206	0.3995	0.081*
C63	0.3336 (9)	0.4926 (6)	0.3665 (6)	0.085 (4)
H63	0.3231	0.4512	0.3877	0.103*
C64	0.2791 (10)	0.5113 (8)	0.3285 (7)	0.099 (6)
H64	0.2320	0.4827	0.3239	0.119*
C65	0.2945 (9)	0.5751 (8)	0.2957 (6)	0.086 (4)
H65	0.2583	0.5882	0.2695	0.103*
C66	0.3647 (8)	0.6170 (6)	0.3040 (5)	0.066 (3)
H66	0.3744	0.6590	0.2837	0.079*
C71	0.8949 (6)	0.6317 (4)	0.3177 (3)	0.0405 (17)
C72	0.9084 (8)	0.6882 (5)	0.3285 (3)	0.051 (2)
H72	0.8646	0.7215	0.3187	0.061*
C73	0.9886 (9)	0.6945 (6)	0.3545 (4)	0.067 (3)
H73	0.9988	0.7323	0.3613	0.080*
C74	1.0520 (8)	0.6447 (6)	0.3697 (4)	0.063 (3)
H74	1.1050	0.6493	0.3868	0.075*
C75	1.0384 (8)	0.5884 (5)	0.3603 (4)	0.062 (3)
H75	1.0807	0.5547	0.3712	0.074*
C76	0.9594 (7)	0.5823 (5)	0.3336 (4)	0.051 (2)
H76	0.9503	0.5445	0.3267	0.061*
C81	0.7131 (7)	0.5724 (4)	0.2411 (3)	0.0430 (18)

C82	0.7677 (8)	0.5718 (5)	0.1945 (4)	0.055 (2)
H82	0.8382	0.5869	0.1839	0.066*
C83	0.7160 (10)	0.5486 (6)	0.1641 (4)	0.076 (4)
H83	0.7518	0.5488	0.1332	0.091*
C84	0.6111 (10)	0.5252 (6)	0.1803 (4)	0.069 (3)
H84	0.5756	0.5112	0.1598	0.083*
C85	0.5603 (8)	0.5229 (5)	0.2264 (4)	0.054 (2)
H85	0.4911	0.5056	0.2376	0.065*
C86	0.6105 (8)	0.5461 (4)	0.2566 (3)	0.048 (2)
H86	0.5745	0.5439	0.2880	0.058*
C91	1.0570 (6)	0.7889 (4)	0.1714 (3)	0.0426 (18)
C92	1.0951 (8)	0.7641 (5)	0.2157 (4)	0.057 (2)
H92	1.0633	0.7273	0.2394	0.068*
C93	1.1799 (8)	0.7950 (6)	0.2235 (4)	0.065 (3)
H93	1.2046	0.7793	0.2529	0.078*
C94	1.2294 (9)	0.8496 (6)	0.1877 (5)	0.070 (3)
H94	1.2878	0.8695	0.1931	0.084*
C95	1.1918 (10)	0.8738 (5)	0.1448 (4)	0.071 (3)
H95	1.2242	0.9107	0.1214	0.085*
C96	1.1056 (8)	0.8438 (4)	0.1356 (4)	0.053 (2)
H96	1.0809	0.8602	0.1062	0.064*
C101	0.8797 (8)	0.7190 (4)	0.1031 (3)	0.048 (2)
C102	0.7785 (8)	0.7347 (5)	0.0919 (4)	0.055 (2)
H102	0.7359	0.7588	0.1082	0.067*
C103	0.7425 (10)	0.7135 (6)	0.0559 (4)	0.068 (3)
H103	0.6742	0.7216	0.0499	0.082*
C104	0.8068 (11)	0.6813 (6)	0.0297 (4)	0.073 (3)
H104	0.7837	0.6697	0.0047	0.087*
C105	0.9062 (11)	0.6662 (6)	0.0404 (4)	0.074 (3)
H105	0.9495	0.6437	0.0228	0.089*
C106	0.9416 (9)	0.6841 (5)	0.0768 (3)	0.061 (3)
H106	1.0082	0.6728	0.0840	0.073*
C111	0.7347 (7)	0.8370 (3)	0.2667 (3)	0.0381 (16)
C112	0.8420 (7)	0.8577 (4)	0.2586 (4)	0.050 (2)
H112	0.8918	0.8432	0.2375	0.059*
C113	0.8751 (9)	0.8988 (5)	0.2812 (4)	0.061 (2)
H113	0.9461	0.9126	0.2751	0.073*
C114	0.8003 (10)	0.9193 (5)	0.3133 (4)	0.062 (3)
H114	0.8225	0.9463	0.3292	0.075*
C115	0.6950 (10)	0.9010 (5)	0.3223 (4)	0.063 (3)
H115	0.6462	0.9160	0.3435	0.076*
C116	0.6616 (7)	0.8593 (4)	0.2989 (3)	0.0464 (19)
H116	0.5902	0.8463	0.3048	0.056*
C121	0.5757 (6)	0.7688 (4)	0.1895 (3)	0.0426 (18)
C122	0.5423 (9)	0.7101 (5)	0.1885 (4)	0.059 (2)
H122	0.5680	0.6731	0.2072	0.071*
C123	0.4694 (10)	0.7072 (7)	0.1589 (5)	0.083 (4)
H123	0.4454	0.6678	0.1584	0.100*

C124	0.4320 (10)	0.7613 (8)	0.1305 (5)	0.087 (4)
H124	0.3832	0.7588	0.1109	0.105*
C125	0.4670 (11)	0.8184 (7)	0.1314 (5)	0.085 (4)
H125	0.4418	0.8550	0.1118	0.102*
C126	0.5386 (7)	0.8246 (5)	0.1601 (3)	0.057 (2)
H126	0.5616	0.8645	0.1602	0.069*
C131	0.6942 (6)	0.1170 (4)	0.1885 (3)	0.0403 (17)
C132	0.6642 (8)	0.0536 (4)	0.2194 (3)	0.050 (2)
H132	0.7000	0.0356	0.2452	0.060*
C133	0.5837 (8)	0.0180 (4)	0.2123 (3)	0.052 (2)
H133	0.5655	−0.0234	0.2327	0.062*
C134	0.5304 (7)	0.0459 (4)	0.1738 (3)	0.049 (2)
C135	0.5584 (7)	0.1073 (4)	0.1414 (3)	0.050 (2)
H135	0.5228	0.1244	0.1155	0.060*
C136	0.6403 (7)	0.1419 (4)	0.1489 (3)	0.0471 (19)
H136	0.6601	0.1825	0.1273	0.057*
C141	1.0062 (7)	0.3733 (4)	0.1241 (3)	0.0422 (18)
C142	1.0027 (10)	0.4290 (5)	0.1361 (4)	0.067 (3)
H142	0.9702	0.4282	0.1676	0.081*
C143	1.0464 (9)	0.4864 (5)	0.1024 (4)	0.060 (3)
H143	1.0469	0.5231	0.1117	0.073*
C144	1.0883 (9)	0.4876 (5)	0.0556 (4)	0.065 (3)
C145	1.0922 (14)	0.4341 (7)	0.0419 (4)	0.109 (6)
H145	1.1220	0.4358	0.0097	0.131*
C146	1.0509 (13)	0.3761 (6)	0.0766 (4)	0.088 (5)
H146	1.0537	0.3392	0.0674	0.105*
C151	1.2490 (6)	0.2693 (4)	0.3237 (3)	0.0384 (16)
C152	1.2898 (6)	0.2426 (4)	0.3669 (3)	0.0412 (17)
H152	1.2587	0.2045	0.3892	0.049*
C153	1.3735 (7)	0.2706 (4)	0.3773 (3)	0.0463 (19)
H153	1.4004	0.2513	0.4057	0.056*
C154	1.4175 (7)	0.3281 (4)	0.3451 (3)	0.0453 (19)
C155	1.3805 (8)	0.3572 (4)	0.3020 (3)	0.053 (2)
H155	1.4119	0.3956	0.2806	0.063*
C156	1.2969 (7)	0.3286 (4)	0.2913 (3)	0.0450 (18)
H156	1.2713	0.3482	0.2626	0.054*
C161	0.8993 (6)	0.0382 (4)	0.3930 (3)	0.0371 (16)
C162	0.9148 (7)	−0.0261 (4)	0.3990 (3)	0.0460 (19)
H162	0.9659	−0.0375	0.3765	0.055*
C163	0.8553 (7)	−0.0731 (5)	0.4378 (4)	0.053 (2)
H163	0.8642	−0.1158	0.4410	0.064*
C164	0.7826 (7)	−0.0550 (5)	0.4718 (3)	0.052 (2)
C165	0.7663 (8)	0.0082 (5)	0.4683 (3)	0.054 (2)
H165	0.7175	0.0192	0.4918	0.065*
C166	0.8253 (7)	0.0546 (4)	0.4284 (3)	0.049 (2)
H166	0.8156	0.0973	0.4252	0.058*
C171	1.1827 (6)	0.2638 (4)	0.1918 (3)	0.0391 (16)
C172	1.2421 (7)	0.3176 (5)	0.1589 (4)	0.060 (3)

H172	1.2168	0.3581	0.1548	0.072*
C173	1.3397 (9)	0.3091 (7)	0.1326 (5)	0.092 (5)
H173	1.3811	0.3444	0.1113	0.110*
C174	1.3762 (10)	0.2487 (7)	0.1376 (5)	0.093 (5)
H174	1.4416	0.2437	0.1197	0.111*
C175	1.3174 (9)	0.1979 (6)	0.1681 (5)	0.079 (4)
H175	1.3415	0.1576	0.1706	0.095*
C176	1.2206 (8)	0.2041 (5)	0.1965 (4)	0.060 (3)
H176	1.1818	0.1683	0.2185	0.072*
C181	0.9551 (7)	0.3364 (3)	0.2637 (3)	0.0391 (17)
C182	1.0012 (8)	0.3577 (4)	0.2963 (3)	0.050 (2)
H182	1.0671	0.3444	0.3032	0.060*
C183	0.9459 (10)	0.3997 (5)	0.3185 (3)	0.062 (3)
H183	0.9759	0.4146	0.3403	0.074*
C184	0.8481 (8)	0.4192 (5)	0.3084 (4)	0.059 (3)
H184	0.8124	0.4467	0.3238	0.071*
C185	0.8021 (8)	0.3985 (5)	0.2758 (4)	0.059 (2)
H185	0.7366	0.4125	0.2686	0.071*
C186	0.8548 (7)	0.3564 (4)	0.2538 (3)	0.0467 (19)
H186	0.8238	0.3413	0.2324	0.056*
C191	0.9507 (8)	0.2102 (4)	0.1035 (3)	0.049 (2)
C192	0.9143 (10)	0.1959 (7)	0.0656 (4)	0.076 (4)
H192	0.8438	0.2020	0.0624	0.091*
C193	0.9803 (11)	0.1729 (7)	0.0324 (4)	0.087 (5)
H193	0.9538	0.1628	0.0077	0.105*
C194	1.0847 (11)	0.1650 (6)	0.0359 (4)	0.078 (4)
H194	1.1290	0.1502	0.0131	0.093*
C195	1.1240 (11)	0.1785 (7)	0.0721 (5)	0.082 (4)
H195	1.1949	0.1726	0.0747	0.098*
C196	1.0575 (9)	0.2014 (6)	0.1055 (4)	0.073 (3)
H196	1.0851	0.2112	0.1301	0.088*
C201	0.7242 (7)	0.2933 (4)	0.1644 (3)	0.0428 (17)
C202	0.7261 (9)	0.3547 (5)	0.1317 (4)	0.062 (3)
H202	0.7847	0.3713	0.1069	0.075*
C203	0.6370 (11)	0.3904 (6)	0.1374 (5)	0.081 (4)
H203	0.6361	0.4313	0.1159	0.097*
C204	0.5510 (11)	0.3661 (7)	0.1741 (6)	0.094 (5)
H204	0.4923	0.3903	0.1772	0.113*
C205	0.5515 (10)	0.3056 (6)	0.2064 (6)	0.086 (4)
H205	0.4935	0.2899	0.2317	0.104*
C206	0.6354 (7)	0.2686 (5)	0.2019 (4)	0.062 (3)
H206	0.6340	0.2275	0.2233	0.074*
C211	0.9909 (7)	0.0667 (4)	0.2439 (3)	0.0443 (18)
C212	1.0872 (7)	0.0462 (4)	0.2574 (4)	0.049 (2)
H212	1.1052	0.0513	0.2857	0.058*
C213	1.1560 (9)	0.0182 (5)	0.2281 (4)	0.062 (3)
H213	1.2203	0.0048	0.2372	0.075*
C214	1.1319 (10)	0.0101 (5)	0.1871 (4)	0.072 (3)

H214	1.1797	−0.0080	0.1677	0.086*
C215	1.0343 (13)	0.0291 (6)	0.1736 (5)	0.083 (4)
H215	1.0160	0.0221	0.1459	0.099*
C216	0.9649 (9)	0.0583 (5)	0.2017 (4)	0.062 (3)
H216	0.9012	0.0722	0.1922	0.074*
C221	0.7505 (6)	0.1336 (4)	0.3154 (3)	0.0341 (15)
C222	0.6784 (7)	0.0820 (5)	0.3385 (4)	0.051 (2)
H222	0.6981	0.0418	0.3377	0.061*
C223	0.5787 (7)	0.0889 (5)	0.3625 (4)	0.058 (2)
H223	0.5310	0.0539	0.3771	0.069*
C224	0.5507 (8)	0.1474 (5)	0.3647 (4)	0.065 (3)
H224	0.4830	0.1528	0.3803	0.078*
C225	0.6214 (10)	0.1981 (5)	0.3440 (5)	0.090 (5)
H225	0.6021	0.2377	0.3467	0.108*
C226	0.7209 (8)	0.1923 (5)	0.3193 (4)	0.063 (3)
H226	0.7680	0.2277	0.3052	0.075*
C231	1.2017 (7)	0.0948 (4)	0.3484 (4)	0.051 (2)
C232	1.2911 (8)	0.1118 (6)	0.3122 (4)	0.063 (3)
H232	1.3010	0.1532	0.2908	0.076*
C233	1.3675 (10)	0.0675 (7)	0.3073 (6)	0.087 (4)
H233	1.4271	0.0789	0.2823	0.105*
C234	1.3527 (12)	0.0057 (7)	0.3406 (7)	0.093 (5)
H234	1.4024	−0.0242	0.3377	0.111*
C235	1.2655 (11)	−0.0104 (6)	0.3774 (6)	0.085 (4)
H235	1.2575	−0.0509	0.4002	0.102*
C236	1.1899 (9)	0.0324 (5)	0.3812 (5)	0.068 (3)
H236	1.1297	0.0201	0.4057	0.081*
C241	0.9942 (7)	0.1796 (5)	0.4103 (3)	0.047 (2)
C242	1.0056 (9)	0.1470 (6)	0.4588 (4)	0.068 (3)
H242	1.0575	0.1176	0.4647	0.081*
C243	0.9389 (10)	0.1589 (8)	0.4981 (4)	0.085 (4)
H243	0.9467	0.1369	0.5301	0.102*
C244	0.8630 (10)	0.2015 (7)	0.4912 (4)	0.079 (4)
H244	0.8190	0.2083	0.5182	0.095*
C245	0.8512 (9)	0.2346 (5)	0.4442 (4)	0.063 (3)
H245	0.8001	0.2647	0.4395	0.076*
C246	0.9144 (8)	0.2240 (5)	0.4033 (4)	0.058 (2)
H246	0.9042	0.2460	0.3717	0.069*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0393 (3)	0.0463 (3)	0.0369 (2)	−0.0038 (2)	−0.0011 (2)	−0.0105 (2)
Sn2	0.0409 (3)	0.0325 (2)	0.0440 (3)	0.00332 (19)	−0.0103 (2)	−0.0128 (2)
Sn3	0.0433 (3)	0.0479 (3)	0.0354 (2)	−0.0048 (2)	0.0008 (2)	−0.0152 (2)
Sn4	0.0445 (3)	0.0325 (2)	0.0388 (2)	0.0047 (2)	−0.0107 (2)	−0.01275 (19)
Sn5	0.0436 (3)	0.0432 (3)	0.0358 (2)	0.0043 (2)	−0.0069 (2)	−0.0149 (2)
Sn6	0.0393 (2)	0.0316 (2)	0.0386 (2)	−0.00328 (19)	0.00257 (19)	−0.01300 (19)

Sn7	0.0387 (3)	0.0444 (3)	0.0370 (2)	0.0014 (2)	−0.0065 (2)	−0.0077 (2)
Sn8	0.0356 (2)	0.0324 (2)	0.0421 (3)	−0.00186 (19)	0.00093 (19)	−0.0123 (2)
Cl1	0.096 (3)	0.193 (5)	0.068 (2)	−0.042 (3)	−0.0097 (18)	0.003 (3)
Cl2	0.0784 (18)	0.103 (2)	0.098 (2)	0.0123 (17)	−0.0334 (17)	−0.059 (2)
Cl3	0.120 (3)	0.0676 (19)	0.120 (3)	−0.0009 (19)	−0.056 (2)	−0.0277 (19)
Cl11	0.0672 (16)	0.108 (2)	0.095 (2)	0.0040 (16)	0.0029 (15)	−0.060 (2)
Cl12	0.095 (2)	0.074 (2)	0.143 (4)	0.0091 (18)	0.021 (2)	−0.035 (2)
Cl13	0.101 (3)	0.213 (6)	0.0637 (19)	0.032 (3)	−0.0133 (19)	−0.008 (3)
Cl21	0.144 (5)	0.207 (7)	0.189 (6)	0.019 (5)	−0.065 (5)	−0.076 (6)
Cl22	0.238 (8)	0.149 (5)	0.204 (7)	0.067 (5)	−0.140 (6)	−0.089 (5)
Cl23	0.171 (5)	0.172 (5)	0.079 (2)	−0.051 (4)	−0.003 (3)	−0.028 (3)
O1	0.033 (2)	0.034 (3)	0.029 (2)	0.002 (2)	0.0024 (19)	−0.0066 (19)
O2	0.035 (3)	0.044 (3)	0.029 (2)	−0.005 (2)	0.007 (2)	−0.007 (2)
O3	0.038 (3)	0.037 (3)	0.033 (2)	−0.004 (2)	−0.007 (2)	−0.014 (2)
O4	0.040 (3)	0.035 (3)	0.031 (2)	−0.009 (2)	−0.005 (2)	−0.006 (2)
O11	0.047 (3)	0.035 (3)	0.038 (3)	0.004 (2)	−0.007 (2)	−0.005 (2)
O18	0.061 (4)	0.069 (5)	0.060 (4)	0.011 (3)	−0.002 (3)	−0.026 (4)
O19	0.066 (5)	0.059 (5)	0.086 (5)	0.018 (4)	−0.006 (4)	−0.017 (4)
O21	0.050 (3)	0.050 (3)	0.036 (3)	−0.002 (3)	−0.009 (2)	−0.011 (2)
O28	0.107 (7)	0.108 (8)	0.051 (4)	0.032 (6)	−0.023 (5)	−0.005 (5)
O29	0.099 (7)	0.058 (5)	0.077 (5)	0.020 (5)	−0.008 (5)	0.009 (4)
O31	0.055 (3)	0.031 (3)	0.046 (3)	0.001 (2)	−0.004 (3)	−0.009 (2)
O38	0.092 (6)	0.066 (5)	0.103 (7)	0.035 (5)	0.001 (5)	−0.005 (5)
O39	0.060 (5)	0.091 (7)	0.127 (8)	0.021 (5)	0.011 (5)	−0.009 (6)
O41	0.051 (3)	0.053 (3)	0.037 (3)	0.004 (3)	−0.005 (2)	−0.014 (3)
O48	0.103 (7)	0.055 (5)	0.080 (6)	0.017 (5)	−0.002 (5)	−0.006 (4)
O49	0.138 (9)	0.074 (6)	0.056 (5)	0.019 (6)	0.011 (5)	0.004 (4)
O131	0.053 (3)	0.035 (3)	0.046 (3)	−0.003 (2)	−0.011 (3)	−0.008 (2)
O138	0.091 (6)	0.059 (5)	0.104 (7)	−0.027 (4)	−0.019 (5)	−0.007 (5)
O139	0.067 (5)	0.084 (6)	0.104 (7)	−0.020 (4)	−0.020 (5)	−0.022 (5)
O141	0.052 (3)	0.043 (3)	0.028 (2)	0.002 (2)	0.000 (2)	−0.009 (2)
O148	0.095 (6)	0.054 (5)	0.089 (6)	−0.016 (4)	0.015 (5)	−0.010 (4)
O149	0.264 (17)	0.099 (8)	0.069 (6)	−0.081 (10)	0.043 (8)	−0.012 (6)
O151	0.046 (3)	0.042 (3)	0.041 (3)	−0.006 (2)	−0.007 (2)	−0.002 (2)
O158	0.072 (5)	0.071 (5)	0.057 (4)	−0.013 (4)	−0.017 (3)	−0.022 (4)
O159	0.069 (4)	0.050 (4)	0.079 (5)	−0.018 (3)	−0.008 (4)	−0.015 (4)
O161	0.047 (3)	0.041 (3)	0.033 (3)	0.003 (2)	−0.005 (2)	−0.008 (2)
O168	0.098 (6)	0.108 (7)	0.051 (4)	−0.048 (6)	0.009 (4)	−0.010 (4)
O169	0.087 (6)	0.060 (5)	0.082 (6)	−0.030 (4)	−0.006 (5)	0.011 (4)
N17	0.060 (5)	0.056 (5)	0.056 (4)	0.014 (4)	−0.011 (4)	−0.029 (4)
N27	0.054 (5)	0.077 (6)	0.051 (5)	0.018 (4)	0.005 (4)	0.006 (4)
N37	0.069 (6)	0.060 (5)	0.072 (6)	0.024 (5)	−0.018 (5)	−0.022 (5)
N47	0.090 (7)	0.063 (6)	0.058 (5)	−0.001 (5)	−0.002 (5)	0.001 (4)
N137	0.056 (5)	0.063 (5)	0.066 (5)	−0.007 (4)	−0.009 (4)	−0.023 (4)
N147	0.114 (9)	0.061 (6)	0.059 (6)	−0.026 (6)	0.008 (6)	−0.001 (5)
N157	0.047 (4)	0.045 (4)	0.056 (4)	−0.004 (3)	0.000 (3)	−0.024 (3)
N167	0.069 (6)	0.078 (7)	0.046 (5)	−0.031 (5)	−0.016 (4)	0.006 (4)
C1	0.053 (5)	0.059 (6)	0.067 (6)	0.006 (4)	−0.018 (5)	−0.024 (5)

C2	0.049 (5)	0.069 (7)	0.059 (6)	0.001 (5)	−0.005 (4)	−0.019 (5)
C3	0.167 (19)	0.137 (16)	0.090 (11)	−0.006 (14)	−0.047 (12)	−0.047 (11)
C11	0.043 (4)	0.033 (4)	0.038 (4)	0.000 (3)	−0.005 (3)	−0.010 (3)
C12	0.050 (5)	0.040 (4)	0.045 (4)	−0.001 (4)	−0.005 (4)	−0.013 (3)
C13	0.049 (4)	0.044 (4)	0.039 (4)	0.005 (4)	−0.005 (3)	−0.016 (3)
C14	0.042 (4)	0.053 (5)	0.041 (4)	0.008 (4)	−0.011 (3)	−0.023 (4)
C15	0.061 (5)	0.044 (5)	0.050 (5)	0.012 (4)	−0.016 (4)	−0.012 (4)
C16	0.049 (5)	0.040 (4)	0.040 (4)	0.001 (4)	−0.008 (3)	−0.002 (3)
C21	0.033 (3)	0.040 (4)	0.037 (4)	0.003 (3)	0.000 (3)	−0.007 (3)
C22	0.039 (4)	0.037 (4)	0.055 (5)	0.005 (3)	−0.005 (3)	−0.018 (4)
C23	0.045 (5)	0.047 (5)	0.059 (5)	−0.001 (4)	0.001 (4)	−0.006 (4)
C24	0.047 (5)	0.057 (5)	0.038 (4)	0.017 (4)	0.004 (4)	0.001 (4)
C25	0.052 (5)	0.069 (6)	0.047 (5)	0.014 (4)	−0.015 (4)	−0.018 (4)
C26	0.044 (4)	0.043 (4)	0.047 (4)	0.003 (3)	−0.008 (3)	−0.013 (4)
C31	0.055 (5)	0.036 (4)	0.046 (4)	−0.001 (4)	−0.005 (4)	−0.018 (3)
C32	0.052 (5)	0.046 (5)	0.057 (5)	−0.003 (4)	−0.008 (4)	−0.010 (4)
C33	0.040 (4)	0.061 (6)	0.057 (5)	0.000 (4)	−0.004 (4)	−0.017 (4)
C34	0.059 (5)	0.046 (5)	0.055 (5)	0.010 (4)	−0.015 (4)	−0.018 (4)
C35	0.064 (6)	0.045 (5)	0.054 (5)	0.006 (4)	−0.008 (4)	−0.010 (4)
C36	0.060 (5)	0.033 (4)	0.057 (5)	0.006 (4)	−0.005 (4)	−0.015 (4)
C41	0.048 (4)	0.044 (4)	0.040 (4)	0.010 (4)	−0.011 (3)	−0.011 (3)
C42	0.057 (5)	0.050 (5)	0.049 (5)	0.000 (4)	0.005 (4)	−0.014 (4)
C43	0.057 (5)	0.055 (6)	0.050 (5)	0.010 (4)	−0.001 (4)	−0.012 (4)
C44	0.064 (6)	0.045 (5)	0.054 (5)	0.002 (4)	−0.001 (4)	−0.007 (4)
C45	0.080 (7)	0.061 (6)	0.046 (5)	−0.003 (5)	0.011 (5)	−0.010 (4)
C46	0.078 (7)	0.053 (5)	0.037 (4)	0.004 (5)	0.003 (4)	−0.008 (4)
C51	0.047 (4)	0.060 (5)	0.036 (4)	0.009 (4)	−0.002 (3)	−0.021 (4)
C52	0.055 (5)	0.057 (5)	0.051 (5)	0.012 (4)	−0.011 (4)	−0.019 (4)
C53	0.065 (6)	0.063 (6)	0.071 (7)	0.010 (5)	−0.017 (5)	−0.030 (5)
C54	0.081 (8)	0.121 (11)	0.059 (6)	0.029 (8)	−0.021 (6)	−0.050 (7)
C55	0.066 (7)	0.123 (11)	0.044 (5)	−0.003 (7)	−0.001 (5)	−0.024 (6)
C56	0.050 (5)	0.090 (8)	0.043 (5)	−0.001 (5)	0.005 (4)	−0.014 (5)
C61	0.037 (4)	0.046 (5)	0.074 (6)	−0.010 (4)	0.003 (4)	−0.027 (4)
C62	0.043 (5)	0.050 (6)	0.099 (8)	−0.003 (4)	0.005 (5)	−0.020 (6)
C63	0.050 (6)	0.053 (6)	0.144 (13)	−0.008 (5)	0.007 (7)	−0.031 (7)
C64	0.048 (6)	0.100 (11)	0.169 (16)	−0.014 (7)	0.010 (8)	−0.086 (11)
C65	0.052 (6)	0.116 (12)	0.111 (10)	0.002 (7)	−0.019 (6)	−0.064 (9)
C66	0.045 (5)	0.076 (7)	0.087 (8)	0.004 (5)	−0.011 (5)	−0.039 (6)
C71	0.036 (4)	0.045 (4)	0.038 (4)	−0.003 (3)	−0.003 (3)	−0.012 (3)
C72	0.064 (6)	0.047 (5)	0.045 (4)	0.001 (4)	−0.010 (4)	−0.016 (4)
C73	0.069 (7)	0.070 (7)	0.066 (6)	−0.015 (5)	−0.021 (5)	−0.022 (5)
C74	0.049 (5)	0.080 (7)	0.060 (6)	−0.001 (5)	−0.021 (4)	−0.017 (5)
C75	0.054 (5)	0.057 (6)	0.076 (7)	0.020 (5)	−0.023 (5)	−0.017 (5)
C76	0.039 (4)	0.049 (5)	0.063 (5)	0.013 (4)	−0.015 (4)	−0.012 (4)
C81	0.046 (4)	0.031 (4)	0.052 (5)	−0.003 (3)	−0.009 (4)	−0.013 (3)
C82	0.061 (5)	0.050 (5)	0.063 (5)	−0.008 (4)	−0.002 (4)	−0.037 (4)
C83	0.086 (8)	0.088 (9)	0.065 (6)	−0.016 (7)	0.002 (6)	−0.048 (6)
C84	0.083 (7)	0.072 (7)	0.061 (6)	−0.020 (6)	−0.005 (5)	−0.037 (5)

C85	0.047 (5)	0.054 (5)	0.063 (6)	−0.008 (4)	−0.013 (4)	−0.019 (4)
C86	0.060 (5)	0.038 (4)	0.051 (5)	−0.005 (4)	−0.009 (4)	−0.022 (4)
C91	0.042 (4)	0.038 (4)	0.050 (4)	−0.007 (3)	0.001 (3)	−0.023 (4)
C92	0.051 (5)	0.057 (6)	0.059 (5)	−0.008 (4)	−0.007 (4)	−0.017 (5)
C93	0.057 (6)	0.076 (7)	0.061 (6)	−0.009 (5)	−0.009 (5)	−0.023 (5)
C94	0.064 (6)	0.068 (7)	0.084 (8)	−0.017 (5)	−0.010 (6)	−0.033 (6)
C95	0.082 (8)	0.060 (6)	0.063 (6)	−0.025 (6)	−0.004 (6)	−0.014 (5)
C96	0.061 (5)	0.041 (5)	0.052 (5)	−0.006 (4)	0.000 (4)	−0.010 (4)
C101	0.062 (5)	0.051 (5)	0.033 (4)	−0.002 (4)	0.003 (4)	−0.019 (4)
C102	0.050 (5)	0.071 (6)	0.058 (5)	0.008 (4)	−0.015 (4)	−0.036 (5)
C103	0.070 (7)	0.092 (8)	0.057 (6)	0.001 (6)	−0.019 (5)	−0.038 (6)
C104	0.093 (8)	0.085 (8)	0.058 (6)	0.009 (7)	−0.027 (6)	−0.040 (6)
C105	0.096 (9)	0.083 (8)	0.052 (6)	0.029 (7)	−0.014 (6)	−0.034 (6)
C106	0.076 (7)	0.067 (6)	0.046 (5)	0.018 (5)	−0.012 (5)	−0.027 (5)
C111	0.054 (4)	0.025 (3)	0.037 (4)	−0.001 (3)	−0.013 (3)	−0.010 (3)
C112	0.052 (5)	0.039 (4)	0.063 (5)	0.002 (4)	−0.011 (4)	−0.025 (4)
C113	0.059 (6)	0.051 (6)	0.076 (7)	−0.002 (4)	−0.020 (5)	−0.021 (5)
C114	0.092 (8)	0.048 (5)	0.059 (6)	0.003 (5)	−0.033 (5)	−0.024 (4)
C115	0.092 (8)	0.052 (6)	0.050 (5)	−0.006 (5)	−0.005 (5)	−0.027 (4)
C116	0.051 (5)	0.039 (4)	0.046 (4)	0.002 (4)	−0.001 (4)	−0.014 (4)
C121	0.039 (4)	0.051 (5)	0.040 (4)	0.005 (3)	−0.007 (3)	−0.018 (4)
C122	0.069 (6)	0.053 (6)	0.065 (6)	−0.009 (5)	−0.022 (5)	−0.026 (5)
C123	0.076 (8)	0.096 (10)	0.095 (9)	−0.005 (7)	−0.042 (7)	−0.041 (8)
C124	0.068 (7)	0.133 (13)	0.075 (8)	0.005 (8)	−0.038 (6)	−0.038 (8)
C125	0.075 (8)	0.104 (11)	0.067 (7)	0.012 (7)	−0.034 (6)	0.000 (7)
C126	0.047 (5)	0.074 (7)	0.051 (5)	0.013 (4)	−0.022 (4)	−0.011 (5)
C131	0.044 (4)	0.040 (4)	0.039 (4)	0.003 (3)	−0.008 (3)	−0.015 (3)
C132	0.067 (6)	0.038 (4)	0.045 (4)	−0.009 (4)	−0.014 (4)	−0.010 (4)
C133	0.057 (5)	0.043 (5)	0.053 (5)	−0.011 (4)	−0.007 (4)	−0.014 (4)
C134	0.046 (4)	0.046 (5)	0.055 (5)	−0.005 (4)	0.004 (4)	−0.023 (4)
C135	0.047 (5)	0.048 (5)	0.051 (5)	0.002 (4)	−0.004 (4)	−0.011 (4)
C136	0.052 (5)	0.032 (4)	0.056 (5)	0.000 (3)	−0.004 (4)	−0.015 (4)
C141	0.044 (4)	0.042 (4)	0.039 (4)	−0.007 (3)	−0.004 (3)	−0.013 (3)
C142	0.105 (9)	0.044 (5)	0.044 (5)	0.003 (5)	0.009 (5)	−0.012 (4)
C143	0.078 (7)	0.039 (5)	0.055 (5)	0.000 (5)	0.005 (5)	−0.012 (4)
C144	0.070 (7)	0.057 (6)	0.055 (6)	−0.017 (5)	0.002 (5)	−0.006 (5)
C145	0.177 (16)	0.085 (9)	0.050 (6)	−0.068 (10)	0.035 (8)	−0.029 (6)
C146	0.142 (12)	0.064 (7)	0.046 (5)	−0.034 (8)	0.020 (7)	−0.023 (5)
C151	0.040 (4)	0.036 (4)	0.037 (4)	0.001 (3)	−0.004 (3)	−0.010 (3)
C152	0.045 (4)	0.034 (4)	0.042 (4)	0.002 (3)	0.000 (3)	−0.011 (3)
C153	0.051 (5)	0.048 (5)	0.040 (4)	0.005 (4)	−0.005 (3)	−0.015 (4)
C154	0.040 (4)	0.049 (5)	0.047 (4)	0.003 (4)	0.002 (3)	−0.021 (4)
C155	0.060 (5)	0.040 (4)	0.048 (5)	−0.014 (4)	0.008 (4)	−0.009 (4)
C156	0.046 (4)	0.040 (4)	0.043 (4)	−0.004 (3)	−0.008 (3)	−0.003 (3)
C161	0.034 (4)	0.038 (4)	0.039 (4)	−0.002 (3)	−0.012 (3)	−0.009 (3)
C162	0.043 (4)	0.047 (5)	0.046 (4)	−0.004 (4)	−0.010 (3)	−0.010 (4)
C163	0.045 (5)	0.049 (5)	0.062 (5)	−0.006 (4)	−0.017 (4)	−0.008 (4)
C164	0.051 (5)	0.056 (5)	0.040 (4)	−0.018 (4)	−0.015 (4)	0.003 (4)

C165	0.056 (5)	0.067 (6)	0.040 (4)	−0.017 (5)	0.001 (4)	−0.023 (4)
C166	0.047 (5)	0.044 (5)	0.053 (5)	−0.004 (4)	−0.002 (4)	−0.017 (4)
C171	0.029 (3)	0.047 (4)	0.040 (4)	−0.001 (3)	−0.005 (3)	−0.012 (3)
C172	0.039 (4)	0.069 (7)	0.057 (5)	−0.014 (4)	0.002 (4)	−0.003 (5)
C173	0.049 (6)	0.092 (10)	0.096 (9)	−0.013 (6)	0.023 (6)	0.008 (8)
C174	0.052 (6)	0.103 (11)	0.100 (10)	0.010 (7)	0.027 (7)	−0.020 (8)
C175	0.056 (6)	0.072 (8)	0.098 (9)	0.025 (6)	0.008 (6)	−0.021 (7)
C176	0.049 (5)	0.053 (5)	0.066 (6)	0.006 (4)	0.012 (4)	−0.016 (5)
C181	0.050 (4)	0.027 (3)	0.040 (4)	−0.004 (3)	0.002 (3)	−0.015 (3)
C182	0.060 (5)	0.034 (4)	0.058 (5)	0.008 (4)	−0.006 (4)	−0.022 (4)
C183	0.097 (8)	0.050 (5)	0.043 (5)	0.004 (5)	−0.006 (5)	−0.024 (4)
C184	0.063 (6)	0.048 (5)	0.062 (6)	0.009 (4)	0.011 (5)	−0.024 (4)
C185	0.056 (5)	0.050 (5)	0.072 (6)	0.007 (4)	−0.002 (5)	−0.024 (5)
C186	0.040 (4)	0.044 (5)	0.056 (5)	0.005 (3)	0.000 (4)	−0.019 (4)
C191	0.063 (5)	0.050 (5)	0.034 (4)	−0.010 (4)	0.000 (4)	−0.017 (4)
C192	0.070 (7)	0.108 (10)	0.057 (6)	−0.017 (7)	0.004 (5)	−0.045 (6)
C193	0.094 (9)	0.123 (11)	0.056 (6)	−0.036 (8)	0.013 (6)	−0.059 (7)
C194	0.099 (9)	0.074 (8)	0.058 (6)	−0.007 (7)	0.021 (6)	−0.036 (6)
C195	0.077 (8)	0.103 (10)	0.078 (8)	0.028 (7)	−0.001 (6)	−0.055 (8)
C196	0.056 (6)	0.104 (10)	0.075 (7)	0.025 (6)	−0.012 (5)	−0.050 (7)
C201	0.045 (4)	0.041 (4)	0.047 (4)	0.009 (3)	−0.013 (3)	−0.018 (3)
C202	0.063 (6)	0.051 (6)	0.066 (6)	0.008 (5)	−0.008 (5)	−0.012 (5)
C203	0.082 (8)	0.066 (7)	0.097 (9)	0.027 (6)	−0.024 (7)	−0.024 (7)
C204	0.077 (8)	0.090 (10)	0.147 (14)	0.042 (8)	−0.033 (9)	−0.073 (10)
C205	0.067 (7)	0.068 (8)	0.121 (11)	0.004 (6)	0.025 (7)	−0.047 (8)
C206	0.041 (5)	0.057 (6)	0.087 (7)	0.009 (4)	−0.003 (5)	−0.027 (5)
C211	0.046 (4)	0.037 (4)	0.051 (4)	0.000 (3)	0.001 (4)	−0.020 (4)
C212	0.049 (5)	0.035 (4)	0.060 (5)	0.003 (3)	−0.003 (4)	−0.016 (4)
C213	0.065 (6)	0.051 (6)	0.063 (6)	0.019 (5)	−0.002 (5)	−0.011 (5)
C214	0.086 (8)	0.056 (6)	0.070 (7)	0.029 (6)	0.001 (6)	−0.023 (5)
C215	0.123 (11)	0.066 (7)	0.066 (7)	0.018 (7)	−0.007 (7)	−0.036 (6)
C216	0.078 (7)	0.054 (6)	0.069 (6)	0.014 (5)	−0.016 (5)	−0.038 (5)
C221	0.029 (3)	0.040 (4)	0.034 (3)	0.007 (3)	−0.008 (3)	−0.012 (3)
C222	0.037 (4)	0.047 (5)	0.065 (5)	−0.004 (4)	−0.003 (4)	−0.015 (4)
C223	0.043 (5)	0.055 (6)	0.064 (6)	−0.009 (4)	0.003 (4)	−0.008 (5)
C224	0.043 (5)	0.071 (7)	0.069 (6)	0.006 (5)	0.007 (4)	−0.014 (5)
C225	0.081 (8)	0.047 (6)	0.119 (10)	0.018 (6)	0.041 (8)	−0.028 (6)
C226	0.058 (6)	0.041 (5)	0.079 (7)	−0.005 (4)	0.023 (5)	−0.022 (5)
C231	0.045 (4)	0.043 (5)	0.072 (6)	0.010 (4)	−0.025 (4)	−0.019 (4)
C232	0.046 (5)	0.070 (7)	0.082 (7)	0.018 (5)	−0.021 (5)	−0.031 (6)
C233	0.055 (6)	0.108 (11)	0.127 (12)	0.025 (7)	−0.026 (7)	−0.074 (10)
C234	0.082 (9)	0.074 (9)	0.156 (15)	0.037 (7)	−0.063 (10)	−0.062 (10)
C235	0.082 (9)	0.049 (6)	0.144 (13)	0.018 (6)	−0.069 (9)	−0.032 (7)
C236	0.062 (6)	0.051 (6)	0.098 (8)	0.006 (5)	−0.041 (6)	−0.020 (6)
C241	0.044 (4)	0.057 (5)	0.037 (4)	−0.010 (4)	−0.003 (3)	−0.014 (4)
C242	0.062 (6)	0.099 (9)	0.044 (5)	0.003 (6)	−0.023 (4)	−0.017 (5)
C243	0.071 (7)	0.144 (13)	0.043 (5)	0.008 (8)	−0.012 (5)	−0.032 (7)
C244	0.067 (7)	0.115 (11)	0.064 (7)	−0.010 (7)	0.008 (5)	−0.054 (7)

C245	0.064 (6)	0.059 (6)	0.070 (6)	−0.003 (5)	0.004 (5)	−0.037 (5)
C246	0.066 (6)	0.052 (5)	0.055 (5)	−0.003 (5)	0.005 (4)	−0.025 (4)

Geometric parameters (Å, º)

Sn1—O1	1.993 (4)	C92—H92	0.9300
Sn1—O11	2.071 (5)	C92—C93	1.372 (14)
Sn1—O21	2.293 (6)	C93—H93	0.9300
Sn1—C51	2.087 (9)	C93—C94	1.395 (15)
Sn1—C61	2.127 (8)	C94—H94	0.9300
Sn2—O1	2.049 (5)	C94—C95	1.369 (17)
Sn2—O2	2.112 (5)	C95—H95	0.9300
Sn2—O21	2.243 (6)	C95—C96	1.395 (14)
Sn2—C71	2.090 (8)	C96—H96	0.9300
Sn2—C81	2.113 (8)	C101—C102	1.409 (14)
Sn3—O2	1.995 (4)	C101—C106	1.394 (13)
Sn3—O31	2.095 (6)	C102—H102	0.9300
Sn3—O41	2.268 (6)	C102—C103	1.409 (13)
Sn3—C91	2.103 (8)	C103—H103	0.9300
Sn3—C101	2.096 (9)	C103—C104	1.366 (16)
Sn4—O1	2.098 (5)	C104—H104	0.9300
Sn4—O2	2.029 (6)	C104—C105	1.380 (17)
Sn4—O41	2.305 (6)	C105—H105	0.9300
Sn4—C111	2.102 (7)	C105—C106	1.381 (15)
Sn4—C121	2.112 (8)	C106—H106	0.9300
Sn5—O3	2.011 (5)	C111—C112	1.408 (12)
Sn5—O131	2.099 (5)	C111—C116	1.398 (11)
Sn5—O141	2.303 (6)	C112—H112	0.9300
Sn5—C191	2.101 (8)	C112—C113	1.377 (13)
Sn5—C201	2.094 (8)	C113—H113	0.9300
Sn6—O3	2.031 (5)	C113—C114	1.388 (16)
Sn6—O4	2.089 (5)	C114—H114	0.9300
Sn6—O141	2.266 (6)	C114—C115	1.367 (16)
Sn6—C171	2.117 (7)	C115—H115	0.9300
Sn6—C181	2.125 (7)	C115—C116	1.407 (13)
Sn7—O4	2.011 (5)	C116—H116	0.9300
Sn7—O151	2.081 (5)	C121—C122	1.378 (13)
Sn7—O161	2.290 (6)	C121—C126	1.406 (13)
Sn7—C231	2.106 (9)	C122—H122	0.9300
Sn7—C241	2.074 (8)	C122—C123	1.389 (15)
Sn8—O3	2.103 (5)	C123—H123	0.9300
Sn8—O4	2.040 (5)	C123—C124	1.370 (19)
Sn8—O161	2.243 (5)	C124—H124	0.9300
Sn8—C211	2.130 (8)	C124—C125	1.35 (2)
Sn8—C221	2.095 (7)	C125—H125	0.9300
Cl1—C1	1.708 (11)	C125—C126	1.377 (15)
Cl2—C1	1.746 (10)	C126—H126	0.9300
Cl3—C1	1.759 (11)	C131—C132	1.427 (11)

Cl11—C2	1.741 (10)	C131—C136	1.412 (12)
Cl12—C2	1.745 (12)	C132—H132	0.9300
Cl13—C2	1.723 (11)	C132—C133	1.380 (12)
Cl21—C3	1.71 (2)	C133—H133	0.9300
Cl22—C3	1.75 (2)	C133—C134	1.394 (14)
Cl23—C3	1.699 (16)	C134—C135	1.401 (12)
O11—C11	1.328 (10)	C135—H135	0.9300
O18—N17	1.231 (11)	C135—C136	1.386 (13)
O19—N17	1.228 (11)	C136—H136	0.9300
O21—C21	1.360 (10)	C141—C142	1.376 (13)
O28—N27	1.215 (14)	C141—C146	1.375 (13)
O29—N27	1.244 (13)	C142—H142	0.9300
O31—C31	1.317 (11)	C142—C143	1.391 (13)
O38—N37	1.225 (12)	C143—H143	0.9300
O39—N37	1.221 (13)	C143—C144	1.358 (14)
O41—C41	1.364 (10)	C144—C145	1.357 (17)
O48—N47	1.227 (13)	C145—H145	0.9300
O49—N47	1.219 (13)	C145—C146	1.403 (15)
O131—C131	1.318 (10)	C146—H146	0.9300
O138—N137	1.214 (12)	C151—C152	1.404 (12)
O139—N137	1.240 (12)	C151—C156	1.424 (10)
O141—C141	1.356 (10)	C152—H152	0.9300
O148—N147	1.215 (13)	C152—C153	1.363 (12)
O149—N147	1.228 (14)	C153—H153	0.9300
O151—C151	1.322 (10)	C153—C154	1.379 (12)
O158—N157	1.231 (11)	C154—C155	1.385 (13)
O159—N157	1.222 (10)	C155—H155	0.9300
O161—C161	1.356 (9)	C155—C156	1.372 (13)
O168—N167	1.226 (14)	C156—H156	0.9300
O169—N167	1.240 (13)	C161—C162	1.395 (12)
N17—C14	1.462 (11)	C161—C166	1.401 (12)
N27—C24	1.447 (12)	C162—H162	0.9300
N37—C34	1.448 (13)	C162—C163	1.386 (12)
N47—C44	1.459 (13)	C163—H163	0.9300
N137—C134	1.437 (12)	C163—C164	1.381 (14)
N147—C144	1.469 (12)	C164—C165	1.389 (14)
N157—C154	1.455 (11)	C165—H165	0.9300
N167—C164	1.465 (11)	C165—C166	1.391 (12)
C1—H1	0.9800	C166—H166	0.9300
C2—H2	0.9800	C171—C172	1.402 (12)
C3—H3	0.9800	C171—C176	1.379 (13)
C11—C12	1.392 (11)	C172—H172	0.9300
C11—C16	1.419 (11)	C172—C173	1.389 (15)
C12—H12	0.9300	C173—H173	0.9300
C12—C13	1.379 (12)	C173—C174	1.388 (19)
C13—H13	0.9300	C174—H174	0.9300
C13—C14	1.374 (12)	C174—C175	1.333 (18)
C14—C15	1.397 (13)	C175—H175	0.9300

C15—H15	0.9300	C175—C176	1.393 (13)
C15—C16	1.376 (13)	C176—H176	0.9300
C16—H16	0.9300	C181—C182	1.387 (12)
C21—C22	1.407 (11)	C181—C186	1.408 (12)
C21—C26	1.395 (12)	C182—H182	0.9300
C22—H22	0.9300	C182—C183	1.407 (12)
C22—C23	1.394 (13)	C183—H183	0.9300
C23—H23	0.9300	C183—C184	1.377 (16)
C23—C24	1.389 (15)	C184—H184	0.9300
C24—C25	1.386 (14)	C184—C185	1.384 (15)
C25—H25	0.9300	C185—H185	0.9300
C25—C26	1.385 (13)	C185—C186	1.390 (12)
C26—H26	0.9300	C186—H186	0.9300
C31—C32	1.402 (12)	C191—C192	1.383 (13)
C31—C36	1.430 (12)	C191—C196	1.391 (14)
C32—H32	0.9300	C192—H192	0.9300
C32—C33	1.410 (13)	C192—C193	1.381 (16)
C33—H33	0.9300	C193—H193	0.9300
C33—C34	1.383 (13)	C193—C194	1.366 (19)
C34—C35	1.380 (14)	C194—H194	0.9300
C35—H35	0.9300	C194—C195	1.351 (18)
C35—C36	1.386 (13)	C195—H195	0.9300
C36—H36	0.9300	C195—C196	1.385 (14)
C41—C42	1.401 (12)	C196—H196	0.9300
C41—C46	1.394 (12)	C201—C202	1.398 (13)
C42—H42	0.9300	C201—C206	1.406 (13)
C42—C43	1.393 (13)	C202—H202	0.9300
C43—H43	0.9300	C202—C203	1.401 (16)
C43—C44	1.389 (13)	C203—H203	0.9300
C44—C45	1.383 (15)	C203—C204	1.37 (2)
C45—H45	0.9300	C204—H204	0.9300
C45—C46	1.368 (14)	C204—C205	1.38 (2)
C46—H46	0.9300	C205—H205	0.9300
C51—C52	1.403 (13)	C205—C206	1.362 (15)
C51—C56	1.406 (12)	C206—H206	0.9300
C52—H52	0.9300	C211—C212	1.394 (13)
C52—C53	1.400 (14)	C211—C216	1.385 (13)
C53—H53	0.9300	C212—H212	0.9300
C53—C54	1.368 (17)	C212—C213	1.390 (13)
C54—H54	0.9300	C213—H213	0.9300
C54—C55	1.376 (18)	C213—C214	1.341 (16)
C55—H55	0.9300	C214—H214	0.9300
C55—C56	1.392 (15)	C214—C215	1.403 (19)
C56—H56	0.9300	C215—H215	0.9300
C61—C62	1.385 (14)	C215—C216	1.390 (15)
C61—C66	1.390 (15)	C216—H216	0.9300
C62—H62	0.9300	C221—C222	1.388 (11)
C62—C63	1.373 (16)	C221—C226	1.383 (12)

C63—H63	0.9300	C222—H222	0.9300
C63—C64	1.37 (2)	C222—C223	1.375 (12)
C64—H64	0.9300	C223—H223	0.9300
C64—C65	1.43 (2)	C223—C224	1.357 (15)
C65—H65	0.9300	C224—H224	0.9300
C65—C66	1.394 (16)	C224—C225	1.358 (15)
C66—H66	0.9300	C225—H225	0.9300
C71—C72	1.395 (12)	C225—C226	1.374 (13)
C71—C76	1.383 (12)	C226—H226	0.9300
C72—H72	0.9300	C231—C232	1.375 (15)
C72—C73	1.408 (14)	C231—C236	1.409 (14)
C73—H73	0.9300	C232—H232	0.9300
C73—C74	1.376 (16)	C232—C233	1.404 (15)
C74—H74	0.9300	C233—H233	0.9300
C74—C75	1.373 (15)	C233—C234	1.40 (2)
C75—H75	0.9300	C234—H234	0.9300
C75—C76	1.407 (14)	C234—C235	1.37 (2)
C76—H76	0.9300	C235—H235	0.9300
C81—C82	1.411 (12)	C235—C236	1.367 (17)
C81—C86	1.382 (12)	C236—H236	0.9300
C82—H82	0.9300	C241—C242	1.406 (13)
C82—C83	1.398 (14)	C241—C246	1.414 (14)
C83—H83	0.9300	C242—H242	0.9300
C83—C84	1.391 (16)	C242—C243	1.389 (16)
C84—H84	0.9300	C243—H243	0.9300
C84—C85	1.362 (14)	C243—C244	1.349 (19)
C85—H85	0.9300	C244—H244	0.9300
C85—C86	1.385 (12)	C244—C245	1.372 (17)
C86—H86	0.9300	C245—H245	0.9300
C91—C92	1.407 (14)	C245—C246	1.392 (13)
C91—C96	1.396 (12)	C246—H246	0.9300

O1—Sn1—O11	79.7 (2)	C81—C86—C85	121.2 (9)
O1—Sn1—O21	71.0 (2)	C81—C86—H86	119.4
O1—Sn1—C51	112.9 (3)	C85—C86—H86	119.4
O1—Sn1—C61	115.4 (3)	C92—C91—Sn3	116.6 (6)
O11—Sn1—O21	150.6 (2)	C96—C91—Sn3	123.2 (7)
O11—Sn1—C51	102.1 (3)	C96—C91—C92	120.3 (8)
O11—Sn1—C61	100.1 (3)	C91—C92—H92	120.4
C51—Sn1—O21	91.7 (3)	C93—C92—C91	119.2 (9)
C51—Sn1—C61	129.5 (4)	C93—C92—H92	120.4
C61—Sn1—O21	90.5 (3)	C92—C93—H93	119.6
O1—Sn2—O2	72.52 (19)	C92—C93—C94	120.8 (11)
O1—Sn2—O21	71.1 (2)	C94—C93—H93	119.6
O1—Sn2—C71	113.0 (3)	C93—C94—H94	120.0
O1—Sn2—C81	105.7 (3)	C95—C94—C93	119.9 (10)
O2—Sn2—O21	143.2 (2)	C95—C94—H94	120.0
O2—Sn2—C81	99.3 (3)	C94—C95—H95	119.6

C71—Sn2—O2	97.5 (3)	C94—C95—C96	120.8 (10)
C71—Sn2—O21	91.1 (3)	C96—C95—H95	119.6
C71—Sn2—C81	140.9 (3)	C91—C96—H96	120.5
C81—Sn2—O21	96.1 (3)	C95—C96—C91	118.9 (10)
O2—Sn3—O31	79.0 (2)	C95—C96—H96	120.5
O2—Sn3—O41	71.3 (2)	C102—C101—Sn3	119.8 (6)
O2—Sn3—C91	113.9 (3)	C106—C101—Sn3	121.8 (8)
O2—Sn3—C101	111.7 (3)	C106—C101—C102	118.0 (9)
O31—Sn3—O41	150.3 (2)	C101—C102—H102	120.2
O31—Sn3—C91	96.1 (3)	C103—C102—C101	119.5 (9)
C91—Sn3—O41	94.0 (3)	C103—C102—H102	120.2
C101—Sn3—O31	98.0 (3)	C102—C103—H103	119.6
C101—Sn3—O41	94.8 (3)	C104—C103—C102	120.8 (11)
C101—Sn3—C91	134.0 (3)	C104—C103—H103	119.6
O1—Sn4—O41	143.2 (2)	C103—C104—H104	120.1
O1—Sn4—C111	102.0 (2)	C103—C104—C105	119.8 (10)
O1—Sn4—C121	101.0 (3)	C105—C104—H104	120.1
O2—Sn4—O1	73.19 (19)	C104—C105—H105	119.8
O2—Sn4—O41	70.0 (2)	C104—C105—C106	120.5 (11)
O2—Sn4—C111	111.7 (3)	C106—C105—H105	119.8
O2—Sn4—C121	112.4 (3)	C101—C106—H106	119.4
C111—Sn4—O41	92.3 (3)	C105—C106—C101	121.3 (11)
C111—Sn4—C121	134.4 (3)	C105—C106—H106	119.4
C121—Sn4—O41	92.2 (3)	C112—C111—Sn4	118.4 (6)
O3—Sn5—O131	79.8 (2)	C116—C111—Sn4	123.7 (6)
O3—Sn5—O141	70.83 (19)	C116—C111—C112	117.9 (8)
O3—Sn5—C191	110.1 (3)	C111—C112—H112	119.1
O3—Sn5—C201	113.8 (3)	C113—C112—C111	121.7 (9)
O131—Sn5—O141	150.4 (2)	C113—C112—H112	119.1
O131—Sn5—C191	98.5 (3)	C112—C113—H113	120.7
C191—Sn5—O141	94.6 (3)	C112—C113—C114	118.6 (10)
C201—Sn5—O131	97.7 (3)	C114—C113—H113	120.7
C201—Sn5—O141	91.4 (3)	C113—C114—H114	119.0
C201—Sn5—C191	135.2 (4)	C115—C114—C113	122.1 (9)
O3—Sn6—O4	72.3 (2)	C115—C114—H114	119.0
O3—Sn6—O141	71.3 (2)	C114—C115—H115	120.5
O3—Sn6—C171	113.7 (3)	C114—C115—C116	119.0 (10)
O3—Sn6—C181	111.1 (3)	C116—C115—H115	120.5
O4—Sn6—O141	143.5 (2)	C111—C116—C115	120.6 (9)
O4—Sn6—C171	100.0 (3)	C111—C116—H116	119.7
O4—Sn6—C181	101.4 (3)	C115—C116—H116	119.7
C171—Sn6—O141	92.8 (3)	C122—C121—Sn4	118.5 (7)
C171—Sn6—C181	134.4 (3)	C122—C121—C126	120.4 (9)
C181—Sn6—O141	93.3 (3)	C126—C121—Sn4	120.9 (7)
O4—Sn7—O151	79.3 (2)	C121—C122—H122	120.6
O4—Sn7—O161	71.32 (19)	C121—C122—C123	118.8 (11)
O4—Sn7—C231	116.1 (3)	C123—C122—H122	120.6
O4—Sn7—C241	113.7 (3)	C122—C123—H123	119.4

O151—Sn7—O161	150.5 (2)	C124—C123—C122	121.2 (12)
O151—Sn7—C231	100.3 (3)	C124—C123—H123	119.4
C231—Sn7—O161	90.5 (3)	C123—C124—H124	120.4
C241—Sn7—O151	102.3 (3)	C125—C124—C123	119.2 (11)
C241—Sn7—O161	91.9 (3)	C125—C124—H124	120.4
C241—Sn7—C231	128.1 (4)	C124—C125—H125	118.8
O3—Sn8—O161	143.2 (2)	C124—C125—C126	122.5 (12)
O3—Sn8—C211	99.1 (3)	C126—C125—H125	118.8
O4—Sn8—O3	71.8 (2)	C121—C126—H126	121.0
O4—Sn8—O161	71.8 (2)	C125—C126—C121	117.9 (11)
O4—Sn8—C211	107.2 (3)	C125—C126—H126	121.0
O4—Sn8—C221	114.5 (3)	O131—C131—C132	118.4 (8)
C211—Sn8—O161	96.6 (3)	O131—C131—C136	124.3 (8)
C221—Sn8—O3	98.0 (2)	C136—C131—C132	117.3 (8)
C221—Sn8—O161	92.1 (2)	C131—C132—H132	118.9
C221—Sn8—C211	138.0 (3)	C133—C132—C131	122.1 (9)
Sn1—O1—Sn2	118.0 (2)	C133—C132—H132	118.9
Sn1—O1—Sn4	135.0 (3)	C132—C133—H133	121.0
Sn2—O1—Sn4	107.0 (2)	C132—C133—C134	118.1 (8)
Sn3—O2—Sn2	132.8 (3)	C134—C133—H133	121.0
Sn3—O2—Sn4	119.5 (3)	C133—C134—N137	118.6 (8)
Sn4—O2—Sn2	107.2 (2)	C133—C134—C135	122.3 (9)
Sn5—O3—Sn6	118.7 (2)	C135—C134—N137	119.1 (9)
Sn5—O3—Sn8	133.2 (2)	C134—C135—H135	120.7
Sn6—O3—Sn8	107.8 (2)	C136—C135—C134	118.6 (9)
Sn7—O4—Sn6	134.7 (3)	C136—C135—H135	120.7
Sn7—O4—Sn8	117.3 (2)	C131—C136—H136	119.3
Sn8—O4—Sn6	108.1 (2)	C135—C136—C131	121.5 (8)
C11—O11—Sn1	127.7 (5)	C135—C136—H136	119.3
Sn2—O21—Sn1	99.6 (2)	O141—C141—C142	121.6 (8)
C21—O21—Sn1	130.2 (5)	O141—C141—C146	120.5 (8)
C21—O21—Sn2	125.2 (5)	C146—C141—C142	117.9 (9)
C31—O31—Sn3	132.6 (5)	C141—C142—H142	119.0
Sn3—O41—Sn4	99.0 (2)	C141—C142—C143	122.0 (9)
C41—O41—Sn3	132.0 (5)	C143—C142—H142	119.0
C41—O41—Sn4	129.0 (5)	C142—C143—H143	120.8
C131—O131—Sn5	132.9 (5)	C144—C143—C142	118.5 (10)
Sn6—O141—Sn5	99.1 (2)	C144—C143—H143	120.8
C141—O141—Sn5	134.5 (5)	C143—C144—N147	118.8 (11)
C141—O141—Sn6	126.0 (5)	C143—C144—C145	121.6 (10)
C151—O151—Sn7	127.8 (5)	C145—C144—N147	119.5 (10)
Sn8—O161—Sn7	99.5 (2)	C144—C145—H145	120.4
C161—O161—Sn7	131.3 (5)	C144—C145—C146	119.3 (10)
C161—O161—Sn8	125.2 (5)	C146—C145—H145	120.4
O18—N17—C14	118.4 (8)	C141—C146—C145	120.7 (11)
O19—N17—O18	122.8 (8)	C141—C146—H146	119.7
O19—N17—C14	118.8 (8)	C145—C146—H146	119.7
O28—N27—O29	121.9 (10)	O151—C151—C152	125.1 (7)

O28—N27—C24	118.7 (11)	O151—C151—C156	117.7 (7)
O29—N27—C24	119.3 (11)	C152—C151—C156	117.1 (8)
O38—N37—C34	118.5 (10)	C151—C152—H152	118.9
O39—N37—O38	122.2 (10)	C153—C152—C151	122.1 (8)
O39—N37—C34	119.3 (10)	C153—C152—H152	118.9
O48—N47—C44	119.0 (9)	C152—C153—H153	120.5
O49—N47—O48	125.2 (10)	C152—C153—C154	119.0 (9)
O49—N47—C44	115.8 (10)	C154—C153—H153	120.5
O138—N137—O139	121.7 (10)	C153—C154—N157	119.7 (8)
O138—N137—C134	120.0 (10)	C153—C154—C155	121.7 (9)
O139—N137—C134	118.2 (9)	C155—C154—N157	118.5 (8)
O148—N147—O149	123.1 (10)	C154—C155—H155	120.4
O148—N147—C144	119.6 (10)	C156—C155—C154	119.3 (8)
O149—N147—C144	117.3 (11)	C156—C155—H155	120.4
O158—N157—C154	118.4 (8)	C151—C156—H156	119.6
O159—N157—O158	122.7 (8)	C155—C156—C151	120.8 (8)
O159—N157—C154	118.9 (8)	C155—C156—H156	119.6
O168—N167—O169	123.4 (9)	O161—C161—C162	119.7 (7)
O168—N167—C164	117.2 (10)	O161—C161—C166	121.7 (7)
O169—N167—C164	119.3 (10)	C162—C161—C166	118.6 (8)
Cl1—C1—Cl2	112.6 (6)	C161—C162—H162	119.4
Cl1—C1—Cl3	111.2 (6)	C163—C162—C161	121.2 (9)
Cl1—C1—H1	108.0	C163—C162—H162	119.4
Cl2—C1—Cl3	108.9 (6)	C162—C163—H163	120.8
Cl2—C1—H1	108.0	C164—C163—C162	118.4 (9)
Cl3—C1—H1	108.0	C164—C163—H163	120.8
Cl11—C2—Cl12	109.5 (6)	C163—C164—N167	117.9 (10)
Cl11—C2—H2	107.8	C163—C164—C165	122.6 (8)
Cl12—C2—H2	107.8	C165—C164—N167	119.5 (10)
Cl13—C2—Cl11	112.0 (6)	C164—C165—H165	121.1
Cl13—C2—Cl12	111.7 (7)	C164—C165—C166	117.9 (9)
Cl13—C2—H2	107.8	C166—C165—H165	121.1
Cl21—C3—Cl22	110.8 (10)	C161—C166—H166	119.4
Cl21—C3—H3	106.7	C165—C166—C161	121.2 (9)
Cl22—C3—H3	106.7	C165—C166—H166	119.4
Cl23—C3—Cl21	114.2 (13)	C172—C171—Sn6	121.2 (7)
Cl23—C3—Cl22	111.3 (11)	C176—C171—Sn6	118.6 (6)
Cl23—C3—H3	106.7	C176—C171—C172	120.0 (8)
O11—C11—C12	123.7 (7)	C171—C172—H172	120.9
O11—C11—C16	117.3 (7)	C173—C172—C171	118.3 (11)
C12—C11—C16	119.0 (8)	C173—C172—H172	120.9
C11—C12—H12	119.3	C172—C173—H173	119.5
C13—C12—C11	121.4 (8)	C174—C173—C172	121.0 (11)
C13—C12—H12	119.3	C174—C173—H173	119.5
C12—C13—H13	120.7	C173—C174—H174	120.1
C14—C13—C12	118.6 (8)	C175—C174—C173	119.8 (10)
C14—C13—H13	120.7	C175—C174—H174	120.1
C13—C14—N17	119.7 (8)	C174—C175—H175	119.3

C13—C14—C15	122.2 (8)	C174—C175—C176	121.4 (12)
C15—C14—N17	118.1 (8)	C176—C175—H175	119.3
C14—C15—H15	120.5	C171—C176—C175	119.6 (10)
C16—C15—C14	119.0 (8)	C171—C176—H176	120.2
C16—C15—H15	120.5	C175—C176—H176	120.2
C11—C16—H16	120.1	C182—C181—Sn6	122.4 (7)
C15—C16—C11	119.8 (8)	C182—C181—C186	120.3 (8)
C15—C16—H16	120.1	C186—C181—Sn6	117.3 (6)
O21—C21—C22	118.8 (8)	C181—C182—H182	120.7
O21—C21—C26	122.2 (8)	C181—C182—C183	118.5 (9)
C26—C21—C22	118.9 (8)	C183—C182—H182	120.7
C21—C22—H22	119.7	C182—C183—H183	119.6
C23—C22—C21	120.6 (9)	C184—C183—C182	120.9 (10)
C23—C22—H22	119.7	C184—C183—H183	119.6
C22—C23—H23	120.9	C183—C184—H184	119.6
C24—C23—C22	118.2 (9)	C183—C184—C185	120.8 (9)
C24—C23—H23	120.9	C185—C184—H184	119.6
C23—C24—N27	117.9 (10)	C184—C185—H185	120.4
C25—C24—N27	119.2 (10)	C184—C185—C186	119.3 (10)
C25—C24—C23	122.8 (9)	C186—C185—H185	120.4
C24—C25—H25	121.0	C181—C186—H186	119.9
C26—C25—C24	118.0 (9)	C185—C186—C181	120.2 (9)
C26—C25—H25	121.0	C185—C186—H186	119.9
C21—C26—H26	119.3	C192—C191—Sn5	124.4 (8)
C25—C26—C21	121.5 (9)	C192—C191—C196	116.4 (10)
C25—C26—H26	119.3	C196—C191—Sn5	119.0 (7)
O31—C31—C32	123.5 (8)	C191—C192—H192	119.3
O31—C31—C36	118.7 (8)	C193—C192—C191	121.4 (12)
C32—C31—C36	117.8 (9)	C193—C192—H192	119.3
C31—C32—H32	119.7	C192—C193—H193	120.0
C31—C32—C33	120.6 (9)	C194—C193—C192	120.1 (11)
C33—C32—H32	119.7	C194—C193—H193	120.0
C32—C33—H33	120.5	C193—C194—H194	119.7
C34—C33—C32	119.0 (9)	C195—C194—C193	120.6 (10)
C34—C33—H33	120.5	C195—C194—H194	119.7
C33—C34—N37	117.9 (9)	C194—C195—H195	120.4
C35—C34—N37	119.7 (9)	C194—C195—C196	119.1 (13)
C35—C34—C33	122.5 (9)	C196—C195—H195	120.4
C34—C35—H35	120.7	C191—C196—H196	118.8
C34—C35—C36	118.7 (9)	C195—C196—C191	122.3 (12)
C36—C35—H35	120.7	C195—C196—H196	118.8
C31—C36—H36	119.3	C202—C201—Sn5	121.3 (7)
C35—C36—C31	121.4 (9)	C202—C201—C206	120.7 (9)
C35—C36—H36	119.3	C206—C201—Sn5	118.0 (7)
O41—C41—C42	121.0 (8)	C201—C202—H202	121.1
O41—C41—C46	120.1 (8)	C201—C202—C203	117.9 (11)
C46—C41—C42	118.9 (8)	C203—C202—H202	121.1
C41—C42—H42	119.7	C202—C203—H203	119.5

C43—C42—C41	120.6 (8)	C204—C203—C202	121.0 (12)
C43—C42—H42	119.7	C204—C203—H203	119.5
C42—C43—H43	120.5	C203—C204—H204	120.0
C44—C43—C42	118.9 (9)	C203—C204—C205	120.0 (12)
C44—C43—H43	120.5	C205—C204—H204	120.0
C43—C44—N47	118.3 (10)	C204—C205—H205	119.4
C45—C44—N47	121.3 (9)	C206—C205—C204	121.2 (12)
C45—C44—C43	120.4 (9)	C206—C205—H205	119.4
C44—C45—H45	119.6	C201—C206—H206	120.4
C46—C45—C44	120.7 (9)	C205—C206—C201	119.2 (11)
C46—C45—H45	119.6	C205—C206—H206	120.4
C41—C46—H46	119.8	C212—C211—Sn8	116.9 (6)
C45—C46—C41	120.3 (10)	C216—C211—Sn8	122.4 (7)
C45—C46—H46	119.8	C216—C211—C212	119.4 (9)
C52—C51—Sn1	118.8 (6)	C211—C212—H212	120.2
C52—C51—C56	118.5 (9)	C213—C212—C211	119.5 (10)
C56—C51—Sn1	122.6 (8)	C213—C212—H212	120.2
C51—C52—H52	119.7	C212—C213—H213	119.2
C53—C52—C51	120.6 (9)	C214—C213—C212	121.6 (11)
C53—C52—H52	119.7	C214—C213—H213	119.2
C52—C53—H53	120.1	C213—C214—H214	120.2
C54—C53—C52	119.9 (11)	C213—C214—C215	119.7 (10)
C54—C53—H53	120.1	C215—C214—H214	120.2
C53—C54—H54	119.8	C214—C215—H215	120.1
C53—C54—C55	120.5 (11)	C216—C215—C214	119.9 (12)
C55—C54—H54	119.8	C216—C215—H215	120.1
C54—C55—H55	119.5	C211—C216—C215	119.9 (12)
C54—C55—C56	121.0 (11)	C211—C216—H216	120.1
C56—C55—H55	119.5	C215—C216—H216	120.1
C51—C56—H56	120.2	C222—C221—Sn8	124.0 (6)
C55—C56—C51	119.6 (11)	C226—C221—Sn8	117.9 (6)
C55—C56—H56	120.2	C226—C221—C222	117.8 (8)
C62—C61—Sn1	121.5 (8)	C221—C222—H222	119.2
C62—C61—C66	120.1 (10)	C223—C222—C221	121.7 (9)
C66—C61—Sn1	118.2 (7)	C223—C222—H222	119.2
C61—C62—H62	119.7	C222—C223—H223	120.4
C63—C62—C61	120.6 (13)	C224—C223—C222	119.3 (9)
C63—C62—H62	119.7	C224—C223—H223	120.4
C62—C63—H63	119.6	C223—C224—H224	120.0
C64—C63—C62	120.7 (13)	C223—C224—C225	120.1 (9)
C64—C63—H63	119.6	C225—C224—H224	120.0
C63—C64—H64	120.0	C224—C225—H225	119.2
C63—C64—C65	119.9 (12)	C224—C225—C226	121.5 (10)
C65—C64—H64	120.0	C226—C225—H225	119.2
C64—C65—H65	120.7	C221—C226—H226	120.2
C66—C65—C64	118.6 (14)	C225—C226—C221	119.6 (9)
C66—C65—H65	120.7	C225—C226—H226	120.2
C61—C66—C65	120.0 (12)	C232—C231—Sn7	119.5 (8)

C61—C66—H66	120.0	C232—C231—C236	118.5 (10)
C65—C66—H66	120.0	C236—C231—Sn7	121.8 (8)
C72—C71—Sn2	116.1 (7)	C231—C232—H232	119.6
C76—C71—Sn2	124.6 (7)	C231—C232—C233	120.7 (12)
C76—C71—C72	119.3 (9)	C233—C232—H232	119.6
C71—C72—H72	120.2	C232—C233—H233	120.5
C71—C72—C73	119.6 (10)	C232—C233—C234	119.0 (14)
C73—C72—H72	120.2	C234—C233—H233	120.5
C72—C73—H73	120.0	C233—C234—H234	119.9
C74—C73—C72	120.0 (10)	C235—C234—C233	120.1 (12)
C74—C73—H73	120.0	C235—C234—H234	119.9
C73—C74—H74	119.4	C234—C235—H235	119.7
C75—C74—C73	121.1 (10)	C234—C235—C236	120.6 (13)
C75—C74—H74	119.4	C236—C235—H235	119.7
C74—C75—H75	120.5	C231—C236—H236	119.5
C74—C75—C76	119.0 (9)	C235—C236—C231	121.0 (13)
C76—C75—H75	120.5	C235—C236—H236	119.5
C71—C76—C75	121.0 (9)	C242—C241—Sn7	122.4 (8)
C71—C76—H76	119.5	C242—C241—C246	118.0 (9)
C75—C76—H76	119.5	C246—C241—Sn7	119.4 (6)
C82—C81—Sn2	121.8 (6)	C241—C242—H242	120.1
C86—C81—Sn2	119.0 (6)	C243—C242—C241	119.7 (12)
C86—C81—C82	118.0 (8)	C243—C242—H242	120.1
C81—C82—H82	119.9	C242—C243—H243	119.0
C83—C82—C81	120.2 (9)	C244—C243—C242	121.9 (11)
C83—C82—H82	119.9	C244—C243—H243	119.0
C82—C83—H83	120.1	C243—C244—H244	120.2
C84—C83—C82	119.8 (10)	C243—C244—C245	119.6 (10)
C84—C83—H83	120.1	C245—C244—H244	120.2
C83—C84—H84	120.1	C244—C245—H245	119.4
C85—C84—C83	119.8 (10)	C244—C245—C246	121.2 (11)
C85—C84—H84	120.1	C246—C245—H245	119.4
C84—C85—H85	119.6	C241—C246—H246	120.2
C84—C85—C86	120.8 (9)	C245—C246—C241	119.6 (10)
C86—C85—H85	119.6	C245—C246—H246	120.2

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C82—H82···O31	0.93	2.35	3.144 (13)	143
C116—H116···O11	0.93	2.55	3.289 (11)	137
C182—H182···O151	0.93	2.52	3.259 (12)	137
C216—H216···O131	0.93	2.37	3.161 (13)	143
C3—H3···O148^{i}	0.98	2.44	3.27 (2)	143
C16—H16···O138^{ii}	0.93	2.60	3.301 (13)	133
C22—H22···O159^{i}	0.93	2.47	3.388 (11)	168
C84—H84···O39^{i}	0.93	2.55	3.264 (16)	134
C94—H94···O138^{iii}	0.93	2.57	3.470 (16)	162

C96—H96···O49^{iv}	0.93	2.53	3.305 (14)	142
C156—H156···O38	0.93	2.53	3.271 (13)	136
C162—H162···O19^{v}	0.93	2.43	3.343 (12)	168
C202—H202···O149^{vi}	0.93	2.53	3.293 (16)	139

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