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Dibutylbis[4-(methylamino)benzoato-κ^2O,O']tin(IV)

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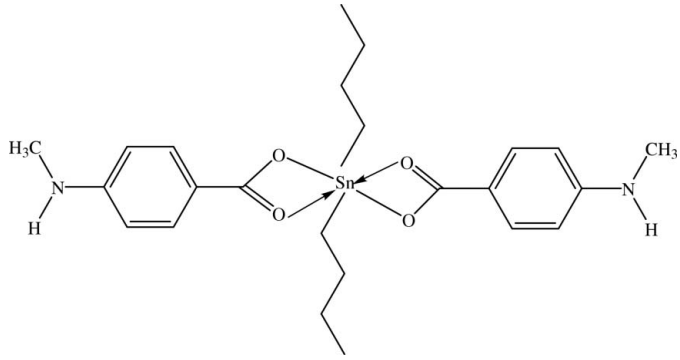
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.029; wR factor = 0.060; data-to-parameter ratio = 35.0.

The monomeric organotin(IV) carboxylate $[Sn(C_4H_9)_2(C_8H_8NO_2)_2]$ has four molecules in the asymmetric unit. The Sn atom exists in a six-coordinated skew-trapezoidal environment in which the carboxylate group chelates in an anisobidentate manner. In one molecule, one of the butyl groups is disordered; the site occupancy factors are *ca* 0.7 and 0.3. In all four molecules, the methylamino substituents are slightly twisted from the mean planes of the phenylene rings, with dihedral angles of 13.43 (13), 11.34 (12), 14.92 (11) and 11.10 (12)°. The crystal structure is stabilized by N—H···O hydrogen bonds and C—H···π interactions. In the crystal packing, the molecules are arranged into chains along the [010] direction. Neighbouring chains are arranged in a *T*-shaped manner. The crystal structure is an inversion twin.

Related literature

For related structures of organotin carboxylates, see: Win *et al.* (2007); Yearwood *et al.* (2002). For literature on the coordination chemistry and bioactivity of organotin compounds, see, for example: Gielen *et al.* (2000); Molloy *et al.* (1984); Novelli *et al.* (1999); Szorcsik *et al.* (2004); Yin *et al.* (2006); Teoh *et al.* (1997); Tian *et al.* (2005); Win *et al.* (2006, 2007); Willem *et al.* (1997); Yin *et al.* (2005).



Experimental

Crystal data

$[Sn(C_4H_9)_2(C_8H_8NO_2)_2]$
M_r = 533.22
Monoclinic, $P2_1$
a = 15.4440 (3) Å
b = 11.7770 (2) Å
c = 27.2069 (5) Å
β = 100.482 (1)°
V = 4865.92 (15) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.08 mm^{-1}
T = 100.0 (1) K
0.57 × 0.50 × 0.35 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.577, T_{max} = 0.701
106321 measured reflections
41599 independent reflections
37515 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.029
$wR(F^2)$ = 0.060
S = 1.04
41599 reflections
1187 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.78 e Å^{-3}
Absolute structure: Flack (1983), 19384 Friedel pairs
Flack parameter: 0.386 (9)

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

*Cg*1 is the centroid of C1*C*–C6*C* benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
N2A—H2AB···O3A^{i}	0.86	2.31	3.146 (3)	164
N2B—H1ND···O3B^{ii}	0.84 (3)	2.13 (3)	2.967 (3)	174 (2)
N1C—H1NE···O4D^{iii}	0.78 (3)	2.32 (3)	3.046 (3)	155 (3)
N2D—H1NH···O1C^{iii}	0.84 (3)	2.20 (2)	2.970 (3)	152 (2)
N2D—H1NH···O4C^{iii}	0.84 (3)	2.45 (3)	3.103 (3)	134 (2)
C8B—H8BC···Cg1	0.96	2.91	3.750 (3)	147

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

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2382).

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supplementary materials

Acta Cryst. (2007). E**63**, m3199-m3200 [**doi:10.1107/S1600536807062411**]

Dibutylbis[4-(methylamino)benzoato-κ^2O,O']tin(IV)

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Comment

The coordination number of organotin(IV) atom vary from four to seven resulting in various kinds of geometric formations (Szorcsik *et al.*, 2004; Yin *et al.*, 2006; Win *et al.*, 2006; Win *et al.*, 2007). In addition, it is well known that organotin(IV) complexes are extensively studied due to their industrial applications as well as biocidal properties (Molloy *et al.*, 1984; Willem *et al.*, 1997; Gielen *et al.*, 2000). Moreover, recent *in vitro* studies of organotin(IV) complexes on cancer cell lines, bacterial and fungal growths have revealed their inhibitory properties (Teoh *et al.*, 1997; Novelli *et al.*, 1999; Gielen *et al.*, 2000; Tian *et al.*, 2005). Generally the complexes obtained from the reaction of dibutyltin(IV) oxide with carboxylic acid in 1:1 ratio are distannoxane-dimer type whereas in 1:2 ratio will produce monomer type (Yin *et al.*, 2005; Win *et al.*, 2006). In this study, the title compound obtained exhibit a normal monomer type from the 1:2 ratio reaction of dibutyltin(IV) oxide with 4-(methylamino)benzoic acid. In addition, the title complex obtained is similar to that found in the dibutylbis[3-(dimethylamino)benzoato]tin(IV) (Win *et al.*, 2007). The only striking difference is that the methylamine group is substituted at *para* position in the titled compound whereas the dimethylamine group is substituted at *meta* position in dibutylbis[3-(dimethylamino)benzoato]tin(IV).

The asymmetric unit of the title complex contains four molecules, *A*, *B*, *C* and *D* of Sn^{IV} complex (Fig. 1). In each molecule, the Sn^{IV} is in a six-coordinated skew-trapezoidal environment and coordinates with the two bidentate 4-methylaminobenzoate ligands through O atoms in the equatorial plane (O1, O2, O3 and O4) and the two butyl ligands in the axial positions. There is a disorder of one butyl ligand in molecule *A* (Fig. 2). In the coordination sphere of Sn^{IV}, two Sn—O bond distances lie in the ranges of 2.1320 (16)–2.1467 (16) Å which are shorter than the other two Sn—O distances [in the ranges of 2.3986 (18)–2.5288 (17) Å]. The Sn—O bond distances observed in the title complex are longer than a typical Sn—O bond distance [Yearwood *et al.*, 2002]. The Sn—C distances, in the ranges of 2.115 (2)–2.13192) Å, are similar to the other six similar coordination Sn^{IV} complexes (Yearwood *et al.*, 2002). The dihedral angles between the two benzene rings (C1–C6) and (C9–C14) are 13.43 (13) °, 11.34 (12) °, 14.92 (11) ° and 11.10 (12) ° in molecules *A*, *B*, *C* and *D*, respectively. In each molecule, the methylamino groups are slightly twisted from the mean planes of the attached benzene rings, as indicated by the torsion angles C8–N1–C3–C4 and C16–N2–C11–C12 of 2.0 (4) ° and 14.4 (4) ° in molecule *A* [3.2 (4) ° and 9.0 (4) ° in molecule *B*; −8.8 (4) ° and −2.9 (4) ° in molecule *C*; −7.4 (4) ° and −15.3 (4) ° in molecule *D*]. Bond lengths and angles observed in the structure are normal.

In the crystal packing (Fig. 3), the molecules are arranged into chains along the [0 1 0] direction. The neighbouring chains are arranged in a T-shape manner (Fig. 3). The crystal is stabilized by N—H···O hydrogen bonds and C—H···π interaction [C8B–H8BC···Cg_1 (Table 1); Cg_1 is the centroid of C1C–C6C benzene ring].

Experimental

The title complex was obtained by heating under reflux a 1:2 molar mixture of dibutyltin(IV) oxide (0.75 g, 3 mmol) and 4-(methylamino)benzoic acid (0.91 g, 6 mmol) in toluene-ethanol (4:1, *v*/*v*) (50 ml) for 4 h. A clear transparent solution

was isolated by filtration and kept in a bottle. After 14 days, colourless crystals (0.54 g, 34% yield) were obtained. *M*.p. 427–428 K. Calculated for $C_{24}H_{34}N_2O_4Sn$: C 54.06, H 6.43, N 5.25 and Sn 22.61%; analysis found C 55.63, H 5.89, N 5.48 and Sn 22.61%.

Refinement

H atoms attached to N atom except for N2A were located from the difference map and isotropically refined. The remainding H atoms were positioned geometrically and allowed to ride on their parent atoms, with N—H distance of 0.82 Å and C—H = 0.93 Å for aromatic rings and in the ranges 0.96–0.97 Å for CH_2 and CH_3. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.58 Å from Sn1C and the deepest hole is located at 0.74 Å from Sn1D. The crystal is a twin and the refined BASF value is 0.396(0.009).

Figures

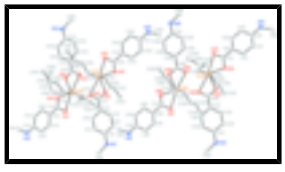

Fig. 1. The asymmetric unit of the title complex, showing 50% probability displacement ellipsoids and the atomic numbering. H atoms were omitted for clarify.

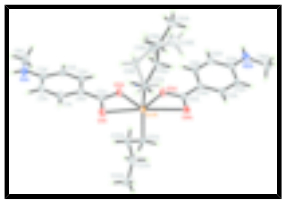

Fig. 2. The molecular structure of the title complex, showing a disorder of one butyl ligand in molecule *A*.

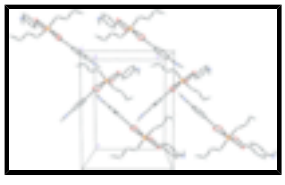

Fig. 3. The crystal packing of the title complex, viewed along the *c* axis.

Dibutylbis[4-(methylamino)benzoato-κ^2O,O']tin(IV)

Crystal data

$[Sn(C_4H_9)_2(C_8H_8NO_2)_2]$	F_{000} = 2192
M_r = 533.22	D_x = 1.456 Mg m^{-3}
Monoclinic, $P2_1$	Melting point = 427–428 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 15.4440 (3) Å	Cell parameters from 41599 reflections
b = 11.7770 (2) Å	θ = 0.8–35.0º
c = 27.2069 (5) Å	μ = 1.08 mm^{-1}
β = 100.482 (1)º	*T* = 100.0 (1) K

V = 4865.92 (15) Å^3	Block, colourless
Z = 8	0.57 × 0.50 × 0.35 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	41599 independent reflections
Radiation source: medium-focus sealed tube	37515 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
Detector resolution: 8.33 pixels mm^{-1}	θ_{max} = 35.0º
T = 100.0(1) K	θ_{min} = 0.8º
φ and ω scans	h = −24→24
Absorption correction: multi-scan (SADABS; Bruker, 2005)	k = −19→19
T_{min} = 0.577, T_{max} = 0.701	l = −43→43
106321 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)]$ = 0.029	$w = 1/[\sigma^2(F_o^2) + (0.0187P)^2 + 1.5089P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.060	$(\Delta/\sigma)_{max}$ = 0.005
S = 1.04	$\Delta\rho_{max}$ = 0.55 e Å^{-3}
41599 reflections	$\Delta\rho_{min}$ = −0.77 e Å^{-3}
1187 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 19384 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.386 (9)
Secondary atom site location: difference Fourier map	

Special details

Experimental. The low-temparture data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1A	0.732628 (10)	0.544969 (10)	0.057900 (5)	0.01736 (3)	
N1A	0.61588 (16)	0.1306 (2)	−0.19094 (9)	0.0326 (5)	
H1AB	0.5711	0.0859	−0.1946	0.039*	
N2A	1.09439 (16)	1.0706 (2)	0.05754 (9)	0.0293 (5)	
H2AB	1.1027	1.0876	0.0280	0.035*	
O1A	0.64204 (13)	0.38967 (17)	0.01865 (7)	0.0251 (4)	
O2A	0.74456 (11)	0.47719 (15)	−0.01322 (6)	0.0215 (3)	
O3A	0.83615 (11)	0.64668 (15)	0.03912 (6)	0.0212 (3)	
O4A	0.81181 (11)	0.71292 (14)	0.11119 (6)	0.0201 (3)	
C1A	0.59769 (18)	0.2520 (3)	−0.06929 (10)	0.0303 (6)	
H1AA	0.5622	0.2443	−0.0453	0.036*	
C2A	0.58154 (19)	0.1864 (3)	−0.11199 (11)	0.0344 (6)	
H2AA	0.5350	0.1352	−0.1164	0.041*	
C3A	0.63355 (17)	0.1954 (2)	−0.14870 (9)	0.0257 (5)	
C4A	0.70370 (16)	0.2726 (2)	−0.14095 (9)	0.0227 (4)	
H4AA	0.7400	0.2792	−0.1646	0.027*	
C5A	0.71934 (16)	0.3392 (2)	−0.09807 (8)	0.0210 (4)	
H5AA	0.7656	0.3910	−0.0936	0.025*	
C6A	0.66712 (16)	0.3297 (2)	−0.06191 (8)	0.0205 (4)	
C7A	0.68368 (16)	0.4004 (2)	−0.01667 (9)	0.0207 (4)	
C8A	0.6677 (2)	0.1329 (3)	−0.22946 (11)	0.0370 (7)	
H8AA	0.6434	0.0810	−0.2555	0.055*	
H8AB	0.7271	0.1109	−0.2158	0.055*	
H8AC	0.6675	0.2082	−0.2429	0.055*	
C9A	0.94627 (17)	0.8284 (2)	0.02603 (9)	0.0203 (4)	
H9AA	0.9277	0.7804	−0.0010	0.024*	
C10A	1.00510 (19)	0.9144 (3)	0.02192 (10)	0.0243 (5)	
H10A	1.0247	0.9249	−0.0081	0.029*	
C11A	1.03589 (17)	0.9862 (2)	0.06248 (10)	0.0218 (5)	
C12A	1.00413 (16)	0.9706 (2)	0.10701 (9)	0.0197 (4)	
H12A	1.0240	1.0171	0.1344	0.024*	
C13A	0.94305 (16)	0.8858 (2)	0.11050 (9)	0.0199 (5)	
H13A	0.9210	0.8777	0.1399	0.024*	
C14A	0.91424 (15)	0.8127 (2)	0.07056 (8)	0.0163 (4)	
C15A	0.85121 (14)	0.7213 (2)	0.07503 (8)	0.0165 (4)	
C16A	1.14278 (17)	1.1324 (2)	0.09923 (11)	0.0331 (6)	
H16A	1.1844	1.1817	0.0878	0.050*	
H16B	1.1735	1.0799	0.1233	0.050*	
H16C	1.1027	1.1767	0.1145	0.050*	
C17A	0.62339 (17)	0.6552 (2)	0.03600 (10)	0.0242 (5)	
H17A	0.6020	0.6805	0.0651	0.029*	0.663 (4)
H17B	0.5768	0.6145	0.0151	0.029*	0.663 (4)
H17I	0.6354	0.7238	0.0551	0.029*	0.337 (4)
H17J	0.5735	0.6201	0.0464	0.029*	0.337 (4)
C18A	0.6501 (2)	0.7609 (3)	0.00678 (14)	0.0213 (8)	0.663 (4)

H18A	0.6966	0.8025	0.0281	0.026*	0.663 (4)
H18B	0.6726	0.7352	−0.0223	0.026*	0.663 (4)
C19A	0.5725 (3)	0.8386 (4)	−0.00959 (14)	0.0237 (8)	0.663 (4)
H19A	0.5478	0.8598	0.0194	0.028*	0.663 (4)
H19B	0.5275	0.7976	−0.0323	0.028*	0.663 (4)
C20A	0.5961 (3)	0.9464 (4)	−0.03543 (18)	0.0348 (10)	0.663 (4)
H20A	0.5446	0.9928	−0.0443	0.052*	0.663 (4)
H20B	0.6182	0.9263	−0.0650	0.052*	0.663 (4)
H20C	0.6404	0.9877	−0.0131	0.052*	0.663 (4)
C18E	0.5968 (4)	0.6871 (6)	−0.0154 (2)	0.0244 (13)	0.337 (4)
H18I	0.5367	0.7149	−0.0208	0.029*	0.337 (4)
H18J	0.5982	0.6208	−0.0364	0.029*	0.337 (4)
C19E	0.6567 (5)	0.7789 (6)	−0.0306 (2)	0.0278 (14)	0.337 (4)
H19I	0.7176	0.7557	−0.0204	0.033*	0.337 (4)
H19J	0.6451	0.7862	−0.0667	0.033*	0.337 (4)
C20E	0.6436 (9)	0.8930 (8)	−0.0076 (4)	0.063 (3)	0.337 (4)
H20M	0.6816	0.9481	−0.0188	0.095*	0.337 (4)
H20N	0.6575	0.8872	0.0282	0.095*	0.337 (4)
H20O	0.5834	0.9164	−0.0176	0.095*	0.337 (4)
C21A	0.80764 (17)	0.4290 (2)	0.10772 (8)	0.0240 (4)	
H21A	0.8527	0.4703	0.1302	0.029*	
H21B	0.7696	0.3926	0.1277	0.029*	
C22A	0.85144 (17)	0.3379 (2)	0.08068 (9)	0.0264 (5)	
H22A	0.8754	0.3733	0.0539	0.032*	
H22B	0.8071	0.2837	0.0657	0.032*	
C23A	0.92530 (18)	0.2743 (2)	0.11496 (11)	0.0378 (6)	
H23A	0.9552	0.2257	0.0946	0.045*	
H23B	0.9678	0.3291	0.1314	0.045*	
C24A	0.8941 (2)	0.2024 (3)	0.15450 (10)	0.0459 (8)	
H24A	0.9441	0.1759	0.1780	0.069*	
H24B	0.8615	0.1385	0.1389	0.069*	
H24C	0.8570	0.2472	0.1717	0.069*	
Sn1B	0.746804 (9)	0.524665 (10)	0.546591 (5)	0.01482 (3)	
N1B	0.60700 (17)	0.1085 (2)	0.29977 (9)	0.0271 (5)	
H1NC	0.5652 (19)	0.062 (3)	0.2985 (11)	0.029 (8)*	
N2B	1.07919 (15)	1.0864 (2)	0.56370 (8)	0.0217 (4)	
H1ND	1.0979 (17)	1.099 (2)	0.5372 (10)	0.019 (7)*	
O1B	0.65559 (12)	0.36903 (17)	0.50943 (7)	0.0205 (3)	
O2B	0.74945 (11)	0.46310 (15)	0.47291 (6)	0.0187 (3)	
O3B	0.84344 (11)	0.63817 (15)	0.52590 (6)	0.0162 (3)	
O4B	0.82446 (11)	0.68014 (14)	0.60184 (6)	0.0164 (3)	
C1B	0.60340 (15)	0.2303 (2)	0.42298 (9)	0.0195 (4)	
H1BA	0.5729	0.2208	0.4492	0.023*	
C2B	0.58297 (17)	0.1630 (2)	0.38097 (9)	0.0216 (5)	
H2BA	0.5389	0.1085	0.3791	0.026*	
C3B	0.62832 (17)	0.1762 (2)	0.34081 (9)	0.0203 (4)	
C4B	0.69498 (16)	0.2586 (2)	0.34474 (9)	0.0213 (4)	
H4BA	0.7257	0.2686	0.3187	0.026*	
C5B	0.71514 (17)	0.3253 (2)	0.38746 (9)	0.0202 (4)	

H5BA	0.7598	0.3790	0.3898	0.024*
C6B	0.66974 (16)	0.3128 (2)	0.42658 (9)	0.0175 (4)
C7B	0.69170 (15)	0.3837 (2)	0.47170 (8)	0.0164 (4)
C8B	0.65333 (19)	0.1111 (3)	0.25801 (10)	0.0311 (6)
H8BA	0.6297	0.0540	0.2342	0.047*
H8BB	0.7148	0.0967	0.2698	0.047*
H8BC	0.6462	0.1845	0.2424	0.047*
C9B	0.95150 (17)	0.8320 (2)	0.52154 (9)	0.0171 (4)
H9BA	0.9377	0.7879	0.4928	0.021*
C10B	1.00553 (17)	0.9246 (2)	0.52179 (9)	0.0183 (4)
H10B	1.0281	0.9421	0.4933	0.022*
C11B	1.02739 (15)	0.9938 (2)	0.56474 (8)	0.0149 (4)
C12B	0.99214 (16)	0.9656 (2)	0.60724 (9)	0.0174 (4)
H12B	1.0053	1.0102	0.6358	0.021*
C13B	0.93774 (16)	0.8717 (2)	0.60676 (8)	0.0165 (4)
H13B	0.9149	0.8540	0.6352	0.020*
C14B	0.91669 (15)	0.8030 (2)	0.56432 (8)	0.0146 (4)
C15B	0.85989 (14)	0.7039 (2)	0.56509 (8)	0.0138 (4)
C16B	1.11244 (16)	1.1539 (2)	0.60725 (9)	0.0255 (5)
H16D	1.1502	1.2124	0.5985	0.038*
H16E	1.1452	1.1063	0.6327	0.038*
H16F	1.0641	1.1879	0.6196	0.038*
C17B	0.63445 (15)	0.6327 (2)	0.53074 (8)	0.0162 (4)
H17C	0.5883	0.5937	0.5080	0.019*
H17D	0.6129	0.6468	0.5615	0.019*
C18B	0.65272 (16)	0.7465 (2)	0.50767 (9)	0.0174 (4)
H18C	0.6999	0.7850	0.5299	0.021*
H18D	0.6723	0.7329	0.4763	0.021*
C19B	0.57196 (16)	0.8227 (2)	0.49833 (9)	0.0188 (4)
H19C	0.5536	0.8387	0.5299	0.023*
H19D	0.5241	0.7833	0.4771	0.023*
C20B	0.59014 (18)	0.9349 (2)	0.47347 (10)	0.0235 (5)
H20D	0.5390	0.9826	0.4701	0.035*
H20E	0.6037	0.9198	0.4410	0.035*
H20F	0.6391	0.9726	0.4937	0.035*
C21B	0.83380 (15)	0.4081 (2)	0.58966 (9)	0.0192 (4)
H21C	0.8753	0.3824	0.5692	0.023*
H21H	0.8673	0.4494	0.6177	0.023*
C22B	0.79490 (14)	0.30345 (17)	0.61032 (8)	0.0189 (4)
H22C	0.7595	0.2620	0.5830	0.023*
H22D	0.7567	0.3270	0.6330	0.023*
C23B	0.86670 (15)	0.2251 (2)	0.63796 (8)	0.0222 (4)
H23C	0.9035	0.1995	0.6148	0.027*
H23D	0.9036	0.2678	0.6643	0.027*
C24B	0.82977 (18)	0.1219 (2)	0.66084 (9)	0.0286 (5)
H24D	0.8768	0.0820	0.6817	0.043*
H24E	0.8016	0.0725	0.6347	0.043*
H24F	0.7876	0.1463	0.6806	0.043*
Sn1C	0.748868 (9)	0.726987 (11)	0.203718 (5)	0.01618 (3)

N1C	0.42110 (15)	0.1625 (2)	0.19635 (8)	0.0220 (4)
H1NE	0.399 (2)	0.166 (3)	0.2201 (11)	0.037 (9)*
N2C	0.88531 (16)	1.1341 (2)	0.45384 (8)	0.0268 (5)
H1NF	0.912 (2)	1.187 (3)	0.4497 (12)	0.037 (9)*
O1C	0.65017 (11)	0.61520 (14)	0.22304 (6)	0.0178 (3)
O2C	0.66822 (11)	0.56898 (14)	0.14741 (6)	0.0178 (3)
O3C	0.83795 (12)	0.88120 (16)	0.24196 (6)	0.0207 (3)
O4C	0.74354 (11)	0.78666 (15)	0.27766 (6)	0.0214 (3)
C1C	0.54797 (16)	0.4209 (2)	0.23189 (8)	0.0178 (4)
H1CA	0.5633	0.4669	0.2599	0.021*
C2C	0.49653 (17)	0.3268 (2)	0.23438 (9)	0.0188 (4)
H2CA	0.4782	0.3095	0.2642	0.023*
C3C	0.47103 (15)	0.2559 (2)	0.19256 (9)	0.0175 (4)
C4C	0.50187 (17)	0.2833 (2)	0.14830 (8)	0.0190 (4)
H4CA	0.4866	0.2375	0.1202	0.023*
C5C	0.55423 (16)	0.3769 (2)	0.14622 (8)	0.0166 (4)
H5CA	0.5745	0.3930	0.1168	0.020*
C6C	0.57769 (14)	0.44852 (19)	0.18754 (8)	0.0145 (4)
C7C	0.63436 (13)	0.54798 (19)	0.18478 (7)	0.0146 (4)
C8C	0.38471 (18)	0.0912 (3)	0.15440 (10)	0.0310 (6)
H8CA	0.3455	0.0367	0.1647	0.046*
H8CB	0.4316	0.0524	0.1426	0.046*
H8CC	0.3530	0.1374	0.1280	0.046*
C9C	0.89113 (15)	1.0156 (2)	0.32983 (8)	0.0198 (4)
H9CA	0.9223	1.0254	0.3039	0.024*
C10C	0.91152 (17)	1.0807 (2)	0.37248 (9)	0.0229 (5)
H10C	0.9568	1.1338	0.3752	0.027*
C11C	0.86433 (16)	1.0677 (2)	0.41202 (8)	0.0198 (4)
C12C	0.79663 (16)	0.9871 (2)	0.40725 (8)	0.0203 (4)
H12C	0.7650	0.9770	0.4329	0.024*
C13C	0.77690 (15)	0.92229 (19)	0.36388 (8)	0.0177 (4)
H13C	0.7314	0.8696	0.3607	0.021*
C14C	0.82366 (15)	0.93458 (19)	0.32534 (8)	0.0172 (4)
C15C	0.80229 (15)	0.86609 (19)	0.27941 (8)	0.0179 (4)
C16C	0.83850 (19)	1.1312 (3)	0.49476 (9)	0.0290 (5)
H16G	0.8632	1.1863	0.5194	0.043*
H16H	0.8434	1.0569	0.5095	0.043*
H16I	0.7776	1.1485	0.4828	0.043*
C17C	0.66119 (16)	0.8437 (2)	0.16031 (9)	0.0224 (4)
H17E	0.6273	0.8019	0.1326	0.027*
H17H	0.6201	0.8699	0.1809	0.027*
C18C	0.69914 (16)	0.94783 (19)	0.13884 (9)	0.0238 (4)
H18E	0.7354	0.9897	0.1657	0.029*
H18F	0.7364	0.9238	0.1157	0.029*
C19C	0.62719 (17)	1.0251 (2)	0.11196 (9)	0.0275 (5)
H19E	0.5916	1.0513	0.1356	0.033*
H19F	0.5893	0.9817	0.0863	0.033*
C20C	0.6624 (2)	1.1279 (2)	0.08780 (11)	0.0391 (6)
H20G	0.6141	1.1707	0.0697	0.059*

H20H	0.6996	1.1028	0.0652	0.059*
H20I	0.6959	1.1748	0.1133	0.059*
C21C	0.85920 (15)	0.6175 (2)	0.22200 (8)	0.0183 (4)
H21D	0.8825	0.6020	0.1919	0.022*
H21E	0.9047	0.6562	0.2453	0.022*
C22C	0.83832 (16)	0.5040 (2)	0.24524 (9)	0.0194 (4)
H22E	0.8172	0.5189	0.2761	0.023*
H22F	0.7916	0.4660	0.2225	0.023*
C23C	0.91833 (16)	0.4259 (2)	0.25620 (9)	0.0217 (5)
H23G	0.9370	0.4069	0.2250	0.026*
H23H	0.9663	0.4659	0.2770	0.026*
C24C	0.89963 (18)	0.3166 (2)	0.28241 (10)	0.0253 (5)
H24G	0.9513	0.2697	0.2877	0.038*
H24H	0.8521	0.2767	0.2620	0.038*
H24I	0.8837	0.3347	0.3140	0.038*
Sn1D	0.766802 (9)	0.699798 (10)	0.695916 (5)	0.01476 (3)
N1D	0.89640 (18)	1.1199 (2)	0.94227 (9)	0.0292 (5)
H1NG	0.921 (2)	1.176 (3)	0.9394 (12)	0.036 (9)*
N2D	0.40765 (14)	0.16751 (19)	0.68114 (8)	0.0216 (4)
H1NH	0.3815 (17)	0.174 (2)	0.7057 (9)	0.017 (6)*
O1D	0.76113 (11)	0.76614 (15)	0.76796 (6)	0.0199 (3)
O2D	0.85658 (12)	0.85973 (17)	0.73252 (6)	0.0200 (3)
O3D	0.69154 (10)	0.53911 (14)	0.64329 (6)	0.0169 (3)
O4D	0.66745 (11)	0.59176 (15)	0.71712 (6)	0.0179 (3)
C1D	0.79077 (17)	0.9059 (2)	0.85288 (9)	0.0209 (4)
H1DA	0.7463	0.8517	0.8500	0.025*
C2D	0.80864 (17)	0.9728 (2)	0.89539 (9)	0.0226 (5)
H2DA	0.7760	0.9637	0.9207	0.027*
C3D	0.87579 (17)	1.0541 (2)	0.90040 (9)	0.0226 (5)
C4D	0.92355 (17)	1.0670 (2)	0.86141 (9)	0.0213 (4)
H4DA	0.9686	1.1203	0.8644	0.026*
C5D	0.90425 (16)	1.0012 (2)	0.81871 (9)	0.0195 (4)
H5DA	0.9352	1.0121	0.7928	0.023*
C6D	0.83835 (15)	0.9183 (2)	0.81423 (8)	0.0158 (4)
C7D	0.81927 (15)	0.8471 (2)	0.76918 (8)	0.0169 (4)
C8D	0.8455 (2)	1.1213 (3)	0.98171 (10)	0.0338 (6)
H8DA	0.8700	1.1759	1.0066	0.051*
H8DB	0.8469	1.0473	0.9967	0.051*
H8DC	0.7857	1.1414	0.9681	0.051*
C9D	0.55920 (16)	0.3671 (2)	0.63677 (8)	0.0163 (4)
H9DA	0.5813	0.3823	0.6078	0.020*
C10D	0.49843 (16)	0.2818 (2)	0.63668 (8)	0.0173 (4)
H10D	0.4790	0.2414	0.6074	0.021*
C11D	0.46515 (15)	0.2546 (2)	0.67969 (8)	0.0166 (4)
C12D	0.49460 (17)	0.3191 (2)	0.72343 (9)	0.0196 (4)
H12D	0.4734	0.3029	0.7525	0.024*
C13D	0.55475 (16)	0.4059 (2)	0.72311 (8)	0.0176 (4)
H13D	0.5732	0.4479	0.7520	0.021*
C14D	0.58832 (15)	0.4315 (2)	0.67989 (8)	0.0143 (4)

C15D	0.65201 (14)	0.5241 (2)	0.67907 (8)	0.0153 (4)
C16D	0.35988 (16)	0.1138 (2)	0.63622 (10)	0.0258 (5)
H16J	0.3179	0.0610	0.6451	0.039*
H16K	0.4005	0.0742	0.6195	0.039*
H16L	0.3296	0.1707	0.6143	0.039*
C17D	0.68483 (18)	0.8130 (2)	0.64780 (9)	0.0243 (5)
H17F	0.7176	0.8430	0.6235	0.029*
H17G	0.6350	0.7711	0.6297	0.029*
C18D	0.65087 (14)	0.91159 (18)	0.67494 (8)	0.0184 (4)
H18G	0.6981	0.9658	0.6847	0.022*
H18H	0.6331	0.8836	0.7051	0.022*
C19D	0.57253 (16)	0.9719 (2)	0.64257 (9)	0.0277 (5)
H19G	0.5281	0.9160	0.6297	0.033*
H19H	0.5468	1.0244	0.6633	0.033*
C20D	0.59772 (19)	1.0368 (2)	0.59901 (9)	0.0354 (6)
H20J	0.5453	1.0598	0.5766	0.053*
H20K	0.6323	0.9888	0.5816	0.053*
H20L	0.6314	1.1027	0.6113	0.053*
C21D	0.87957 (15)	0.5952 (2)	0.71526 (9)	0.0173 (4)
H21F	0.9028	0.5781	0.6853	0.021*
H21G	0.9245	0.6367	0.7378	0.021*
C22D	0.86077 (16)	0.4838 (2)	0.74013 (9)	0.0199 (4)
H22G	0.8356	0.5007	0.7695	0.024*
H22H	0.8175	0.4409	0.7171	0.024*
C23D	0.94273 (16)	0.4110 (2)	0.75557 (9)	0.0205 (4)
H23E	0.9683	0.3943	0.7263	0.025*
H23F	0.9859	0.4532	0.7789	0.025*
C24D	0.92202 (19)	0.3005 (2)	0.77969 (10)	0.0266 (5)
H24J	0.9748	0.2561	0.7881	0.040*
H24K	0.8790	0.2587	0.7567	0.040*
H24L	0.8991	0.3166	0.8095	0.040*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1A	0.01956 (6)	0.01543 (6)	0.01708 (6)	−0.00260 (5)	0.00330 (5)	−0.00235 (5)
N1A	0.0289 (11)	0.0323 (12)	0.0341 (11)	−0.0020 (9)	−0.0013 (9)	−0.0172 (10)
N2A	0.0278 (10)	0.0237 (10)	0.0408 (12)	−0.0058 (8)	0.0177 (9)	−0.0011 (9)
O1A	0.0294 (9)	0.0232 (9)	0.0237 (8)	−0.0080 (8)	0.0074 (7)	−0.0035 (7)
O2A	0.0250 (8)	0.0198 (7)	0.0202 (7)	−0.0088 (6)	0.0055 (6)	−0.0057 (6)
O3A	0.0211 (7)	0.0194 (7)	0.0237 (7)	−0.0052 (6)	0.0057 (6)	−0.0061 (6)
O4A	0.0203 (7)	0.0186 (8)	0.0222 (7)	−0.0044 (6)	0.0059 (5)	0.0006 (6)
C1A	0.0287 (12)	0.0328 (14)	0.0307 (12)	−0.0101 (11)	0.0084 (9)	−0.0098 (10)
C2A	0.0294 (12)	0.0350 (14)	0.0386 (13)	−0.0144 (12)	0.0061 (10)	−0.0136 (12)
C3A	0.0259 (10)	0.0222 (10)	0.0263 (10)	0.0036 (9)	−0.0029 (8)	−0.0092 (9)
C4A	0.0236 (10)	0.0214 (10)	0.0223 (9)	0.0001 (8)	0.0021 (8)	−0.0047 (8)
C5A	0.0203 (9)	0.0196 (9)	0.0216 (9)	−0.0031 (8)	0.0001 (8)	−0.0034 (8)
C6A	0.0229 (10)	0.0175 (9)	0.0196 (9)	−0.0029 (8)	−0.0006 (8)	−0.0026 (8)

C7A	0.0228 (10)	0.0174 (9)	0.0208 (9)	−0.0030 (8)	0.0014 (8)	−0.0025 (8)
C8A	0.0375 (14)	0.0373 (15)	0.0332 (13)	0.0117 (12)	−0.0015 (11)	−0.0200 (11)
C9A	0.0215 (10)	0.0186 (9)	0.0223 (10)	0.0008 (8)	0.0079 (8)	−0.0021 (8)
C10A	0.0267 (12)	0.0239 (11)	0.0262 (10)	0.0001 (9)	0.0152 (9)	−0.0007 (8)
C11A	0.0188 (10)	0.0155 (9)	0.0335 (11)	0.0012 (8)	0.0107 (8)	0.0015 (8)
C12A	0.0189 (10)	0.0163 (9)	0.0234 (9)	−0.0035 (8)	0.0029 (8)	−0.0011 (8)
C13A	0.0190 (10)	0.0223 (11)	0.0185 (9)	−0.0016 (9)	0.0037 (7)	0.0003 (8)
C14A	0.0155 (9)	0.0144 (9)	0.0191 (9)	0.0000 (8)	0.0037 (7)	−0.0002 (8)
C15A	0.0165 (8)	0.0152 (9)	0.0170 (8)	0.0009 (8)	0.0005 (7)	0.0006 (8)
C16A	0.0216 (11)	0.0234 (11)	0.0545 (16)	−0.0070 (9)	0.0079 (11)	−0.0021 (11)
C17A	0.0224 (11)	0.0202 (10)	0.0277 (11)	−0.0006 (9)	−0.0015 (8)	−0.0002 (9)
C18A	0.0189 (14)	0.0187 (15)	0.0257 (16)	0.0017 (12)	0.0025 (12)	0.0070 (12)
C19A	0.0214 (15)	0.0255 (17)	0.0225 (15)	0.0005 (13)	−0.0007 (12)	0.0013 (13)
C20A	0.034 (2)	0.0236 (17)	0.043 (2)	−0.0023 (16)	−0.0024 (17)	0.0124 (16)
C18E	0.025 (3)	0.029 (3)	0.017 (2)	−0.005 (2)	−0.001 (2)	−0.004 (2)
C19E	0.031 (3)	0.032 (3)	0.021 (3)	0.004 (3)	0.006 (2)	0.000 (2)
C20E	0.124 (10)	0.034 (4)	0.045 (5)	−0.011 (5)	0.051 (6)	−0.007 (4)
C21A	0.0314 (12)	0.0193 (10)	0.0196 (9)	0.0054 (9)	0.0001 (8)	−0.0052 (8)
C22A	0.0301 (12)	0.0229 (10)	0.0280 (11)	0.0026 (9)	0.0097 (9)	−0.0026 (9)
C23A	0.0272 (12)	0.0313 (13)	0.0515 (16)	0.0096 (10)	−0.0017 (11)	−0.0131 (12)
C24A	0.066 (2)	0.0389 (16)	0.0269 (11)	0.0265 (15)	−0.0066 (12)	−0.0031 (13)
Sn1B	0.01493 (6)	0.01194 (6)	0.01787 (6)	−0.00171 (5)	0.00371 (5)	−0.00083 (5)
N1B	0.0307 (11)	0.0225 (10)	0.0264 (10)	−0.0025 (9)	0.0007 (9)	−0.0085 (9)
N2B	0.0256 (9)	0.0184 (8)	0.0234 (8)	−0.0076 (7)	0.0109 (7)	−0.0009 (7)
O1B	0.0208 (8)	0.0171 (8)	0.0238 (8)	−0.0029 (6)	0.0046 (6)	−0.0023 (7)
O2B	0.0223 (8)	0.0139 (6)	0.0205 (7)	−0.0052 (6)	0.0055 (6)	−0.0051 (6)
O3B	0.0169 (7)	0.0139 (6)	0.0187 (7)	−0.0027 (6)	0.0059 (5)	−0.0030 (5)
O4B	0.0163 (7)	0.0145 (7)	0.0192 (7)	−0.0008 (6)	0.0050 (5)	0.0024 (5)
C1B	0.0178 (9)	0.0159 (9)	0.0242 (9)	−0.0016 (9)	0.0026 (7)	−0.0009 (9)
C2B	0.0211 (10)	0.0158 (9)	0.0263 (10)	−0.0035 (9)	−0.0002 (8)	−0.0016 (9)
C3B	0.0208 (10)	0.0143 (9)	0.0232 (10)	0.0022 (8)	−0.0029 (8)	−0.0019 (8)
C4B	0.0206 (10)	0.0204 (10)	0.0230 (10)	0.0009 (8)	0.0037 (8)	−0.0019 (8)
C5B	0.0206 (10)	0.0154 (9)	0.0245 (10)	−0.0007 (8)	0.0038 (8)	0.0007 (8)
C6B	0.0169 (9)	0.0115 (8)	0.0229 (10)	0.0002 (7)	0.0010 (8)	−0.0016 (8)
C7B	0.0163 (9)	0.0128 (8)	0.0198 (9)	0.0009 (7)	0.0028 (7)	0.0002 (7)
C8B	0.0326 (13)	0.0311 (13)	0.0265 (11)	0.0091 (11)	−0.0026 (10)	−0.0104 (11)
C9B	0.0204 (10)	0.0162 (9)	0.0159 (8)	−0.0015 (8)	0.0062 (8)	−0.0010 (8)
C10B	0.0216 (11)	0.0161 (9)	0.0197 (9)	−0.0021 (8)	0.0103 (8)	0.0009 (8)
C11B	0.0164 (9)	0.0105 (8)	0.0183 (8)	−0.0009 (7)	0.0042 (7)	0.0006 (7)
C12B	0.0194 (10)	0.0169 (9)	0.0164 (8)	−0.0040 (8)	0.0048 (7)	−0.0006 (7)
C13B	0.0175 (9)	0.0166 (9)	0.0163 (8)	−0.0037 (8)	0.0051 (7)	−0.0009 (8)
C14B	0.0140 (9)	0.0123 (8)	0.0181 (9)	0.0000 (7)	0.0040 (7)	0.0010 (7)
C15B	0.0112 (7)	0.0119 (8)	0.0184 (8)	0.0022 (7)	0.0029 (6)	0.0027 (7)
C16B	0.0223 (10)	0.0234 (10)	0.0311 (11)	−0.0095 (9)	0.0058 (9)	−0.0054 (9)
C17B	0.0145 (9)	0.0163 (9)	0.0177 (9)	−0.0007 (7)	0.0024 (7)	−0.0015 (7)
C18B	0.0171 (9)	0.0181 (10)	0.0174 (9)	−0.0006 (8)	0.0043 (7)	0.0019 (8)
C19B	0.0179 (9)	0.0187 (9)	0.0201 (9)	0.0019 (8)	0.0038 (7)	0.0033 (8)
C20B	0.0238 (11)	0.0212 (10)	0.0261 (10)	0.0028 (9)	0.0061 (8)	0.0046 (9)
C21B	0.0171 (9)	0.0161 (9)	0.0247 (10)	−0.0005 (8)	0.0041 (8)	0.0012 (8)

C22B	0.0190 (9)	0.0153 (8)	0.0231 (9)	0.0010 (7)	0.0060 (7)	0.0004 (7)
C23B	0.0245 (10)	0.0175 (9)	0.0247 (9)	0.0015 (9)	0.0045 (8)	0.0022 (8)
C24B	0.0372 (13)	0.0206 (10)	0.0293 (11)	0.0019 (9)	0.0090 (9)	0.0061 (9)
Sn1C	0.01712 (6)	0.01329 (6)	0.01889 (5)	−0.00262 (5)	0.00528 (5)	−0.00213 (5)
N1C	0.0252 (9)	0.0181 (8)	0.0246 (9)	−0.0066 (7)	0.0094 (7)	0.0007 (7)
N2C	0.0300 (11)	0.0250 (10)	0.0227 (9)	−0.0033 (9)	−0.0023 (8)	−0.0075 (8)
O1C	0.0193 (7)	0.0169 (7)	0.0183 (6)	−0.0036 (6)	0.0060 (5)	−0.0042 (5)
O2C	0.0189 (7)	0.0173 (7)	0.0183 (7)	−0.0036 (6)	0.0064 (5)	0.0001 (6)
O3C	0.0211 (8)	0.0206 (8)	0.0209 (8)	−0.0048 (7)	0.0053 (6)	−0.0034 (7)
O4C	0.0219 (8)	0.0202 (7)	0.0229 (7)	−0.0083 (6)	0.0059 (6)	−0.0060 (6)
C1C	0.0218 (10)	0.0144 (9)	0.0189 (9)	0.0016 (8)	0.0079 (8)	−0.0017 (7)
C2C	0.0232 (11)	0.0168 (9)	0.0190 (9)	−0.0014 (8)	0.0105 (8)	−0.0007 (7)
C3C	0.0143 (9)	0.0148 (9)	0.0243 (9)	−0.0005 (7)	0.0058 (7)	0.0033 (8)
C4C	0.0219 (10)	0.0177 (9)	0.0174 (9)	−0.0033 (8)	0.0035 (7)	−0.0026 (8)
C5C	0.0195 (9)	0.0156 (9)	0.0150 (8)	−0.0040 (8)	0.0040 (7)	0.0022 (7)
C6C	0.0131 (8)	0.0135 (8)	0.0169 (8)	0.0001 (7)	0.0027 (7)	−0.0002 (7)
C7C	0.0137 (8)	0.0125 (9)	0.0178 (8)	−0.0004 (7)	0.0034 (6)	−0.0012 (7)
C8C	0.0279 (12)	0.0300 (12)	0.0334 (12)	−0.0146 (10)	0.0013 (10)	0.0034 (10)
C9C	0.0186 (9)	0.0183 (10)	0.0224 (9)	−0.0046 (8)	0.0033 (7)	−0.0017 (8)
C10C	0.0226 (11)	0.0199 (10)	0.0244 (10)	−0.0057 (9)	−0.0003 (8)	−0.0044 (9)
C11C	0.0209 (10)	0.0164 (9)	0.0199 (9)	0.0016 (8)	−0.0024 (8)	−0.0033 (8)
C12C	0.0228 (10)	0.0183 (9)	0.0195 (9)	0.0014 (8)	0.0032 (8)	−0.0034 (8)
C13C	0.0166 (9)	0.0133 (8)	0.0231 (9)	−0.0014 (7)	0.0036 (7)	−0.0016 (7)
C14C	0.0182 (9)	0.0131 (8)	0.0194 (9)	−0.0014 (7)	0.0006 (7)	−0.0016 (7)
C15C	0.0190 (9)	0.0137 (8)	0.0208 (9)	−0.0016 (8)	0.0031 (7)	−0.0032 (7)
C16C	0.0327 (13)	0.0298 (12)	0.0221 (10)	0.0061 (11)	−0.0012 (9)	−0.0077 (10)
C17C	0.0233 (10)	0.0148 (9)	0.0281 (11)	0.0000 (8)	0.0019 (8)	0.0002 (8)
C18C	0.0275 (11)	0.0177 (9)	0.0275 (10)	−0.0006 (8)	0.0084 (8)	0.0007 (8)
C19C	0.0336 (12)	0.0222 (10)	0.0253 (10)	0.0040 (10)	0.0016 (9)	0.0020 (9)
C20C	0.0494 (17)	0.0286 (13)	0.0408 (14)	0.0065 (12)	0.0121 (12)	0.0118 (11)
C21C	0.0189 (10)	0.0175 (9)	0.0194 (9)	−0.0005 (8)	0.0059 (7)	−0.0009 (8)
C22C	0.0189 (10)	0.0194 (10)	0.0208 (9)	−0.0020 (8)	0.0056 (8)	0.0000 (8)
C23C	0.0193 (10)	0.0242 (11)	0.0218 (9)	−0.0026 (9)	0.0042 (8)	0.0016 (8)
C24C	0.0260 (12)	0.0237 (11)	0.0256 (10)	0.0014 (9)	0.0031 (9)	0.0056 (9)
Sn1D	0.01570 (6)	0.01273 (6)	0.01571 (5)	−0.00063 (5)	0.00253 (5)	−0.00088 (5)
N1D	0.0342 (12)	0.0244 (10)	0.0276 (10)	−0.0052 (9)	0.0020 (9)	−0.0126 (9)
N2D	0.0231 (9)	0.0174 (8)	0.0272 (9)	−0.0052 (7)	0.0121 (7)	−0.0018 (7)
O1D	0.0227 (8)	0.0168 (7)	0.0200 (7)	−0.0043 (6)	0.0034 (6)	−0.0048 (6)
O2D	0.0234 (8)	0.0183 (8)	0.0186 (7)	−0.0013 (7)	0.0047 (6)	−0.0020 (6)
O3D	0.0178 (6)	0.0150 (7)	0.0184 (6)	−0.0019 (6)	0.0047 (5)	0.0000 (5)
O4D	0.0179 (7)	0.0158 (7)	0.0202 (7)	−0.0022 (6)	0.0042 (6)	−0.0041 (6)
C1D	0.0212 (10)	0.0202 (10)	0.0200 (9)	−0.0033 (8)	0.0004 (7)	−0.0003 (8)
C2D	0.0252 (11)	0.0236 (11)	0.0192 (9)	−0.0006 (9)	0.0050 (8)	−0.0037 (8)
C3D	0.0244 (10)	0.0188 (10)	0.0222 (9)	0.0028 (9)	−0.0019 (8)	−0.0058 (9)
C4D	0.0214 (10)	0.0157 (9)	0.0249 (10)	−0.0036 (8)	−0.0003 (8)	−0.0057 (8)
C5D	0.0189 (9)	0.0167 (9)	0.0224 (9)	−0.0015 (8)	0.0028 (8)	−0.0019 (8)
C6D	0.0161 (9)	0.0141 (9)	0.0163 (8)	−0.0007 (7)	0.0006 (7)	−0.0023 (7)
C7D	0.0169 (9)	0.0146 (9)	0.0182 (9)	0.0011 (8)	0.0004 (7)	−0.0011 (8)
C8D	0.0394 (15)	0.0362 (14)	0.0236 (11)	0.0075 (12)	0.0000 (10)	−0.0118 (11)

C9D	0.0181 (9)	0.0157 (9)	0.0155 (8)	0.0000 (8)	0.0040 (7)	0.0001 (8)
C10D	0.0198 (9)	0.0157 (9)	0.0171 (8)	−0.0015 (8)	0.0047 (7)	−0.0003 (7)
C11D	0.0162 (9)	0.0125 (8)	0.0214 (9)	0.0015 (7)	0.0046 (7)	−0.0001 (7)
C12D	0.0241 (11)	0.0188 (10)	0.0180 (9)	0.0010 (9)	0.0094 (8)	0.0018 (8)
C13D	0.0194 (10)	0.0167 (9)	0.0165 (9)	0.0014 (8)	0.0031 (7)	−0.0014 (8)
C14D	0.0134 (9)	0.0137 (9)	0.0157 (8)	0.0027 (7)	0.0023 (7)	0.0015 (7)
C15D	0.0139 (8)	0.0125 (8)	0.0191 (8)	0.0016 (8)	0.0017 (7)	−0.0004 (8)
C16D	0.0203 (10)	0.0207 (10)	0.0367 (12)	−0.0052 (8)	0.0062 (9)	−0.0022 (9)
C17D	0.0342 (13)	0.0194 (10)	0.0174 (9)	0.0078 (9)	−0.0002 (8)	−0.0017 (8)
C18D	0.0178 (9)	0.0170 (8)	0.0214 (9)	0.0039 (7)	0.0057 (7)	−0.0043 (7)
C19D	0.0235 (10)	0.0272 (11)	0.0299 (11)	0.0095 (9)	−0.0021 (8)	−0.0087 (9)
C20D	0.0462 (15)	0.0286 (13)	0.0277 (11)	0.0168 (12)	−0.0035 (10)	−0.0031 (11)
C21D	0.0164 (9)	0.0182 (10)	0.0178 (9)	0.0002 (8)	0.0045 (7)	0.0010 (8)
C22D	0.0192 (10)	0.0192 (10)	0.0221 (10)	−0.0021 (8)	0.0055 (8)	0.0033 (8)
C23D	0.0190 (10)	0.0195 (9)	0.0229 (9)	0.0032 (8)	0.0033 (7)	0.0008 (8)
C24D	0.0297 (12)	0.0216 (10)	0.0280 (11)	0.0019 (9)	0.0043 (9)	0.0043 (9)

Geometric parameters (Å, °)

Sn1A—C21A	2.115 (2)	C23B—C24B	1.522 (3)
Sn1A—C17A	2.126 (3)	C23B—H23C	0.9700
Sn1A—O2A	2.1320 (16)	C23B—H23D	0.9700
Sn1A—O3A	2.1329 (17)	C24B—H24D	0.9600
Sn1A—O1A	2.4288 (19)	C24B—H24E	0.9600
N1A—C3A	1.366 (3)	C24B—H24F	0.9600
N1A—C8A	1.430 (4)	Sn1C—C21C	2.123 (2)
N1A—H1AB	0.8600	Sn1C—C17C	2.129 (2)
N2A—C11A	1.366 (3)	Sn1C—O4C	2.1467 (16)
N2A—C16A	1.437 (4)	Sn1C—O1C	2.1505 (16)
N2A—H2AB	0.8600	Sn1C—O3C	2.3986 (18)
O1A—C7A	1.256 (3)	N1C—C3C	1.358 (3)
O2A—C7A	1.296 (3)	N1C—C8C	1.446 (3)
O3A—C15A	1.303 (3)	N1C—H1NE	0.79 (3)
O4A—C15A	1.251 (3)	N2C—C11C	1.370 (3)
C1A—C2A	1.379 (4)	N2C—C16C	1.434 (4)
C1A—C6A	1.397 (4)	N2C—H1NF	0.77 (3)
C1A—H1AA	0.9300	O1C—C7C	1.295 (3)
C2A—C3A	1.395 (4)	O2C—C7C	1.250 (2)
C2A—H2AA	0.9300	O3C—C15C	1.256 (3)
C3A—C4A	1.400 (4)	O4C—C15C	1.298 (3)
C4A—C5A	1.391 (3)	C1C—C2C	1.372 (3)
C4A—H4AA	0.9300	C1C—C6C	1.405 (3)
C5A—C6A	1.386 (3)	C1C—H1CA	0.9300
C5A—H5AA	0.9300	C2C—C3C	1.408 (3)
C6A—C7A	1.469 (3)	C2C—H2CA	0.9300
C8A—H8AA	0.9600	C3C—C4C	1.411 (3)
C8A—H8AB	0.9600	C4C—C5C	1.375 (3)
C8A—H8AC	0.9600	C4C—H4CA	0.9300
C9A—C10A	1.378 (4)	C5C—C6C	1.399 (3)

C9A—C14A	1.402 (3)	C5C—H5CA	0.9300
C9A—H9AA	0.9300	C6C—C7C	1.472 (3)
C10A—C11A	1.403 (4)	C8C—H8CA	0.9600
C10A—H10A	0.9300	C8C—H8CB	0.9600
C11A—C12A	1.400 (3)	C8C—H8CC	0.9600
C12A—C13A	1.388 (4)	C9C—C10C	1.379 (3)
C12A—H12A	0.9300	C9C—C14C	1.401 (3)
C13A—C14A	1.394 (3)	C9C—H9CA	0.9300
C13A—H13A	0.9300	C10C—C11C	1.413 (3)
C14A—C15A	1.472 (3)	C10C—H10C	0.9300
C16A—H16A	0.9600	C11C—C12C	1.401 (3)
C16A—H16B	0.9600	C12C—C13C	1.392 (3)
C16A—H16C	0.9600	C12C—H12C	0.9300
C17A—C18E	1.435 (6)	C13C—C14C	1.385 (3)
C17A—C18A	1.572 (5)	C13C—H13C	0.9300
C17A—H17A	0.9601	C14C—C15C	1.473 (3)
C17A—H17B	0.9600	C16C—H16G	0.9600
C17A—H17I	0.9599	C16C—H16H	0.9600
C17A—H17J	0.9599	C16C—H16I	0.9600
C18A—C19A	1.510 (5)	C17C—C18C	1.521 (3)
C18A—H18A	0.9700	C17C—H17E	0.9700
C18A—H18B	0.9700	C17C—H17H	0.9700
C19A—C20A	1.527 (6)	C18C—C19C	1.517 (3)
C19A—H19A	0.9700	C18C—H18E	0.9700
C19A—H19B	0.9700	C18C—H18F	0.9700
C20A—H20A	0.9600	C19C—C20C	1.524 (4)
C20A—H20B	0.9600	C19C—H19E	0.9700
C20A—H20C	0.9600	C19C—H19F	0.9700
C18E—C19E	1.528 (9)	C20C—H20G	0.9600
C18E—H17B	1.2682	C20C—H20H	0.9600
C18E—H18I	0.9700	C20C—H20I	0.9600
C18E—H18J	0.9700	C21C—C22C	1.537 (3)
C19E—C20E	1.512 (11)	C21C—H21D	0.9700
C19E—H19I	0.9700	C21C—H21E	0.9700
C19E—H19J	0.9700	C22C—C23C	1.526 (4)
C20E—H20M	0.9600	C22C—H22E	0.9700
C20E—H20N	0.9600	C22C—H22F	0.9700
C20E—H20O	0.9600	C23C—C24C	1.524 (4)
C21A—C22A	1.526 (4)	C23C—H23G	0.9700
C21A—H21A	0.9700	C23C—H23H	0.9700
C21A—H21B	0.9700	C24C—H24G	0.9600
C22A—C23A	1.532 (4)	C24C—H24H	0.9600
C22A—H22A	0.9700	C24C—H24I	0.9600
C22A—H22B	0.9700	Sn1D—C17D	2.119 (2)
C23A—C24A	1.515 (4)	Sn1D—C21D	2.120 (2)
C23A—H23A	0.9700	Sn1D—O1D	2.1266 (16)
C23A—H23B	0.9700	Sn1D—O4D	2.1514 (17)
C24A—H24A	0.9600	Sn1D—O2D	2.4412 (19)
C24A—H24B	0.9600	Sn1D—O3D	2.5252 (17)

C24A—H24C	0.9600	N1D—C3D	1.366 (3)
Sn1B—C21B	2.119 (2)	N1D—C8D	1.441 (4)
Sn1B—C17B	2.131 (2)	N1D—H1NG	0.77 (4)
Sn1B—O2B	2.1390 (16)	N2D—C11D	1.362 (3)
Sn1B—O3B	2.1534 (16)	N2D—C16D	1.453 (3)
Sn1B—O1B	2.4182 (19)	N2D—H1NH	0.84 (3)
Sn1B—O4B	2.5288 (17)	O1D—C7D	1.306 (3)
N1B—C3B	1.362 (3)	O2D—C7D	1.248 (3)
N1B—C8B	1.449 (4)	O3D—C15D	1.252 (3)
N1B—H1NC	0.84 (3)	O4D—C15D	1.294 (3)
N2B—C11B	1.356 (3)	C1D—C2D	1.386 (3)
N2B—C16B	1.441 (3)	C1D—C6D	1.396 (3)
N2B—H1ND	0.84 (3)	C1D—H1DA	0.9300
O1B—C7B	1.266 (3)	C2D—C3D	1.400 (4)
O2B—C7B	1.288 (3)	C2D—H2DA	0.9300
O3B—C15B	1.305 (3)	C3D—C4D	1.406 (4)
O4B—C15B	1.256 (2)	C4D—C5D	1.383 (3)
C1B—C2B	1.379 (3)	C4D—H4DA	0.9300
C1B—C6B	1.403 (3)	C5D—C6D	1.400 (3)
C1B—H1BA	0.9300	C5D—H5DA	0.9300
C2B—C3B	1.410 (4)	C6D—C7D	1.470 (3)
C2B—H2BA	0.9300	C8D—H8DA	0.9600
C3B—C4B	1.405 (4)	C8D—H8DB	0.9600
C4B—C5B	1.390 (3)	C8D—H8DC	0.9600
C4B—H4BA	0.9300	C9D—C10D	1.375 (3)
C5B—C6B	1.385 (3)	C9D—C14D	1.400 (3)
C5B—H5BA	0.9300	C9D—H9DA	0.9300
C6B—C7B	1.473 (3)	C10D—C11D	1.398 (3)
C8B—H8BA	0.9600	C10D—H10D	0.9300
C8B—H8BB	0.9600	C11D—C12D	1.415 (3)
C8B—H8BC	0.9600	C12D—C13D	1.382 (4)
C9B—C10B	1.372 (3)	C12D—H12D	0.9300
C9B—C14B	1.410 (3)	C13D—C14D	1.401 (3)
C9B—H9BA	0.9300	C13D—H13D	0.9300
C10B—C11B	1.414 (3)	C14D—C15D	1.472 (3)
C10B—H10B	0.9300	C16D—H16J	0.9600
C11B—C12B	1.404 (3)	C16D—H16K	0.9600
C12B—C13B	1.388 (3)	C16D—H16L	0.9600
C12B—H12B	0.9300	C17D—C18D	1.520 (3)
C13B—C14B	1.399 (3)	C17D—H17F	0.9700
C13B—H13B	0.9300	C17D—H17G	0.9700
C14B—C15B	1.462 (3)	C18D—C19D	1.535 (3)
C16B—H16D	0.9600	C18D—H18G	0.9700
C16B—H16E	0.9600	C18D—H18H	0.9700
C16B—H16F	0.9600	C19D—C20D	1.519 (4)
C17B—C18B	1.528 (4)	C19D—H19G	0.9700
C17B—H17C	0.9700	C19D—H19H	0.9700
C17B—H17D	0.9700	C20D—H20J	0.9600
C18B—C19B	1.520 (4)	C20D—H20K	0.9600

C18B—H18C	0.9700	C20D—H20L	0.9600
C18B—H18D	0.9700	C21D—C22D	1.528 (3)
C19B—C20B	1.533 (4)	C21D—H21F	0.9700
C19B—H19C	0.9700	C21D—H21G	0.9700
C19B—H19D	0.9700	C22D—C23D	1.523 (3)
C20B—H20D	0.9600	C22D—H22G	0.9700
C20B—H20E	0.9600	C22D—H22H	0.9700
C20B—H20F	0.9600	C23D—C24D	1.518 (4)
C21B—C22B	1.523 (3)	C23D—H23E	0.9700
C21B—H21C	0.9700	C23D—H23F	0.9700
C21B—H21H	0.9700	C24D—H24J	0.9600
C22B—C23B	1.531 (3)	C24D—H24K	0.9600
C22B—H22C	0.9700	C24D—H24L	0.9600
C22B—H22D	0.9700		
C21A—Sn1A—C17A	152.63 (10)	C23B—C22B—H22C	109.3
C21A—Sn1A—O2A	102.24 (8)	C21B—C22B—H22D	109.3
C17A—Sn1A—O2A	99.76 (9)	C23B—C22B—H22D	109.3
C21A—Sn1A—O3A	99.74 (9)	H22C—C22B—H22D	107.9
C17A—Sn1A—O3A	100.45 (9)	C24B—C23B—C22B	112.96 (19)
O2A—Sn1A—O3A	78.49 (6)	C24B—C23B—H23C	109.0
C21A—Sn1A—O1A	90.00 (8)	C22B—C23B—H23C	109.0
C17A—Sn1A—O1A	88.41 (9)	C24B—C23B—H23D	109.0
O2A—Sn1A—O1A	57.11 (6)	C22B—C23B—H23D	109.0
O3A—Sn1A—O1A	135.60 (6)	H23C—C23B—H23D	107.8
C21A—Sn1A—C7A	97.02 (8)	C23B—C24B—H24D	109.5
C17A—Sn1A—C7A	94.38 (9)	C23B—C24B—H24E	109.5
O2A—Sn1A—C7A	28.92 (7)	H24D—C24B—H24E	109.5
O3A—Sn1A—C7A	107.41 (7)	C23B—C24B—H24F	109.5
O1A—Sn1A—C7A	28.19 (7)	H24D—C24B—H24F	109.5
C3A—N1A—C8A	123.6 (3)	H24E—C24B—H24F	109.5
C3A—N1A—H1AB	118.2	C21C—Sn1C—C17C	157.58 (9)
C8A—N1A—H1AB	118.2	C21C—Sn1C—O4C	98.36 (8)
C11A—N2A—C16A	123.3 (2)	C17C—Sn1C—O4C	100.35 (9)
C11A—N2A—H2AB	118.4	C21C—Sn1C—O1C	98.34 (8)
C16A—N2A—H2AB	118.4	C17C—Sn1C—O1C	97.07 (8)
C7A—O1A—Sn1A	85.80 (14)	O4C—Sn1C—O1C	79.72 (6)
C7A—O2A—Sn1A	98.38 (14)	C21C—Sn1C—O3C	89.19 (8)
C15A—O3A—Sn1A	103.79 (13)	C17C—Sn1C—O3C	90.50 (8)
C2A—C1A—C6A	120.3 (2)	O4C—Sn1C—O3C	57.47 (6)
C2A—C1A—H1AA	119.9	O1C—Sn1C—O3C	137.19 (6)
C6A—C1A—H1AA	119.9	C21C—Sn1C—C15C	94.05 (8)
C1A—C2A—C3A	121.4 (3)	C17C—Sn1C—C15C	96.26 (8)
C1A—C2A—H2AA	119.3	O4C—Sn1C—C15C	29.16 (6)
C3A—C2A—H2AA	119.3	O1C—Sn1C—C15C	108.88 (6)
N1A—C3A—C2A	120.5 (3)	O3C—Sn1C—C15C	28.32 (6)
N1A—C3A—C4A	121.3 (2)	C3C—N1C—C8C	123.7 (2)
C2A—C3A—C4A	118.2 (2)	C3C—N1C—H1NE	111 (2)
C5A—C4A—C3A	120.3 (2)	C8C—N1C—H1NE	121 (2)
C5A—C4A—H4AA	119.9	C11C—N2C—C16C	123.7 (2)

C3A—C4A—H4AA	119.9	C11C—N2C—H1NF	113 (2)
C6A—C5A—C4A	121.0 (2)	C16C—N2C—H1NF	120 (2)
C6A—C5A—H5AA	119.5	C7C—O1C—Sn1C	102.48 (12)
C4A—C5A—H5AA	119.5	C15C—O3C—Sn1C	86.73 (13)
C5A—C6A—C1A	118.8 (2)	C15C—O4C—Sn1C	97.16 (13)
C5A—C6A—C7A	120.9 (2)	C2C—C1C—C6C	120.8 (2)
C1A—C6A—C7A	120.3 (2)	C2C—C1C—H1CA	119.6
O1A—C7A—O2A	118.7 (2)	C6C—C1C—H1CA	119.6
O1A—C7A—C6A	123.3 (2)	C1C—C2C—C3C	121.2 (2)
O2A—C7A—C6A	118.0 (2)	C1C—C2C—H2CA	119.4
O1A—C7A—Sn1A	66.00 (13)	C3C—C2C—H2CA	119.4
O2A—C7A—Sn1A	52.70 (11)	N1C—C3C—C2C	119.9 (2)
C6A—C7A—Sn1A	170.69 (17)	N1C—C3C—C4C	122.3 (2)
N1A—C8A—H8AA	109.5	C2C—C3C—C4C	117.8 (2)
N1A—C8A—H8AB	109.5	C5C—C4C—C3C	120.7 (2)
H8AA—C8A—H8AB	109.5	C5C—C4C—H4CA	119.6
N1A—C8A—H8AC	109.5	C3C—C4C—H4CA	119.6
H8AA—C8A—H8AC	109.5	C4C—C5C—C6C	121.2 (2)
H8AB—C8A—H8AC	109.5	C4C—C5C—H5CA	119.4
C10A—C9A—C14A	120.5 (2)	C6C—C5C—H5CA	119.4
C10A—C9A—H9AA	119.7	C5C—C6C—C1C	118.2 (2)
C14A—C9A—H9AA	119.7	C5C—C6C—C7C	120.53 (19)
C9A—C10A—C11A	120.9 (2)	C1C—C6C—C7C	121.2 (2)
C9A—C10A—H10A	119.6	O2C—C7C—O1C	119.2 (2)
C11A—C10A—H10A	119.6	O2C—C7C—C6C	122.65 (19)
N2A—C11A—C12A	121.6 (2)	O1C—C7C—C6C	118.18 (18)
N2A—C11A—C10A	119.8 (2)	N1C—C8C—H8CA	109.5
C12A—C11A—C10A	118.6 (2)	N1C—C8C—H8CB	109.5
C13A—C12A—C11A	120.2 (2)	H8CA—C8C—H8CB	109.5
C13A—C12A—H12A	119.9	N1C—C8C—H8CC	109.5
C11A—C12A—H12A	119.9	H8CA—C8C—H8CC	109.5
C12A—C13A—C14A	121.0 (2)	H8CB—C8C—H8CC	109.5
C12A—C13A—H13A	119.5	C10C—C9C—C14C	120.3 (2)
C14A—C13A—H13A	119.5	C10C—C9C—H9CA	119.8
C13A—C14A—C9A	118.7 (2)	C14C—C9C—H9CA	119.8
C13A—C14A—C15A	120.6 (2)	C9C—C10C—C11C	120.6 (2)
C9A—C14A—C15A	120.7 (2)	C9C—C10C—H10C	119.7
O4A—C15A—O3A	119.4 (2)	C11C—C10C—H10C	119.7
O4A—C15A—C14A	123.1 (2)	N2C—C11C—C12C	121.6 (2)
O3A—C15A—C14A	117.52 (19)	N2C—C11C—C10C	119.6 (2)
N2A—C16A—H16A	109.5	C12C—C11C—C10C	118.8 (2)
N2A—C16A—H16B	109.5	C13C—C12C—C11C	119.7 (2)
H16A—C16A—H16B	109.5	C13C—C12C—H12C	120.2
N2A—C16A—H16C	109.5	C11C—C12C—H12C	120.2
H16A—C16A—H16C	109.5	C14C—C13C—C12C	121.4 (2)
H16B—C16A—H16C	109.5	C14C—C13C—H13C	119.3
C18E—C17A—C18A	49.8 (3)	C12C—C13C—H13C	119.3
C18E—C17A—Sn1A	120.3 (3)	C13C—C14C—C9C	119.1 (2)
C18A—C17A—Sn1A	110.95 (19)	C13C—C14C—C15C	121.2 (2)

C18E—C17A—H17A	130.1	C9C—C14C—C15C	119.7 (2)
C18A—C17A—H17A	109.5	O3C—C15C—O4C	118.6 (2)
Sn1A—C17A—H17A	109.4	O3C—C15C—C14C	123.1 (2)
C18E—C17A—H17B	60.1	O4C—C15C—C14C	118.2 (2)
C18A—C17A—H17B	109.4	O3C—C15C—Sn1C	64.95 (12)
Sn1A—C17A—H17B	109.4	O4C—C15C—Sn1C	53.69 (11)
H17A—C17A—H17B	108.1	C14C—C15C—Sn1C	171.90 (16)
C18E—C17A—H17I	107.4	N2C—C16C—H16G	109.5
C18A—C17A—H17I	64.1	N2C—C16C—H16H	109.5
Sn1A—C17A—H17I	107.3	H16G—C16C—H16H	109.5
H17A—C17A—H17I	49.8	N2C—C16C—H16I	109.5
H17B—C17A—H17I	142.2	H16G—C16C—H16I	109.5
C18E—C17A—H17J	107.2	H16H—C16C—H16I	109.5
C18A—C17A—H17J	141.9	C18C—C17C—Sn1C	118.86 (16)
Sn1A—C17A—H17J	107.1	C18C—C17C—H17E	107.6
H17A—C17A—H17J	58.4	Sn1C—C17C—H17E	107.6
H17B—C17A—H17J	53.5	C18C—C17C—H17H	107.6
H17I—C17A—H17J	106.9	Sn1C—C17C—H17H	107.6
C19A—C18A—C17A	111.2 (3)	H17E—C17C—H17H	107.0
C19A—C18A—H17I	101.8	C19C—C18C—C17C	111.7 (2)
C19A—C18A—H18A	109.4	C19C—C18C—H18E	109.3
C17A—C18A—H18A	109.4	C17C—C18C—H18E	109.3
H17I—C18A—H18A	80.2	C19C—C18C—H18F	109.3
C19A—C18A—H18B	109.4	C17C—C18C—H18F	109.3
C17A—C18A—H18B	109.4	H18E—C18C—H18F	107.9
H17I—C18A—H18B	142.1	C18C—C19C—C20C	113.4 (2)
H18A—C18A—H18B	108.0	C18C—C19C—H19E	108.9
C18A—C19A—C20A	113.3 (3)	C20C—C19C—H19E	108.9
C18A—C19A—H19A	108.9	C18C—C19C—H19F	108.9
C20A—C19A—H19A	108.9	C20C—C19C—H19F	108.9
C18A—C19A—H19B	108.9	H19E—C19C—H19F	107.7
C20A—C19A—H19B	108.9	C19C—C20C—H20G	109.5
H19A—C19A—H19B	107.7	C19C—C20C—H20H	109.5
C17A—C18E—C19E	111.6 (4)	H20G—C20C—H20H	109.5
C19E—C18E—H17B	152.2	C19C—C20C—H20I	109.5
C17A—C18E—H18I	109.3	H20G—C20C—H20I	109.5
C19E—C18E—H18I	109.3	H20H—C20C—H20I	109.5
H17B—C18E—H18I	89.2	C22C—C21C—Sn1C	113.89 (15)
C17A—C18E—H18J	109.3	C22C—C21C—H21D	108.8
C19E—C18E—H18J	109.3	Sn1C—C21C—H21D	108.8
H17B—C18E—H18J	83.0	C22C—C21C—H21E	108.8
H18I—C18E—H18J	108.0	Sn1C—C21C—H21E	108.8
C20E—C19E—C18E	112.6 (6)	H21D—C21C—H21E	107.7
C20E—C19E—H19I	109.1	C23C—C22C—C21C	112.4 (2)
C18E—C19E—H19I	109.1	C23C—C22C—H22E	109.1
C20E—C19E—H19J	109.1	C21C—C22C—H22E	109.1
C18E—C19E—H19J	109.1	C23C—C22C—H22F	109.1
H19I—C19E—H19J	107.8	C21C—C22C—H22F	109.1
C19E—C20E—H20M	109.5	H22E—C22C—H22F	107.8

C19E—C20E—H20N	109.5	C24C—C23C—C22C	112.6 (2)
H20M—C20E—H20N	109.5	C24C—C23C—H23G	109.1
C19E—C20E—H20O	109.5	C22C—C23C—H23G	109.1
H20M—C20E—H20O	109.5	C24C—C23C—H23H	109.1
H20N—C20E—H20O	109.5	C22C—C23C—H23H	109.1
C22A—C21A—Sn1A	112.58 (15)	H23G—C23C—H23H	107.8
C22A—C21A—H21A	109.1	C23C—C24C—H24G	109.5
Sn1A—C21A—H21A	109.1	C23C—C24C—H24H	109.5
C22A—C21A—H21B	109.1	H24G—C24C—H24H	109.5
Sn1A—C21A—H21B	109.1	C23C—C24C—H24I	109.5
H21A—C21A—H21B	107.8	H24G—C24C—H24I	109.5
C21A—C22A—C23A	113.4 (2)	H24H—C24C—H24I	109.5
C21A—C22A—H22A	108.9	C17D—Sn1D—C21D	152.92 (10)
C23A—C22A—H22A	108.9	C17D—Sn1D—O1D	102.60 (8)
C21A—C22A—H22B	108.9	C21D—Sn1D—O1D	98.89 (8)
C23A—C22A—H22B	108.9	C17D—Sn1D—O4D	99.36 (9)
H22A—C22A—H22B	107.7	C21D—Sn1D—O4D	100.57 (8)
C24A—C23A—C22A	114.1 (2)	O1D—Sn1D—O4D	79.58 (6)
C24A—C23A—H23A	108.7	C17D—Sn1D—O2D	89.87 (8)
C22A—C23A—H23A	108.7	C21D—Sn1D—O2D	88.12 (8)
C24A—C23A—H23B	108.7	O1D—Sn1D—O2D	57.05 (6)
C22A—C23A—H23B	108.7	O4D—Sn1D—O2D	136.62 (6)
H23A—C23A—H23B	107.6	C17D—Sn1D—O3D	87.68 (8)
C23A—C24A—H24A	109.5	C21D—Sn1D—O3D	88.73 (8)
C23A—C24A—H24B	109.5	O1D—Sn1D—O3D	134.91 (6)
H24A—C24A—H24B	109.5	O4D—Sn1D—O3D	55.36 (5)
C23A—C24A—H24C	109.5	O2D—Sn1D—O3D	168.02 (5)
H24A—C24A—H24C	109.5	C17D—Sn1D—C7D	96.85 (8)
H24B—C24A—H24C	109.5	C21D—Sn1D—C7D	93.93 (8)
C21B—Sn1B—C17B	155.44 (9)	O1D—Sn1D—C7D	29.10 (7)
C21B—Sn1B—O2B	100.39 (8)	O4D—Sn1D—C7D	108.67 (7)
C17B—Sn1B—O2B	99.57 (8)	O2D—Sn1D—C7D	27.95 (6)
C21B—Sn1B—O3B	98.44 (8)	O3D—Sn1D—C7D	164.00 (6)
C17B—Sn1B—O3B	98.86 (8)	C3D—N1D—C8D	123.5 (3)
O2B—Sn1B—O3B	80.39 (6)	C3D—N1D—H1NG	116 (2)
C21B—Sn1B—O1B	90.16 (8)	C8D—N1D—H1NG	114 (2)
C17B—Sn1B—O1B	88.68 (8)	C11D—N2D—C16D	122.5 (2)
O2B—Sn1B—O1B	57.34 (6)	C11D—N2D—H1NH	111.3 (19)
O3B—Sn1B—O1B	137.72 (6)	C16D—N2D—H1NH	117.5 (18)
C21B—Sn1B—O4B	87.47 (8)	C7D—O1D—Sn1D	98.52 (13)
C17B—Sn1B—O4B	88.21 (7)	C7D—O2D—Sn1D	85.60 (15)
O2B—Sn1B—O4B	135.61 (6)	C15D—O3D—Sn1D	84.50 (14)
O3B—Sn1B—O4B	55.22 (6)	C15D—O4D—Sn1D	100.73 (13)
O1B—Sn1B—O4B	167.04 (5)	C2D—C1D—C6D	121.2 (2)
C21B—Sn1B—C7B	95.87 (8)	C2D—C1D—H1DA	119.4
C17B—Sn1B—C7B	94.74 (8)	C6D—C1D—H1DA	119.4
O2B—Sn1B—C7B	28.83 (6)	C1D—C2D—C3D	120.1 (2)
O3B—Sn1B—C7B	109.22 (7)	C1D—C2D—H2DA	119.9
O1B—Sn1B—C7B	28.51 (6)	C3D—C2D—H2DA	119.9

O4B—Sn1B—C7B	164.44 (6)	N1D—C3D—C2D	121.7 (2)
C3B—N1B—C8B	123.4 (3)	N1D—C3D—C4D	119.6 (2)
C3B—N1B—H1NC	119 (2)	C2D—C3D—C4D	118.8 (2)
C8B—N1B—H1NC	118 (2)	C5D—C4D—C3D	120.7 (2)
C11B—N2B—C16B	123.3 (2)	C5D—C4D—H4DA	119.6
C11B—N2B—H1ND	117.0 (19)	C3D—C4D—H4DA	119.6
C16B—N2B—H1ND	119.1 (19)	C4D—C5D—C6D	120.4 (2)
C7B—O1B—Sn1B	85.78 (14)	C4D—C5D—H5DA	119.8
C7B—O2B—Sn1B	97.98 (13)	C6D—C5D—H5DA	119.8
C15B—O3B—Sn1B	101.30 (13)	C1D—C6D—C5D	118.8 (2)
C15B—O4B—Sn1B	85.21 (14)	C1D—C6D—C7D	121.0 (2)
C2B—C1B—C6B	120.7 (2)	C5D—C6D—C7D	120.2 (2)
C2B—C1B—H1BA	119.7	O2D—C7D—O1D	118.8 (2)
C6B—C1B—H1BA	119.7	O2D—C7D—C6D	123.1 (2)
C1B—C2B—C3B	120.5 (2)	O1D—C7D—C6D	118.0 (2)
C1B—C2B—H2BA	119.7	O2D—C7D—Sn1D	66.45 (13)
C3B—C2B—H2BA	119.7	O1D—C7D—Sn1D	52.38 (11)
N1B—C3B—C4B	122.1 (2)	C6D—C7D—Sn1D	170.42 (17)
N1B—C3B—C2B	119.4 (2)	N1D—C8D—H8DA	109.5
C4B—C3B—C2B	118.5 (2)	N1D—C8D—H8DB	109.5
C5B—C4B—C3B	120.2 (2)	H8DA—C8D—H8DB	109.5
C5B—C4B—H4BA	119.9	N1D—C8D—H8DC	109.5
C3B—C4B—H4BA	119.9	H8DA—C8D—H8DC	109.5
C6B—C5B—C4B	121.0 (2)	H8DB—C8D—H8DC	109.5
C6B—C5B—H5BA	119.5	C10D—C9D—C14D	120.8 (2)
C4B—C5B—H5BA	119.5	C10D—C9D—H9DA	119.6
C5B—C6B—C1B	119.0 (2)	C14D—C9D—H9DA	119.6
C5B—C6B—C7B	120.6 (2)	C9D—C10D—C11D	121.4 (2)
C1B—C6B—C7B	120.4 (2)	C9D—C10D—H10D	119.3
O1B—C7B—O2B	118.9 (2)	C11D—C10D—H10D	119.3
O1B—C7B—C6B	122.0 (2)	N2D—C11D—C10D	122.5 (2)
O2B—C7B—C6B	119.1 (2)	N2D—C11D—C12D	119.4 (2)
O1B—C7B—Sn1B	65.72 (13)	C10D—C11D—C12D	118.0 (2)
O2B—C7B—Sn1B	53.19 (11)	C13D—C12D—C11D	120.3 (2)
C6B—C7B—Sn1B	172.28 (17)	C13D—C12D—H12D	119.8
N1B—C8B—H8BA	109.5	C11D—C12D—H12D	119.8
N1B—C8B—H8BB	109.5	C12D—C13D—C14D	121.1 (2)
H8BA—C8B—H8BB	109.5	C12D—C13D—H13D	119.5
N1B—C8B—H8BC	109.5	C14D—C13D—H13D	119.5
H8BA—C8B—H8BC	109.5	C9D—C14D—C13D	118.4 (2)
H8BB—C8B—H8BC	109.5	C9D—C14D—C15D	120.1 (2)
C10B—C9B—C14B	120.7 (2)	C13D—C14D—C15D	121.5 (2)
C10B—C9B—H9BA	119.6	O3D—C15D—O4D	119.4 (2)
C14B—C9B—H9BA	119.6	O3D—C15D—C14D	122.6 (2)
C9B—C10B—C11B	121.0 (2)	O4D—C15D—C14D	118.07 (19)
C9B—C10B—H10B	119.5	N2D—C16D—H16J	109.5
C11B—C10B—H10B	119.5	N2D—C16D—H16K	109.5
N2B—C11B—C12B	121.7 (2)	H16J—C16D—H16K	109.5
N2B—C11B—C10B	120.0 (2)	N2D—C16D—H16L	109.5

C12B—C11B—C10B	118.3 (2)	H16J—C16D—H16L	109.5
C13B—C12B—C11B	120.4 (2)	H16K—C16D—H16L	109.5
C13B—C12B—H12B	119.8	C18D—C17D—Sn1D	113.62 (15)
C11B—C12B—H12B	119.8	C18D—C17D—H17F	108.8
C12B—C13B—C14B	121.2 (2)	Sn1D—C17D—H17F	108.8
C12B—C13B—H13B	119.4	C18D—C17D—H17G	108.8
C14B—C13B—H13B	119.4	Sn1D—C17D—H17G	108.8
C13B—C14B—C9B	118.4 (2)	H17F—C17D—H17G	107.7
C13B—C14B—C15B	120.0 (2)	C17D—C18D—C19D	112.37 (19)
C9B—C14B—C15B	121.7 (2)	C17D—C18D—H18G	109.1
O4B—C15B—O3B	118.0 (2)	C19D—C18D—H18G	109.1
O4B—C15B—C14B	122.6 (2)	C17D—C18D—H18H	109.1
O3B—C15B—C14B	119.34 (18)	C19D—C18D—H18H	109.1
N2B—C16B—H16D	109.5	H18G—C18D—H18H	107.9
N2B—C16B—H16E	109.5	C20D—C19D—C18D	113.2 (2)
H16D—C16B—H16E	109.5	C20D—C19D—H19G	108.9
N2B—C16B—H16F	109.5	C18D—C19D—H19G	108.9
H16D—C16B—H16F	109.5	C20D—C19D—H19H	108.9
H16E—C16B—H16F	109.5	C18D—C19D—H19H	108.9
C18B—C17B—Sn1B	113.72 (15)	H19G—C19D—H19H	107.8
C18B—C17B—H17C	108.8	C19D—C20D—H20J	109.5
Sn1B—C17B—H17C	108.8	C19D—C20D—H20K	109.5
C18B—C17B—H17D	108.8	H20J—C20D—H20K	109.5
Sn1B—C17B—H17D	108.8	C19D—C20D—H20L	109.5
H17C—C17B—H17D	107.7	H20J—C20D—H20L	109.5
C19B—C18B—C17B	112.31 (19)	H20K—C20D—H20L	109.5
C19B—C18B—H18C	109.1	C22D—C21D—Sn1D	113.27 (15)
C17B—C18B—H18C	109.1	C22D—C21D—H21F	108.9
C19B—C18B—H18D	109.1	Sn1D—C21D—H21F	108.9
C17B—C18B—H18D	109.1	C22D—C21D—H21G	108.9
H18C—C18B—H18D	107.9	Sn1D—C21D—H21G	108.9
C18B—C19B—C20B	111.9 (2)	H21F—C21D—H21G	107.7
C18B—C19B—H19C	109.2	C23D—C22D—C21D	112.9 (2)
C20B—C19B—H19C	109.2	C23D—C22D—H22G	109.0
C18B—C19B—H19D	109.2	C21D—C22D—H22G	109.0
C20B—C19B—H19D	109.2	C23D—C22D—H22H	109.0
H19C—C19B—H19D	107.9	C21D—C22D—H22H	109.0
C19B—C20B—H20D	109.5	H22G—C22D—H22H	107.8
C19B—C20B—H20E	109.5	C24D—C23D—C22D	111.8 (2)
H20D—C20B—H20E	109.5	C24D—C23D—H23E	109.2
C19B—C20B—H20F	109.5	C22D—C23D—H23E	109.2
H20D—C20B—H20F	109.5	C24D—C23D—H23F	109.2
H20E—C20B—H20F	109.5	C22D—C23D—H23F	109.2
C22B—C21B—Sn1B	118.39 (15)	H23E—C23D—H23F	107.9
C22B—C21B—H21C	107.7	C23D—C24D—H24J	109.5
Sn1B—C21B—H21C	107.7	C23D—C24D—H24K	109.5
C22B—C21B—H21H	107.7	H24J—C24D—H24K	109.5
Sn1B—C21B—H21H	107.7	C23D—C24D—H24L	109.5
H21C—C21B—H21H	107.1	H24J—C24D—H24L	109.5

C21B—C22B—C23B	111.73 (17)	H24K—C24D—H24L	109.5
C21B—C22B—H22C	109.3		
C21A—Sn1A—O1A—C7A	−104.99 (16)	O4B—Sn1B—C21B—C22B	129.92 (18)
C17A—Sn1A—O1A—C7A	102.34 (16)	C7B—Sn1B—C21B—C22B	−65.32 (18)
O2A—Sn1A—O1A—C7A	−0.36 (14)	Sn1B—C21B—C22B—C23B	176.83 (15)
O3A—Sn1A—O1A—C7A	−1.01 (19)	C21B—C22B—C23B—C24B	177.7 (2)
C21A—Sn1A—O2A—C7A	82.29 (16)	C21C—Sn1C—O1C—C7C	−78.75 (14)
C17A—Sn1A—O2A—C7A	−81.32 (16)	C17C—Sn1C—O1C—C7C	84.92 (14)
O3A—Sn1A—O2A—C7A	179.89 (16)	O4C—Sn1C—O1C—C7C	−175.79 (14)
O1A—Sn1A—O2A—C7A	0.35 (14)	O3C—Sn1C—O1C—C7C	−176.64 (12)
C21A—Sn1A—O3A—C15A	−84.75 (15)	C15C—Sn1C—O1C—C7C	−175.96 (13)
C17A—Sn1A—O3A—C15A	76.66 (16)	C21C—Sn1C—O3C—C15C	−100.08 (15)
O2A—Sn1A—O3A—C15A	174.61 (15)	C17C—Sn1C—O3C—C15C	102.34 (15)
O1A—Sn1A—O3A—C15A	175.16 (13)	O4C—Sn1C—O3C—C15C	0.37 (13)
C7A—Sn1A—O3A—C15A	174.66 (14)	O1C—Sn1C—O3C—C15C	1.35 (18)
C6A—C1A—C2A—C3A	0.1 (5)	C21C—Sn1C—O4C—C15C	83.29 (15)
C8A—N1A—C3A—C2A	−178.2 (3)	C17C—Sn1C—O4C—C15C	−84.28 (15)
C8A—N1A—C3A—C4A	2.0 (4)	O1C—Sn1C—O4C—C15C	−179.68 (15)
C1A—C2A—C3A—N1A	−179.3 (3)	O3C—Sn1C—O4C—C15C	−0.36 (13)
C1A—C2A—C3A—C4A	0.5 (5)	C6C—C1C—C2C—C3C	−0.8 (4)
N1A—C3A—C4A—C5A	178.8 (2)	C8C—N1C—C3C—C2C	173.8 (3)
C2A—C3A—C4A—C5A	−1.1 (4)	C8C—N1C—C3C—C4C	−8.8 (4)
C3A—C4A—C5A—C6A	1.0 (4)	C1C—C2C—C3C—N1C	179.1 (2)
C4A—C5A—C6A—C1A	−0.3 (4)	C1C—C2C—C3C—C4C	1.5 (4)
C4A—C5A—C6A—C7A	−179.9 (2)	N1C—C3C—C4C—C5C	−178.3 (2)
C2A—C1A—C6A—C5A	−0.3 (4)	C2C—C3C—C4C—C5C	−0.7 (4)
C2A—C1A—C6A—C7A	179.3 (3)	C3C—C4C—C5C—C6C	−0.8 (4)
Sn1A—O1A—C7A—O2A	0.6 (2)	C4C—C5C—C6C—C1C	1.5 (4)
Sn1A—O1A—C7A—C6A	−179.6 (2)	C4C—C5C—C6C—C7C	179.6 (2)
Sn1A—O2A—C7A—O1A	−0.7 (3)	C2C—C1C—C6C—C5C	−0.7 (4)
Sn1A—O2A—C7A—C6A	179.52 (19)	C2C—C1C—C6C—C7C	−178.8 (2)
C5A—C6A—C7A—O1A	−175.1 (2)	Sn1C—O1C—C7C—O2C	−7.4 (2)
C1A—C6A—C7A—O1A	5.3 (4)	Sn1C—O1C—C7C—C6C	171.81 (16)
C5A—C6A—C7A—O2A	4.7 (4)	C5C—C6C—C7C—O2C	−4.6 (3)
C1A—C6A—C7A—O2A	−174.9 (2)	C1C—C6C—C7C—O2C	173.4 (2)
C21A—Sn1A—C7A—O1A	76.72 (16)	C5C—C6C—C7C—O1C	176.2 (2)
C17A—Sn1A—C7A—O1A	−78.35 (16)	C1C—C6C—C7C—O1C	−5.8 (3)
O2A—Sn1A—C7A—O1A	179.4 (2)	C14C—C9C—C10C—C11C	−0.6 (4)
O3A—Sn1A—C7A—O1A	179.26 (14)	C16C—N2C—C11C—C12C	−2.9 (4)
C21A—Sn1A—C7A—O2A	−102.65 (16)	C16C—N2C—C11C—C10C	176.8 (2)
C17A—Sn1A—C7A—O2A	102.28 (16)	C9C—C10C—C11C—N2C	−179.4 (2)
O3A—Sn1A—C7A—O2A	−0.11 (16)	C9C—C10C—C11C—C12C	0.2 (4)
O1A—Sn1A—C7A—O2A	−179.4 (2)	N2C—C11C—C12C—C13C	179.3 (2)
C14A—C9A—C10A—C11A	1.6 (4)	C10C—C11C—C12C—C13C	−0.4 (3)
C16A—N2A—C11A—C12A	14.4 (4)	C11C—C12C—C13C—C14C	0.9 (3)
C16A—N2A—C11A—C10A	−166.8 (3)	C12C—C13C—C14C—C9C	−1.2 (3)
C9A—C10A—C11A—N2A	179.8 (3)	C12C—C13C—C14C—C15C	−179.7 (2)
C9A—C10A—C11A—C12A	−1.4 (4)	C10C—C9C—C14C—C13C	1.1 (4)
N2A—C11A—C12A—C13A	178.4 (3)	C10C—C9C—C14C—C15C	179.6 (2)

C10A—C11A—C12A—C13A	−0.4 (4)	Sn1C—O3C—C15C—O4C	−0.6 (2)
C11A—C12A—C13A—C14A	2.0 (4)	Sn1C—O3C—C15C—C14C	179.7 (2)
C12A—C13A—C14A—C9A	−1.8 (4)	Sn1C—O4C—C15C—O3C	0.7 (2)
C12A—C13A—C14A—C15A	178.4 (2)	Sn1C—O4C—C15C—C14C	−179.57 (17)
C10A—C9A—C14A—C13A	0.0 (4)	C13C—C14C—C15C—O3C	173.8 (2)
C10A—C9A—C14A—C15A	179.8 (2)	C9C—C14C—C15C—O3C	−4.7 (4)
Sn1A—O3A—C15A—O4A	5.5 (2)	C13C—C14C—C15C—O4C	−6.0 (3)
Sn1A—O3A—C15A—C14A	−174.05 (17)	C9C—C14C—C15C—O4C	175.5 (2)
C13A—C14A—C15A—O4A	9.6 (4)	C21C—Sn1C—C15C—O3C	80.72 (15)
C9A—C14A—C15A—O4A	−170.2 (2)	C17C—Sn1C—C15C—O3C	−79.33 (15)
C13A—C14A—C15A—O3A	−170.9 (2)	O4C—Sn1C—C15C—O3C	−179.4 (2)
C9A—C14A—C15A—O3A	9.4 (3)	O1C—Sn1C—C15C—O3C	−179.03 (13)
C21A—Sn1A—C17A—C18E	−159.5 (3)	C21C—Sn1C—C15C—O4C	−99.91 (15)
O2A—Sn1A—C17A—C18E	−16.4 (3)	C17C—Sn1C—C15C—O4C	100.03 (15)
O3A—Sn1A—C17A—C18E	63.6 (3)	O1C—Sn1C—C15C—O4C	0.34 (15)
O1A—Sn1A—C17A—C18E	−72.6 (3)	O3C—Sn1C—C15C—O4C	179.4 (2)
C7A—Sn1A—C17A—C18E	−45.1 (3)	C21C—Sn1C—C17C—C18C	−49.9 (3)
C21A—Sn1A—C17A—C18A	145.7 (2)	O4C—Sn1C—C17C—C18C	96.15 (19)
O2A—Sn1A—C17A—C18A	−71.2 (2)	O1C—Sn1C—C17C—C18C	176.93 (18)
O3A—Sn1A—C17A—C18A	8.8 (2)	O3C—Sn1C—C17C—C18C	39.17 (19)
O1A—Sn1A—C17A—C18A	−127.4 (2)	C15C—Sn1C—C17C—C18C	66.96 (19)
C7A—Sn1A—C17A—C18A	−99.8 (2)	Sn1C—C17C—C18C—C19C	−176.28 (17)
C18E—C17A—C18A—C19A	66.5 (4)	C17C—C18C—C19C—C20C	−177.3 (2)
Sn1A—C17A—C18A—C19A	179.1 (2)	C17C—Sn1C—C21C—C22C	−136.9 (2)
C17A—C18A—C19A—C20A	176.5 (3)	O4C—Sn1C—C21C—C22C	76.80 (17)
C18A—C17A—C18E—C19E	14.8 (4)	O1C—Sn1C—C21C—C22C	−3.95 (17)
Sn1A—C17A—C18E—C19E	−78.0 (5)	O3C—Sn1C—C21C—C22C	133.74 (16)
C17A—C18E—C19E—C20E	−71.2 (8)	C15C—Sn1C—C21C—C22C	105.82 (16)
C17A—Sn1A—C21A—C22A	145.9 (2)	Sn1C—C21C—C22C—C23C	177.99 (16)
O2A—Sn1A—C21A—C22A	3.11 (19)	C21C—C22C—C23C—C24C	176.2 (2)
O3A—Sn1A—C21A—C22A	−77.10 (18)	C17D—Sn1D—O1D—C7D	−81.36 (16)
O1A—Sn1A—C21A—C22A	59.36 (18)	C21D—Sn1D—O1D—C7D	82.05 (15)
C7A—Sn1A—C21A—C22A	31.98 (19)	O4D—Sn1D—O1D—C7D	−178.74 (15)
Sn1A—C21A—C22A—C23A	163.91 (18)	O2D—Sn1D—O1D—C7D	0.15 (13)
C21A—C22A—C23A—C24A	66.3 (3)	O3D—Sn1D—O1D—C7D	179.18 (12)
C21B—Sn1B—O1B—C7B	−102.08 (15)	C17D—Sn1D—O2D—C7D	104.99 (15)
C17B—Sn1B—O1B—C7B	102.45 (15)	C21D—Sn1D—O2D—C7D	−102.02 (15)
O2B—Sn1B—O1B—C7B	0.19 (13)	O1D—Sn1D—O2D—C7D	−0.16 (13)
O3B—Sn1B—O1B—C7B	0.70 (19)	O4D—Sn1D—O2D—C7D	1.42 (18)
O4B—Sn1B—O1B—C7B	178.6 (2)	O3D—Sn1D—O2D—C7D	−176.8 (2)
C21B—Sn1B—O2B—C7B	83.26 (15)	C17D—Sn1D—O3D—C15D	−104.21 (15)
C17B—Sn1B—O2B—C7B	−82.38 (15)	C21D—Sn1D—O3D—C15D	102.63 (14)
O3B—Sn1B—O2B—C7B	−179.84 (15)	O1D—Sn1D—O3D—C15D	1.32 (17)
O1B—Sn1B—O2B—C7B	−0.19 (13)	O4D—Sn1D—O3D—C15D	−1.16 (13)
O4B—Sn1B—O2B—C7B	−179.67 (12)	O2D—Sn1D—O3D—C15D	177.4 (3)
C21B—Sn1B—O3B—C15B	−83.73 (15)	C7D—Sn1D—O3D—C15D	2.8 (3)
C17B—Sn1B—O3B—C15B	78.77 (14)	C17D—Sn1D—O4D—C15D	81.72 (15)
O2B—Sn1B—O3B—C15B	177.07 (14)	C21D—Sn1D—O4D—C15D	−79.87 (15)
O1B—Sn1B—O3B—C15B	176.63 (12)	O1D—Sn1D—O4D—C15D	−177.08 (15)

O4B—Sn1B—O3B—C15B	−2.79 (12)	O2D—Sn1D—O4D—C15D	−178.43 (13)
C7B—Sn1B—O3B—C15B	176.98 (13)	O3D—Sn1D—O4D—C15D	1.14 (12)
C21B—Sn1B—O4B—C15B	104.95 (14)	C7D—Sn1D—O4D—C15D	−177.72 (13)
C17B—Sn1B—O4B—C15B	−99.23 (14)	C6D—C1D—C2D—C3D	−0.5 (4)
O2B—Sn1B—O4B—C15B	2.66 (17)	C8D—N1D—C3D—C2D	−7.4 (4)
O3B—Sn1B—O4B—C15B	2.86 (12)	C8D—N1D—C3D—C4D	173.3 (3)
O1B—Sn1B—O4B—C15B	−175.4 (2)	C1D—C2D—C3D—N1D	−178.6 (3)
C7B—Sn1B—O4B—C15B	2.1 (3)	C1D—C2D—C3D—C4D	0.7 (4)
C6B—C1B—C2B—C3B	−0.1 (4)	N1D—C3D—C4D—C5D	179.7 (3)
C8B—N1B—C3B—C4B	3.2 (4)	C2D—C3D—C4D—C5D	0.4 (4)
C8B—N1B—C3B—C2B	−176.2 (3)	C3D—C4D—C5D—C6D	−1.8 (4)
C1B—C2B—C3B—N1B	179.9 (2)	C2D—C1D—C6D—C5D	−0.9 (4)
C1B—C2B—C3B—C4B	0.4 (4)	C2D—C1D—C6D—C7D	180.0 (2)
N1B—C3B—C4B—C5B	−179.5 (2)	C4D—C5D—C6D—C1D	2.0 (4)
C2B—C3B—C4B—C5B	0.0 (4)	C4D—C5D—C6D—C7D	−178.8 (2)
C3B—C4B—C5B—C6B	−0.7 (4)	Sn1D—O2D—C7D—O1D	0.2 (2)
C4B—C5B—C6B—C1B	1.0 (4)	Sn1D—O2D—C7D—C6D	179.5 (2)
C4B—C5B—C6B—C7B	179.9 (2)	Sn1D—O1D—C7D—O2D	−0.3 (2)
C2B—C1B—C6B—C5B	−0.6 (4)	Sn1D—O1D—C7D—C6D	−179.58 (17)
C2B—C1B—C6B—C7B	−179.5 (2)	C1D—C6D—C7D—O2D	175.7 (2)
Sn1B—O1B—C7B—O2B	−0.3 (2)	C5D—C6D—C7D—O2D	−3.5 (4)
Sn1B—O1B—C7B—C6B	179.6 (2)	C1D—C6D—C7D—O1D	−5.1 (3)
Sn1B—O2B—C7B—O1B	0.3 (2)	C5D—C6D—C7D—O1D	175.8 (2)
Sn1B—O2B—C7B—C6B	−179.57 (18)	C17D—Sn1D—C7D—O2D	−76.64 (16)
C5B—C6B—C7B—O1B	−175.0 (2)	C21D—Sn1D—C7D—O2D	78.48 (15)
C1B—C6B—C7B—O1B	3.9 (4)	O1D—Sn1D—C7D—O2D	179.7 (2)
C5B—C6B—C7B—O2B	4.9 (3)	O4D—Sn1D—C7D—O2D	−178.97 (13)
C1B—C6B—C7B—O2B	−176.2 (2)	O3D—Sn1D—C7D—O2D	177.63 (19)
C21B—Sn1B—C7B—O1B	79.43 (15)	C17D—Sn1D—C7D—O1D	103.64 (15)
C17B—Sn1B—C7B—O1B	−78.40 (15)	C21D—Sn1D—C7D—O1D	−101.24 (15)
O2B—Sn1B—C7B—O1B	−179.7 (2)	O4D—Sn1D—C7D—O1D	1.31 (16)
O3B—Sn1B—C7B—O1B	−179.50 (13)	O2D—Sn1D—C7D—O1D	−179.7 (2)
O4B—Sn1B—C7B—O1B	−178.81 (19)	O3D—Sn1D—C7D—O1D	−2.1 (3)
C21B—Sn1B—C7B—O2B	−100.91 (15)	C14D—C9D—C10D—C11D	−1.5 (4)
C17B—Sn1B—C7B—O2B	101.27 (15)	C16D—N2D—C11D—C10D	−15.3 (4)
O3B—Sn1B—C7B—O2B	0.17 (16)	C16D—N2D—C11D—C12D	166.3 (2)
O1B—Sn1B—C7B—O2B	179.7 (2)	C9D—C10D—C11D—N2D	−177.2 (2)
O4B—Sn1B—C7B—O2B	0.9 (3)	C9D—C10D—C11D—C12D	1.2 (4)
C14B—C9B—C10B—C11B	−0.4 (4)	N2D—C11D—C12D—C13D	178.3 (2)
C16B—N2B—C11B—C12B	9.0 (4)	C10D—C11D—C12D—C13D	−0.2 (4)
C16B—N2B—C11B—C10B	−172.9 (2)	C11D—C12D—C13D—C14D	−0.5 (4)
C9B—C10B—C11B—N2B	−178.4 (2)	C10D—C9D—C14D—C13D	0.8 (4)
C9B—C10B—C11B—C12B	−0.2 (4)	C10D—C9D—C14D—C15D	−178.7 (2)
N2B—C11B—C12B—C13B	178.6 (2)	C12D—C13D—C14D—C9D	0.2 (4)
C10B—C11B—C12B—C13B	0.4 (4)	C12D—C13D—C14D—C15D	179.7 (2)
C11B—C12B—C13B—C14B	0.0 (4)	Sn1D—O3D—C15D—O4D	1.8 (2)
C12B—C13B—C14B—C9B	−0.6 (4)	Sn1D—O3D—C15D—C14D	−177.9 (2)
C12B—C13B—C14B—C15B	179.4 (2)	Sn1D—O4D—C15D—O3D	−2.2 (2)
C10B—C9B—C14B—C13B	0.8 (4)	Sn1D—O4D—C15D—C14D	177.53 (17)

C10B—C9B—C14B—C15B	−179.2 (2)	C9D—C14D—C15D—O3D	−10.2 (3)
Sn1B—O4B—C15B—O3B	−4.39 (19)	C13D—C14D—C15D—O3D	170.4 (2)
Sn1B—O4B—C15B—C14B	174.2 (2)	C9D—C14D—C15D—O4D	170.1 (2)
Sn1B—O3B—C15B—O4B	5.2 (2)	C13D—C14D—C15D—O4D	−9.3 (3)
Sn1B—O3B—C15B—C14B	−173.44 (17)	C21D—Sn1D—C17D—C18D	−137.4 (2)
C13B—C14B—C15B—O4B	3.9 (3)	O1D—Sn1D—C17D—C18D	4.26 (19)
C9B—C14B—C15B—O4B	−176.1 (2)	O4D—Sn1D—C17D—C18D	85.58 (18)
C13B—C14B—C15B—O3B	−177.5 (2)	O2D—Sn1D—C17D—C18D	−51.83 (18)
C9B—C14B—C15B—O3B	2.5 (3)	O3D—Sn1D—C17D—C18D	139.90 (18)
C21B—Sn1B—C17B—C18B	138.2 (2)	C7D—Sn1D—C17D—C18D	−24.70 (19)
O2B—Sn1B—C17B—C18B	−77.79 (17)	Sn1D—C17D—C18D—C19D	−163.65 (16)
O3B—Sn1B—C17B—C18B	3.87 (17)	C17D—C18D—C19D—C20D	−69.0 (3)
O1B—Sn1B—C17B—C18B	−134.32 (16)	C17D—Sn1D—C21D—C22D	−140.3 (2)
O4B—Sn1B—C17B—C18B	58.25 (16)	O1D—Sn1D—C21D—C22D	77.46 (17)
C7B—Sn1B—C17B—C18B	−106.44 (16)	O4D—Sn1D—C21D—C22D	−3.50 (18)
Sn1B—C17B—C18B—C19B	−178.24 (16)	O2D—Sn1D—C21D—C22D	133.69 (16)
C17B—C18B—C19B—C20B	−178.0 (2)	O3D—Sn1D—C21D—C22D	−57.88 (17)
C17B—Sn1B—C21B—C22B	49.8 (3)	C7D—Sn1D—C21D—C22D	106.33 (17)
O2B—Sn1B—C21B—C22B	−94.09 (18)	Sn1D—C21D—C22D—C23D	−177.97 (16)
O3B—Sn1B—C21B—C22B	−175.79 (17)	C21D—C22D—C23D—C24D	−179.4 (2)
O1B—Sn1B—C21B—C22B	−37.34 (18)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2A—H2AB···O3A^{i}	0.86	2.31	3.146 (3)	164
N2B—H1ND···O3B^{ii}	0.84 (3)	2.13 (3)	2.967 (3)	174 (2)
N1C—H1NE···O4D^{iii}	0.78 (3)	2.32 (3)	3.046 (3)	155 (3)
N2D—H1NH···O1C^{iii}	0.84 (3)	2.20 (2)	2.970 (3)	152 (2)
N2D—H1NH···O4C^{iii}	0.84 (3)	2.45 (3)	3.103 (3)	134 (2)
C8B—H8BC···Cg1	0.96	2.91	3.750 (3)	147

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

Fig. 1

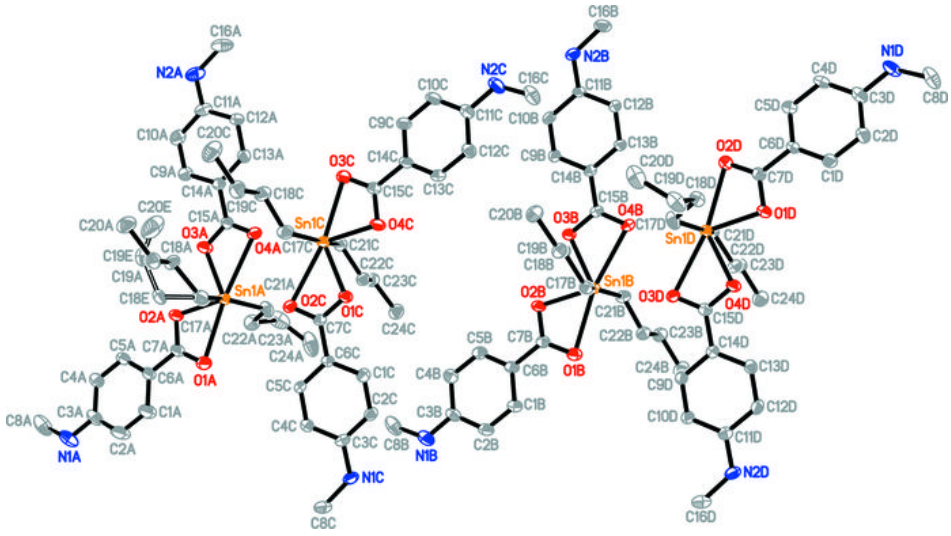
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Fig. 2

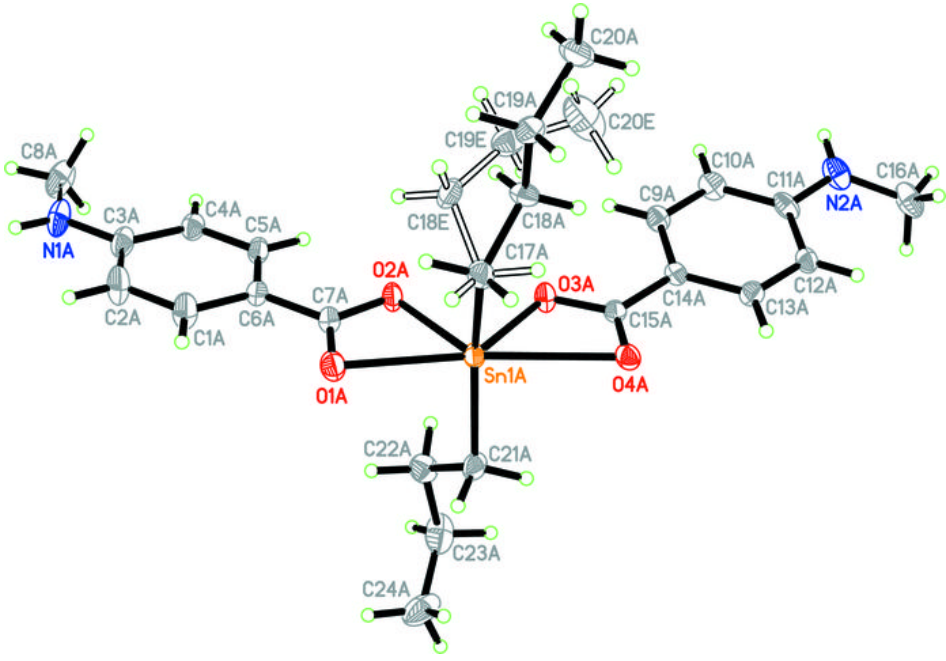
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Fig. 3