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Bis{μ-2-hydroxy-5-[(*E*)-2-(2-methoxyphenyl)diazenyl]benzoato}bis(di-*n*-butyl-{2-hydroxy-5-[(*E*)-2-(2-methoxyphenyl)-diazenyl]benzoato}tin(IV))

Anthony Linden,[a]* David Wolstenholme,[b] Tushar S. Basu Baul[c] and Wandondor Rynjah[c]

[a]Institute of Organic Chemistry, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland, [b]Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, Canada B3H 4J3, and [c]Department of Chemistry, North Eastern Hill University, NEHU Permanent Campus, Umshing, Shillong 793 022, India
Correspondence e-mail: alinden@oci.uzh.ch

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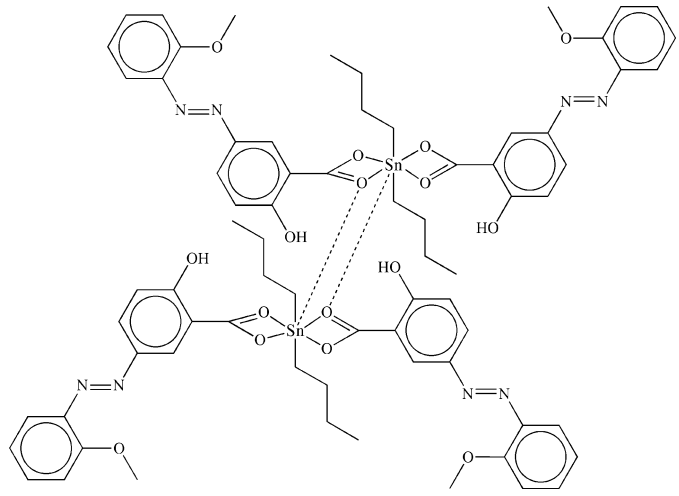
Key indicators: single-crystal X-ray study; T = 160 K; mean σ(C–C) = 0.009 Å; H-atom completeness 103%; disorder in main residue; R factor = 0.057; wR factor = 0.148; data-to-parameter ratio = 12.1.

The title compound, $[Sn_2(C_{14}H_{11}N_2O_4)_4(C_4H_9)_4]$, is a further example from a series of 5-[(*E*)-aryldiazenyl]-2-hydroxybenzoate complexes with di-*n*-butyltin(IV). The structure consists of centrosymmetric dimers formed by the linking of two monomers *via* long Sn···O interactions of 3.192 (5) Å. Each Sn atom has a skewed trapezoidal bipyramidal inner-sphere coordination geometry with the O atoms from two carboxylate ligands in the equatorial plane and disordered butyl groups occupying axial positions. The singly-bonded carboxyl O atoms from each ligand form coordination Sn—O bonds (*ca* 2.11 Å) and are *cis* to one another, while the carbonyl O atoms from the ligands have one lone pair donating into empty orbitals on the Sn atom in a dative fashion, which results in significantly longer Sn—O bonds of *ca* 2.56 Å. The long Sn···O interactions complete a pentagonal bipyramidal coordination geometry at the Sn atom. Several types of O—H···O hydrogen bonds and C—H···O close contacts are present.

Related literature

For related literature, see: Basu Baul, Dhar & Tiekink (2001); Basu Baul, Dhar, Pyke *et al.* (2001); Basu Baul *et al.* (2003, 2004, 2005); Desiraju *et al.* (1993); Evans & Karpel (1984); Lockhart *et al.* (1987); Munshi & Guru Row (2005).



Experimental

Crystal data

$[Sn_2(C_{14}H_{11}N_2O_4)_4(C_4H_9)_4]$
M_r = 1550.66
Monoclinic, $C2/c$
a = 35.6311 (7) Å
b = 10.6333 (2) Å
c = 19.5551 (4) Å
β = 104.0634 (11)°
V = 7186.9 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.77 mm^{-1}
T = 160 (1) K
0.20 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.805, T_{max} = 0.892
70128 measured reflections
6348 independent reflections
4601 reflections with $I > 2\sigma(I)$
R_{int} = 0.104

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.057
$wR(F^2)$ = 0.148
S = 1.09
6347 reflections
524 parameters
147 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.73 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.109 (3)	Sn1—C29*B*	2.139 (10)
Sn1—C29*A*	2.112 (11)	Sn1—O6	2.517 (4)
Sn1—O5	2.116 (3)	Sn1—O2	2.597 (4)
Sn1—C33*B*	2.122 (10)	Sn1—O7^{i}	3.192 (4)
Sn1—C33*A*	2.127 (10)		
C29*A*—Sn1—C33*A*	132.7 (11)	O6—Sn1—O2	168.28 (13)
O5—Sn1—O6	55.23 (12)	O1—Sn1—O5	81.86 (13)
O1—Sn1—O2	54.41 (13)		

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

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Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.84	1.93	2.613 (6)	138
O7—H7···O6	0.84	2.01	2.603 (6)	127
O7—H7···O6^{i}	0.84	2.39	2.871 (6)	117
C22—H22···O8^{ii}	0.95	2.62	3.334 (7)	134
C27—H271···O8^{ii}	0.98	2.62	3.449 (8)	142
C27—H272···O4^{iii}	0.98	2.67	3.434 (8)	136
C32B—H326···O3^{iv}	0.98	2.69	3.67 (2)	170
C33B—H333···O7^{i}	0.99	2.64	3.33 (3)	127

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

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *DENZO-SMN* (Otwinowski & Minor, 1997); data reduction: *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2373).

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supplementary materials

Acta Cryst. (2007). E**63**, m1547-m1548 [**doi:10.1107/S1600536807020302**]

Bis{μ-2-hydroxy-5-[(*E*)-2-(2-methoxyphenyl)diazenyl]benzoato}bis(di-*n*-butyl{2-hydroxy-5-[(*E*)-2-(2-methoxyphenyl)diazenyl]benzoato}tin(IV))

A. Linden, D. Wolstenholme, T. S. Basu Baul and W. Rynjah

Comment

The di-n-butyltin(IV) dicarboxylates are widely used as homogeneous catalysts for polyurethane and RTV silicone polymerization and for *trans* esterification reactions (Evans & Karpel, 1984; Lockhart *et al.*, 1987). We have been studying a series of $^{n}Bu_2Sn(LH)_2$ complexes (LH = 5-[(*E*)-2-(aryl)-1-diazenyl]-2-hydroxybenzoate) (Basu Baul, Dhar & Tiekink, 2001; Basu Baul *et al.*, 2003, 2004, 2005). Some of these complexes exhibit significant biological activity towards Aedes aegypti mosquito larvae (Basu Baul *et al.*, 2003) and *in vitro* cytotoxicity against human tumor cell lines (Basu Baul *et al.*, 2004). The title compound, (I), whose structure is reported here, is a further member of the $^{n}Bu_2Sn(LH)_2$ series.

The structure of (I) is related to those several other Sn-complexes built from similar azo-carboxylate ligands (references above). The coordination geometry about the Sn atom is best described as that of a skewed trapezoidal bipyramid (Fig. 1). The carboxylate groups on the two azo-carboxylate ligands act as bidentate chelating ligands, giving rise to an equatorial plane around the Sn atom. The carboxyl O atoms (O1 and O5) from each ligand form coordination bonds and take up a *cis* arrangement to each other. The carbonyl O atoms (O2 and O6) from the ligands have one lone pair donating into empty orbitals on the Sn atom in a dative fashion, which results in significantly longer Sn—O bonds (Table 1). The O2—Sn1—O6 bond angle between the two carbonyl O atoms is only slightly distorted from linearity by 11.72 (13)°, resulting in one side of the Sn-complex being open for additional coordination. The two butyl groups coordinate to the Sn atom in axial positions, thereby completing the six-coordinate geometry around the Sn atom. The average C—Sn—C angle involving the butyl groups deviates by approximately 47° from linearity. Both of the butyl groups are disordered, with two conformations being present for all atoms in each group. The open side of the Sn1 coordination sphere allows one of the O7 hydroxy atom lone pairs to donate in a weak intermolecular interaction to the Sn1 atom of an adjacent centrosymmetrically related molecule. The internuclear Sn1···O7($1-x$, $1-y$,$1-z$) distance is 3.192 (5) Å, which is significantly shorter then the sum of the van der Waals radii for the two atoms. When this weak interaction is considered in the description of the coordination geometry of the Sn atom, a distorted pentagonal bipyramidal geometry is obtained. The centre of inversion between the two molecules involved in this weak interaction means that there are two identical two bridges between the two molecules, so that this Sn-complex exists as a dimer in its crystalline state (Fig. 1).

In (I), the C—N═N—C step present in both azo-carboxylate ligands points in the same direction. The only difference between the two ligands, is that the plane of the methoxyphenyl group of one ligand is tilted 52.7 (3)° out of the plane of the remainder of the carboxylate ligand, whereas the other methoxyphenyl group is oriented more normally and is only tilted by 9.3 (3)° from the remainder of the ligand.

The 2-hydroxybenzoate hydroxy group from both LHH' ligands in compound (I) form classical O—H···O hydrogen bonds with the carboxylate carbonyl oxygen atom on the same ligand (Table 2). The hydroxy oxygen atom involved in the bridging Sn···O interaction can also make an intermolecular O—H···O hydrogen bond with the carboxylate carbonyl oxygen atom in the other ligand across the bridge. The crystal packing in this Sn-complex also affords a geometry that produces

several close contacts of the form C—H···O. These interactions have been shown to play an important role in the packing and stability of many organic molecules (Munshi & Guru Row, 2005; Desiraju *et al.*, 1993). For example, the methyl hydrogen (H272) in the more non-planar methoxyphenyl group forms a close contact with the methoxy O atom (O4) in a symmetry related molecule to help stabilize the crystalline state of molecule (I).

Experimental

5-[(*E*)-2-(2-methoxyphenyl)-1-diazenyl]-2-hydroxybenzoic acid (LHH') was prepared according to the method of Basu Baul, Dhar, Pyke *et al.* (2001) by a diazo-coupling reaction using *o*-anisidine and salicylic acid in alkaline medium. The brown coloured precipitate was recrystallized from methanol to give pure LHH' (31.5% yield, m.p. 458–460 K). Analysis calculated for $C_{14}H_{12}N_2O_4Sn$: C, 43.01; H, 3.09; N, 7.17%; found: C, 43.09; H, 3.03; N, 7.12%.

The title compound was prepared by refluxing LHH' (0.75 g, 2.75 mmol) and Bu_2SnO (0.35 g, 1.40 mmol) in anhydrous toluene (50 ml) in a Dean and Stark apparatus for 3 h. The orange colored solution was filtered, concentrated to one tenth of its initial solvent volume and precipitated with petroleum-ether (333–353 K). The orange coloured precipitate was separated by filtration, washed with hexane (2 *x* 5 ml) and dried *in vacuo*. The dried residue was dissolved in hexane and filtered to remove any particles. The filtrate was allowed to evaporate at room temperature, which afforded orange prismatic crystals of (I) (0.75 g, 70% yield, m.p. 352–354 K). Analysis calculated for $C_{36}H_{40}N_4O_8Sn$: C, 55.77; H, 5.20; N, 7.23%; found: C, 55.80; H, 5.24; N, 7.20%.

Spectroscopic details for the ligand and for (I) are given in the _exptl_special_details section of the CIF.

Refinement

All atoms of each butyl group are disordered over two conformations. Refinement of constrained site occupation factors for the two orientations of the C29 to C32 group yielded a value of 0.599 (8) for the major conformation. The two conformations of the C33 to C36 butyl moiety are necessarily equally occupied, because each conformation of this group makes short contacts with itself in a neighbouring molecule related by a twofold axis. Similarity restraints were applied to the chemically equivalent bond lengths and angles involving disordered C atoms, while neighbouring atoms within and between each conformation of the disordered groups were restrained to have similar atomic displacement parameters. The methyl and hydroxy H atoms were constrained to an ideal geometry with C—H and O—H distances of 0.98 and 0.84 Å, respectively, and with $U_{iso}(H) = 1.5U_{eq}$(parent atom), but were allowed to rotate freely about the parent C—C or C—O bonds. All other H atoms were placed geometrically and refined using a riding model with C—H distances of 0.95 Å (phenyl) or 0.99 Å (methylene) and with $U_{iso}(H) = 1.2U_{eq}(C)$. One low angle reflection was omitted from the final cycles of refinement because its observed intensity was much lower than the calculated value as a result of being partially obscured by the beam stop.

Figures

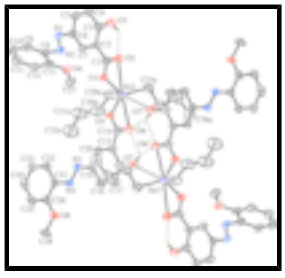

Fig. 1. View of the dimeric molecule of (I) showing the atom-labelling scheme, the long Sn1—O7^{i} interaction (unfilled bonds) and the hydrogen bonds (dashed lines). Displacement ellipsoids are drawn at the 30% probability level. H atoms are represented by circles of arbitrary size. Symmetry code: (i) 1 − *x*, 1 − *y*, 1 − *z*. only one component of the disorder is shown

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Crystal data

$[Sn_2(C_{14}H_{11}N_2O_4)_4(C_4H_9)_4]$	F_{000} = 3184
M_r = 1550.66	D_x = 1.433 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 353 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 35.6311 (7) Å	Cell parameters from 84575 reflections
b = 10.6333 (2) Å	θ = 2.0–25.0º
c = 19.5551 (4) Å	μ = 0.77 mm^{-1}
β = 104.0634 (11)º	*T* = 160 (1) K
V = 7186.9 (2) Å^3	Prism, orange–red
Z = 4	0.20 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer	6348 independent reflections
Radiation source: Nonius FR590 sealed tube generator	4601 reflections with $I > 2\sigma(I)$
Monochromator: horizontally mounted graphite crystal	R_{int} = 0.104
Detector resolution: 9 pixels mm^{-1}	θ_{max} = 25.0º
T = 160(1) K	θ_{min} = 2.0º
φ and ω scans with κ offsets	*h* = −42→42
Absorption correction: multi-scan (Blessing, 1995)	*k* = −12→12
T_{min} = 0.805, T_{max} = 0.892	*l* = −23→22
70128 measured reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.148$	$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 33.1175P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$
6347 reflections	$\Delta\rho_{max} = 0.73$ e Å^{-3}
524 parameters	$\Delta\rho_{min} = -1.12$ e Å^{-3}
147 restraints	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.00054 (9)

Special details

Experimental. Solvent used: hexane Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: glued on a glass fibre Mosaicity (°.): 0.591 (1) Frames collected: 567 Seconds exposure per frame: 10 Degrees rotation per frame: 1.0 Crystal-Detector distance (mm): 30.0

Spectroscopic data for the ligand (LHH') IR (KBr, cm^{-1}): 1661 ν(OCO)$_{asym}$; ^{1}H NMR (DMSO-d^6, 300.13 MHz); δ_H: Ligand skeleton: 4.04 [s, 3H, OCH_3], 7.04 [ddd,1*H*, H-3], 7.11 [dd, 2H, H-3' & H-4'], 7.45 [ddd, 1H, H-5'], 7.68 [dd, 1H, H-6'], 8.14 [dd, 1H, H-4], 8.54 [d, 1H, H-6] p.p.m.. Signals for the phenol and carboxylic acid were exchanged due to presence of water in the solvent; ^{13}C NMR (DMSO-d^6, 75.47 MHz); δ_C: Ligand skeleton: 56.0 [OCH_3], 112.7 [C-6'], 112.9 [C-1], 116.6 [C-3], 118.9 [C-6], 120.6 [C-5'], 127.4 [C-4], 128.2 [C-4'], 132.2 [C-3'], 141.8 [C-2'], 145.4 [C-5], 156.5 [C-1'], 164.0 [C-2], 172.3 [CO_2] p.p.m..

Spectroscopic data for (I) IR (KBr, cm^{-1}): 1622 ν(OCO)$_{asym}$; ^{1}H NMR ($CDCl_3$, 300.13 MHz); δ_H: Ligand skeleton: 4.02 [s, 3H, OCH_3], 7.02 [ddd,1*H*, H-3], 7.10 [dd, 2H, H-3' & H-4'], 7.43 [ddd, 1H, H-5'], 7.69 [dd, 1H, H-6'], 8.13 [dd, 1H, H-4], 8.65 [d, 1H, H-6], 10.98 [s, 1H, OH]; Sn-^{n}Bu skeleton: 0.93 [t, 3H, H-4*], 1.45 [m, 2H, H-3*], 1.79 [m, 2H, H-2*], 1.93 [t, 2H, H-1*], p.p.m.. ^{13}C NMR ($CDCl_3$, 75.47 MHz); δ_C: Ligand skeleton: 56.3 [OCH_3], 112.6 [C-6'], 112.8 [C-1], 116.9 [C-3], 118.3 [C-6], 120.7 [C-5'], 128.7 [C-4], 129.2 [C-4'], 132.2 [C-3'], 142.1 [C-2'], 146.1 [C-5], 156.8 [C-1'], 163.7 [C-2], 177.2 [CO_2]; Sn-^{n}Bu skeleton: 13.5 [C-4*], 26.3 [C-3*], 26.4 [C-2*], 26.5 [C-1*], p.p.m.. ^{119}Sn NMR ($CDCl_3$, 111.92 MHz); δ_{Sn}: −112.9 p.p.m., ^{119}Sn Mössbauer: $\delta = 1.52$, $\Delta = 3.69$, $\Gamma_1 = 0.85$, $\Gamma_2 = 0.86$ mm s^{-1}, C—Sn—C = 152°.

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)

Sn1	0.440621 (10)	0.23007 (4)	0.50793 (3)	0.0626 (2)
O1	0.38955 (10)	0.1216 (3)	0.4884 (2)	0.0622 (11)
O2	0.43609 (12)	−0.0038 (4)	0.5434 (3)	0.0775 (13)
O3	0.42002 (13)	−0.2343 (4)	0.5729 (3)	0.0739 (12)
H3	0.4325	−0.1672	0.5840	0.089*
O4	0.21361 (11)	0.1554 (3)	0.4502 (2)	0.0595 (10)
O5	0.40166 (9)	0.3689 (3)	0.4550 (2)	0.0546 (10)
O6	0.45967 (11)	0.4485 (4)	0.4800 (3)	0.0801 (14)
O7	0.47184 (11)	0.6766 (5)	0.4421 (4)	0.104 (2)
H7	0.4759	0.6295	0.4776	0.124*
O8	0.28023 (12)	0.9501 (4)	0.1671 (2)	0.0615 (10)
N1	0.26745 (13)	−0.1497 (4)	0.4320 (2)	0.0515 (11)
N2	0.25529 (13)	−0.0380 (4)	0.4257 (2)	0.0518 (11)
N3	0.31623 (12)	0.6859 (4)	0.3049 (2)	0.0478 (10)
N4	0.30688 (12)	0.7685 (4)	0.2575 (2)	0.0462 (10)
C1	0.40120 (16)	0.0127 (6)	0.5147 (3)	0.0614 (16)
C2	0.37205 (16)	−0.0880 (5)	0.5096 (3)	0.0541 (14)
C3	0.38338 (17)	−0.2071 (6)	0.5400 (3)	0.0589 (15)
C4	0.35504 (19)	−0.2998 (5)	0.5339 (3)	0.0611 (16)
H4	0.3622	−0.3799	0.5545	0.073*
C5	0.31803 (17)	−0.2796 (5)	0.4998 (3)	0.0556 (14)
H5	0.2995	−0.3451	0.4967	0.067*
C6	0.30644 (16)	−0.1620 (5)	0.4686 (3)	0.0499 (13)
C7	0.33387 (15)	−0.0672 (5)	0.4743 (3)	0.0507 (13)
H71	0.3264	0.0127	0.4537	0.061*
C8	0.21665 (16)	−0.0261 (5)	0.3836 (3)	0.0513 (13)
C9	0.20017 (18)	−0.1081 (5)	0.3296 (3)	0.0598 (15)
H9	0.2145	−0.1785	0.3201	0.072*
C10	0.16311 (18)	−0.0885 (7)	0.2896 (3)	0.0700 (18)
H10	0.1520	−0.1452	0.2527	0.084*
C11	0.14208 (19)	0.0138 (6)	0.3031 (4)	0.0701 (17)
H11	0.1165	0.0271	0.2757	0.084*
C12	0.15840 (17)	0.0967 (6)	0.3567 (3)	0.0608 (15)
H12	0.1439	0.1668	0.3661	0.073*
C13	0.19547 (16)	0.0780 (5)	0.3962 (3)	0.0525 (14)
C14	0.42436 (14)	0.4608 (5)	0.4515 (3)	0.0551 (14)
C15	0.40969 (14)	0.5758 (5)	0.4136 (3)	0.0476 (13)
C16	0.43376 (16)	0.6769 (6)	0.4106 (4)	0.0676 (18)
C17	0.41870 (17)	0.7851 (6)	0.3733 (4)	0.0729 (19)
H17	0.4351	0.8550	0.3721	0.087*
C18	0.38074 (16)	0.7911 (5)	0.3388 (3)	0.0573 (15)
H18	0.3709	0.8647	0.3131	0.069*
C19	0.35611 (14)	0.6903 (5)	0.3410 (3)	0.0425 (11)
C20	0.37058 (14)	0.5844 (5)	0.3788 (3)	0.0457 (12)
H20	0.3537	0.5162	0.3813	0.055*
C21	0.26767 (15)	0.7612 (5)	0.2192 (3)	0.0457 (12)
C22	0.24313 (15)	0.6617 (5)	0.2244 (3)	0.0516 (13)
H22	0.2525	0.5938	0.2555	0.062*
C23	0.20544 (17)	0.6604 (6)	0.1849 (3)	0.0596 (15)

H23	0.1886	0.5930	0.1891	0.072*	
C24	0.19255 (19)	0.7583 (7)	0.1393 (3)	0.0735 (19)	
H24	0.1665	0.7585	0.1124	0.088*	
C25	0.21640 (19)	0.8555 (6)	0.1317 (3)	0.0660 (17)	
H25	0.2068	0.9212	0.0992	0.079*	
C26	0.25438 (17)	0.8588 (5)	0.1710 (3)	0.0531 (14)	
C27	0.19379 (19)	0.2689 (5)	0.4603 (4)	0.0676 (17)	
H271	0.1876	0.3172	0.4163	0.101*	
H272	0.2104	0.3193	0.4976	0.101*	
H273	0.1698	0.2477	0.4738	0.101*	
C28	0.2687 (2)	1.0449 (6)	0.1137 (3)	0.081 (2)	
H281	0.2592	1.0045	0.0677	0.121*	
H282	0.2909	1.0983	0.1125	0.121*	
H283	0.2481	1.0965	0.1244	0.121*	
C29A	0.4745 (7)	0.151 (3)	0.4441 (9)	0.104 (5)	0.401 (8)
H291	0.5022	0.1578	0.4687	0.125*	0.401 (8)
H292	0.4682	0.0605	0.4367	0.125*	0.401 (8)
C30A	0.4676 (6)	0.217 (2)	0.3722 (10)	0.123 (4)	0.401 (8)
H301	0.4757	0.3057	0.3814	0.147*	0.401 (8)
H302	0.4854	0.1786	0.3464	0.147*	0.401 (8)
C31A	0.4272 (6)	0.219 (3)	0.3217 (12)	0.147 (4)	0.401 (8)
H311	0.4082	0.2621	0.3430	0.176*	0.401 (8)
H312	0.4179	0.1323	0.3081	0.176*	0.401 (8)
C32A	0.4340 (9)	0.292 (3)	0.2580 (13)	0.166 (7)	0.401 (8)
H321	0.4400	0.3800	0.2714	0.249*	0.401 (8)
H322	0.4107	0.2883	0.2193	0.249*	0.401 (8)
H323	0.4558	0.2547	0.2428	0.249*	0.401 (8)
C29B	0.4633 (5)	0.1640 (18)	0.4227 (7)	0.110 (4)	0.599 (8)
H293	0.4836	0.2228	0.4158	0.132*	0.599 (8)
H294	0.4755	0.0809	0.4353	0.132*	0.599 (8)
C30B	0.4318 (5)	0.1520 (17)	0.3524 (8)	0.135 (4)	0.599 (8)
H303	0.4102	0.1032	0.3631	0.161*	0.599 (8)
H304	0.4217	0.2379	0.3396	0.161*	0.599 (8)
C31B	0.4400 (6)	0.0947 (19)	0.2865 (9)	0.171 (5)	0.599 (8)
H313	0.4490	0.0067	0.2948	0.205*	0.599 (8)
H314	0.4595	0.1442	0.2699	0.205*	0.599 (8)
C32B	0.3996 (6)	0.101 (2)	0.2330 (11)	0.188 (6)	0.599 (8)
H324	0.3816	0.1488	0.2539	0.282*	0.599 (8)
H325	0.3897	0.0160	0.2217	0.282*	0.599 (8)
H326	0.4023	0.1434	0.1898	0.282*	0.599 (8)
C33A	0.4517 (10)	0.2667 (15)	0.6180 (5)	0.096 (4)	0.50
H331	0.4307	0.2293	0.6366	0.115*	0.50
H332	0.4763	0.2255	0.6421	0.115*	0.50
C34A	0.4544 (5)	0.4080 (13)	0.6348 (6)	0.098 (3)	0.50
H341	0.4752	0.4474	0.6165	0.118*	0.50
H342	0.4297	0.4503	0.6131	0.118*	0.50
C35A	0.4636 (6)	0.4189 (14)	0.7155 (7)	0.123 (4)	0.50
H351	0.4431	0.3766	0.7333	0.147*	0.50
H352	0.4885	0.3767	0.7365	0.147*	0.50

C36A	0.4660 (6)	0.5578 (15)	0.7375 (10)	0.134 (5)	0.50
H361	0.4558	0.6104	0.6960	0.200*	0.50
H362	0.4931	0.5803	0.7581	0.200*	0.50
H363	0.4508	0.5715	0.7724	0.200*	0.50
C33B	0.4473 (9)	0.2926 (16)	0.6133 (6)	0.098 (4)	0.50
H333	0.4732	0.3318	0.6275	0.118*	0.50
H334	0.4283	0.3612	0.6114	0.118*	0.50
C34B	0.4437 (5)	0.2066 (16)	0.6743 (9)	0.109 (4)	0.50
H343	0.4216	0.1481	0.6591	0.131*	0.50
H344	0.4397	0.2569	0.7146	0.131*	0.50
C35B	0.4821 (5)	0.1337 (17)	0.6950 (10)	0.130 (5)	0.50
H353	0.4877	0.0947	0.6526	0.156*	0.50
H354	0.5034	0.1921	0.7157	0.156*	0.50
C36B	0.4791 (6)	0.0312 (18)	0.7489 (11)	0.149 (6)	0.50
H364	0.4785	0.0706	0.7939	0.223*	0.50
H365	0.5016	−0.0245	0.7558	0.223*	0.50
H366	0.4554	−0.0177	0.7314	0.223*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0315 (2)	0.0532 (3)	0.0955 (4)	−0.00124 (17)	0.00051 (19)	0.0235 (2)
O1	0.039 (2)	0.047 (2)	0.097 (3)	−0.0048 (17)	0.009 (2)	0.015 (2)
O2	0.050 (3)	0.059 (3)	0.118 (4)	−0.005 (2)	0.008 (2)	0.022 (3)
O3	0.064 (3)	0.060 (3)	0.094 (3)	−0.001 (2)	0.013 (2)	0.020 (2)
O4	0.056 (2)	0.047 (2)	0.078 (3)	−0.0057 (18)	0.023 (2)	−0.015 (2)
O5	0.0328 (18)	0.045 (2)	0.081 (3)	−0.0064 (16)	0.0025 (17)	0.0121 (18)
O6	0.032 (2)	0.061 (3)	0.137 (4)	−0.0022 (18)	−0.002 (2)	0.039 (3)
O7	0.027 (2)	0.084 (3)	0.184 (6)	−0.015 (2)	−0.005 (3)	0.062 (4)
O8	0.072 (3)	0.049 (2)	0.062 (2)	0.019 (2)	0.014 (2)	0.0153 (19)
N1	0.053 (3)	0.043 (3)	0.065 (3)	−0.009 (2)	0.026 (2)	−0.011 (2)
N2	0.052 (3)	0.041 (3)	0.070 (3)	−0.009 (2)	0.030 (2)	−0.010 (2)
N3	0.044 (2)	0.044 (2)	0.050 (3)	0.0077 (19)	0.002 (2)	0.002 (2)
N4	0.046 (3)	0.043 (2)	0.048 (3)	0.0108 (19)	0.007 (2)	0.004 (2)
C1	0.043 (3)	0.051 (3)	0.089 (5)	−0.001 (3)	0.014 (3)	0.012 (3)
C2	0.051 (3)	0.044 (3)	0.071 (4)	−0.004 (2)	0.020 (3)	0.004 (3)
C3	0.053 (3)	0.057 (4)	0.068 (4)	0.002 (3)	0.018 (3)	0.009 (3)
C4	0.079 (4)	0.040 (3)	0.072 (4)	−0.007 (3)	0.033 (3)	0.005 (3)
C5	0.051 (3)	0.041 (3)	0.083 (4)	−0.007 (2)	0.031 (3)	0.003 (3)
C6	0.058 (3)	0.041 (3)	0.057 (3)	−0.007 (2)	0.026 (3)	−0.011 (2)
C7	0.046 (3)	0.041 (3)	0.072 (4)	−0.002 (2)	0.027 (3)	−0.003 (3)
C8	0.049 (3)	0.048 (3)	0.062 (3)	−0.015 (2)	0.024 (3)	−0.006 (3)
C9	0.064 (4)	0.051 (3)	0.070 (4)	−0.012 (3)	0.027 (3)	−0.016 (3)
C10	0.059 (4)	0.080 (5)	0.070 (4)	−0.018 (3)	0.015 (3)	−0.015 (3)
C11	0.058 (4)	0.077 (5)	0.075 (4)	−0.005 (3)	0.016 (3)	0.004 (4)
C12	0.056 (4)	0.058 (4)	0.075 (4)	−0.006 (3)	0.027 (3)	0.003 (3)
C13	0.051 (3)	0.047 (3)	0.065 (4)	−0.014 (3)	0.025 (3)	−0.007 (3)
C14	0.032 (3)	0.050 (3)	0.078 (4)	−0.001 (2)	0.003 (3)	0.010 (3)

C15	0.032 (3)	0.043 (3)	0.067 (3)	0.003 (2)	0.009 (2)	0.014 (2)
C16	0.034 (3)	0.058 (4)	0.105 (5)	0.000 (3)	0.007 (3)	0.029 (3)
C17	0.042 (3)	0.060 (4)	0.113 (5)	−0.006 (3)	0.011 (3)	0.032 (4)
C18	0.053 (3)	0.043 (3)	0.075 (4)	0.006 (2)	0.013 (3)	0.014 (3)
C19	0.041 (3)	0.040 (3)	0.044 (3)	0.007 (2)	0.008 (2)	0.002 (2)
C20	0.035 (3)	0.041 (3)	0.057 (3)	−0.001 (2)	0.004 (2)	0.004 (2)
C21	0.047 (3)	0.047 (3)	0.040 (3)	0.015 (2)	0.006 (2)	−0.001 (2)
C22	0.052 (3)	0.052 (3)	0.048 (3)	0.012 (3)	0.008 (3)	−0.001 (2)
C23	0.052 (3)	0.069 (4)	0.054 (3)	0.000 (3)	0.004 (3)	−0.007 (3)
C24	0.054 (4)	0.102 (6)	0.056 (4)	0.024 (4)	−0.004 (3)	−0.004 (4)
C25	0.068 (4)	0.072 (4)	0.053 (4)	0.027 (3)	0.005 (3)	0.012 (3)
C26	0.060 (4)	0.052 (3)	0.045 (3)	0.022 (3)	0.010 (3)	0.005 (3)
C27	0.067 (4)	0.050 (3)	0.093 (5)	0.000 (3)	0.034 (4)	−0.010 (3)
C28	0.115 (6)	0.058 (4)	0.072 (4)	0.034 (4)	0.029 (4)	0.027 (3)
C29A	0.094 (9)	0.072 (8)	0.169 (11)	0.039 (8)	0.076 (8)	0.039 (9)
C30A	0.131 (8)	0.090 (7)	0.170 (10)	0.039 (7)	0.082 (8)	0.031 (7)
C31A	0.166 (9)	0.112 (8)	0.177 (10)	0.046 (8)	0.072 (8)	0.026 (8)
C32A	0.179 (13)	0.136 (12)	0.191 (13)	0.041 (11)	0.059 (12)	0.024 (11)
C29B	0.108 (8)	0.070 (6)	0.172 (10)	0.041 (6)	0.076 (7)	0.049 (7)
C30B	0.159 (8)	0.098 (7)	0.169 (9)	0.035 (7)	0.082 (7)	0.028 (7)
C31B	0.192 (10)	0.125 (8)	0.201 (11)	0.032 (8)	0.060 (8)	0.036 (8)
C32B	0.209 (13)	0.143 (11)	0.205 (13)	0.020 (11)	0.038 (11)	0.053 (10)
C33A	0.087 (7)	0.095 (7)	0.091 (6)	−0.017 (6)	−0.005 (5)	0.029 (6)
C34A	0.091 (7)	0.097 (7)	0.096 (6)	−0.012 (6)	0.002 (6)	0.014 (6)
C35A	0.120 (9)	0.119 (9)	0.110 (8)	0.002 (8)	−0.009 (8)	−0.004 (8)
C36A	0.136 (11)	0.129 (11)	0.119 (10)	−0.009 (10)	0.000 (9)	−0.010 (10)
C33B	0.088 (7)	0.098 (7)	0.097 (6)	−0.021 (6)	−0.001 (6)	0.023 (6)
C34B	0.106 (7)	0.105 (7)	0.108 (7)	−0.007 (6)	0.009 (6)	0.023 (6)
C35B	0.141 (10)	0.114 (9)	0.122 (9)	0.006 (8)	0.010 (8)	0.026 (8)
C36B	0.171 (12)	0.130 (11)	0.132 (11)	0.011 (10)	0.012 (11)	0.028 (10)

Geometric parameters (Å, °)

Sn1—O1	2.109 (3)	C23—C24	1.375 (9)
Sn1—C29A	2.112 (11)	C23—H23	0.9500
Sn1—O5	2.116 (3)	C24—C25	1.369 (9)
Sn1—C33B	2.122 (10)	C24—H24	0.9500
Sn1—C33A	2.127 (10)	C25—C26	1.385 (8)
Sn1—C29B	2.139 (10)	C25—H25	0.9500
Sn1—O6	2.517 (4)	C27—H271	0.9800
Sn1—O2	2.597 (4)	C27—H272	0.9800
Sn1—O7^{i}	3.192 (4)	C27—H273	0.9800
O1—C1	1.294 (7)	C28—H281	0.9800
O2—C1	1.246 (7)	C28—H282	0.9800
O3—C3	1.339 (7)	C28—H283	0.9800
O3—H3	0.8400	C29A—C30A	1.538 (8)
O4—C13	1.371 (6)	C29A—H291	0.9900
O4—C27	1.436 (7)	C29A—H292	0.9900
O5—C14	1.281 (6)	C30A—C31A	1.535 (8)

O6—C14	1.253 (6)	C30A—H301	0.9900
O7—C16	1.347 (7)	C30A—H302	0.9900
O7—H7	0.8400	C31A—C32A	1.539 (9)
O8—C26	1.353 (7)	C31A—H311	0.9900
O8—C28	1.439 (7)	C31A—H312	0.9900
N1—N2	1.261 (6)	C32A—H321	0.9800
N1—C6	1.406 (7)	C32A—H322	0.9800
N2—C8	1.427 (7)	C32A—H323	0.9800
N3—N4	1.261 (6)	C29B—C30B	1.556 (12)
N3—C19	1.426 (6)	C29B—H293	0.9900
N4—C21	1.418 (6)	C29B—H294	0.9900
C1—C2	1.478 (8)	C30B—C31B	1.517 (12)
C2—C7	1.386 (8)	C30B—H303	0.9900
C2—C3	1.415 (8)	C30B—H304	0.9900
C3—C4	1.395 (8)	C31B—C32B	1.560 (12)
C4—C5	1.342 (8)	C31B—H313	0.9900
C4—H4	0.9500	C31B—H314	0.9900
C5—C6	1.409 (8)	C32B—H324	0.9800
C5—H5	0.9500	C32B—H325	0.9800
C6—C7	1.390 (7)	C32B—H326	0.9800
C7—H71	0.9500	C33A—C34A	1.536 (9)
C8—C9	1.385 (7)	C33A—H331	0.9900
C8—C13	1.395 (8)	C33A—H332	0.9900
C9—C10	1.378 (8)	C34A—C35A	1.536 (8)
C9—H9	0.9500	C34A—H341	0.9900
C10—C11	1.382 (9)	C34A—H342	0.9900
C10—H10	0.9500	C35A—C36A	1.535 (8)
C11—C12	1.384 (9)	C35A—H351	0.9900
C11—H11	0.9500	C35A—H352	0.9900
C12—C13	1.373 (8)	C36A—H361	0.9800
C12—H12	0.9500	C36A—H362	0.9800
C14—C15	1.459 (7)	C36A—H363	0.9800
C15—C16	1.386 (7)	C33B—C34B	1.533 (12)
C15—C20	1.397 (7)	C33B—H333	0.9900
C16—C17	1.397 (8)	C33B—H334	0.9900
C17—C18	1.358 (8)	C34B—C35B	1.538 (12)
C17—H17	0.9500	C34B—H343	0.9900
C18—C19	1.393 (7)	C34B—H344	0.9900
C18—H18	0.9500	C35B—C36B	1.537 (12)
C19—C20	1.377 (7)	C35B—H353	0.9900
C20—H20	0.9500	C35B—H354	0.9900
C21—C22	1.392 (8)	C36B—H364	0.9800
C21—C26	1.405 (7)	C36B—H365	0.9800
C22—C23	1.377 (7)	C36B—H366	0.9800
C22—H22	0.9500		
O1—Sn1—C29A	105.5 (9)	C23—C22—H22	119.6
O1—Sn1—O5	81.84 (14)	C21—C22—H22	119.6
C29A—Sn1—O5	113.0 (5)	C24—C23—C22	118.8 (6)
O1—Sn1—C33B	103.6 (8)	C24—C23—H23	120.6

O5—Sn1—C33B	99.3 (6)	C22—C23—H23	120.6
O1—Sn1—C33A	102.9 (8)	C25—C24—C23	121.6 (6)
C29A—Sn1—C33A	132.7 (11)	C25—C24—H24	119.2
O5—Sn1—C33A	107.8 (6)	C23—C24—H24	119.2
O1—Sn1—C29B	98.8 (6)	C24—C25—C26	120.5 (6)
O5—Sn1—C29B	100.1 (4)	C24—C25—H25	119.7
C33B—Sn1—C29B	152.2 (10)	C26—C25—H25	119.7
O1—Sn1—O6	137.01 (13)	O8—C26—C25	125.0 (5)
C29A—Sn1—O6	90.9 (8)	O8—C26—C21	116.4 (5)
O5—Sn1—O6	55.23 (12)	C25—C26—C21	118.6 (6)
C33B—Sn1—O6	87.1 (6)	O4—C27—H271	109.5
C33A—Sn1—O6	93.3 (5)	O4—C27—H272	109.5
C29B—Sn1—O6	87.7 (6)	H271—C27—H272	109.5
O1—Sn1—O2	54.41 (13)	O4—C27—H273	109.5
C29A—Sn1—O2	81.8 (8)	H271—C27—H273	109.5
O5—Sn1—O2	136.25 (13)	H272—C27—H273	109.5
C33B—Sn1—O2	92.3 (5)	O8—C28—H281	109.5
C33A—Sn1—O2	85.0 (5)	O8—C28—H282	109.5
C29B—Sn1—O2	87.3 (6)	H281—C28—H282	109.5
O6—Sn1—O2	168.28 (13)	O8—C28—H283	109.5
O1—Sn1—O5	81.86 (13)	H281—C28—H283	109.5
O1—Sn1—O7^{i}	164.01 (13)	H282—C28—H283	109.5
C29A—Sn1—O7^{i}	69.4 (9)	C30A—C29A—Sn1	111.7 (12)
O5—Sn1—O7^{i}	114.15 (12)	C30A—C29A—H291	109.3
C33B—Sn1—O7^{i}	74.6 (9)	Sn1—C29A—H291	109.3
C33A—Sn1—O7^{i}	72.9 (9)	C30A—C29A—H292	109.3
C29B—Sn1—O7^{i}	79.3 (6)	Sn1—C29A—H292	109.3
O6—Sn1—O7^{i}	58.97 (12)	H291—C29A—H292	107.9
O2—Sn1—O7^{i}	109.60 (12)	C31A—C30A—C29A	120.7 (14)
C1—O1—Sn1	103.8 (3)	C31A—C30A—H301	107.1
C1—O2—Sn1	82.2 (3)	C29A—C30A—H301	107.1
C3—O3—H3	109.5	C31A—C30A—H302	107.1
C13—O4—C27	117.1 (5)	C29A—C30A—H302	107.1
C14—O5—Sn1	102.2 (3)	H301—C30A—H302	106.8
C14—O6—Sn1	84.2 (3)	C30A—C31A—C32A	102.6 (14)
C16—O7—Sn1^{i}	160.1 (4)	C30A—C31A—H311	111.3
C16—O7—H7	109.5	C32A—C31A—H311	111.3
Sn1^{i}—O7—H7	88.4	C30A—C31A—H312	111.3
C26—O8—C28	117.7 (5)	C32A—C31A—H312	111.3
N2—N1—C6	114.3 (4)	H311—C31A—H312	109.2
N1—N2—C8	113.6 (4)	C30B—C29B—Sn1	112.7 (10)
N4—N3—C19	113.2 (4)	C30B—C29B—H293	109.0
N3—N4—C21	113.6 (4)	Sn1—C29B—H293	109.0
O2—C1—O1	119.6 (5)	C30B—C29B—H294	109.0
O2—C1—C2	122.4 (5)	Sn1—C29B—H294	109.0
O1—C1—C2	118.0 (5)	H293—C29B—H294	107.8
C7—C2—C3	119.8 (5)	C31B—C30B—C29B	122.5 (12)

C7—C2—C1	120.4 (5)	C31B—C30B—H303	106.7
C3—C2—C1	119.7 (5)	C29B—C30B—H303	106.7
O3—C3—C4	119.3 (5)	C31B—C30B—H304	106.7
O3—C3—C2	122.7 (5)	C29B—C30B—H304	106.7
C4—C3—C2	118.0 (6)	H303—C30B—H304	106.6
C5—C4—C3	122.2 (6)	C30B—C31B—C32B	102.4 (14)
C5—C4—H4	118.9	C30B—C31B—H313	111.3
C3—C4—H4	118.9	C32B—C31B—H313	111.3
C4—C5—C6	120.4 (5)	C30B—C31B—H314	111.3
C4—C5—H5	119.8	C32B—C31B—H314	111.3
C6—C5—H5	119.8	H313—C31B—H314	109.2
C7—C6—N1	124.2 (5)	C31B—C32B—H324	109.5
C7—C6—C5	118.9 (5)	C31B—C32B—H325	109.5
N1—C6—C5	116.9 (5)	H324—C32B—H325	109.5
C2—C7—C6	120.7 (5)	C31B—C32B—H326	109.5
C2—C7—H71	119.7	H324—C32B—H326	109.5
C6—C7—H71	119.7	H325—C32B—H326	109.5
C9—C8—C13	119.1 (5)	C34A—C33A—Sn1	112.5 (9)
C9—C8—N2	123.7 (5)	C34A—C33A—H331	109.1
C13—C8—N2	117.1 (5)	Sn1—C33A—H331	109.1
C10—C9—C8	120.5 (6)	C34A—C33A—H332	109.1
C10—C9—H9	119.7	Sn1—C33A—H332	109.1
C8—C9—H9	119.7	H331—C33A—H332	107.8
C9—C10—C11	120.0 (6)	C35A—C34A—C33A	106.3 (10)
C9—C10—H10	120.0	C35A—C34A—H341	110.5
C11—C10—H10	120.0	C33A—C34A—H341	110.5
C10—C11—C12	119.9 (6)	C35A—C34A—H342	110.5
C10—C11—H11	120.1	C33A—C34A—H342	110.5
C12—C11—H11	120.1	H341—C34A—H342	108.7
C13—C12—C11	120.2 (6)	C36A—C35A—C34A	110.1 (12)
C13—C12—H12	119.9	C36A—C35A—H351	109.6
C11—C12—H12	119.9	C34A—C35A—H351	109.6
O4—C13—C12	123.8 (5)	C36A—C35A—H352	109.6
O4—C13—C8	116.0 (5)	C34A—C35A—H352	109.6
C12—C13—C8	120.2 (5)	H351—C35A—H352	108.2
O6—C14—O5	118.4 (5)	C34B—C33B—Sn1	123.9 (13)
O6—C14—C15	120.7 (5)	C34B—C33B—H333	106.4
O5—C14—C15	120.9 (4)	Sn1—C33B—H333	106.4
C16—C15—C20	118.9 (5)	C34B—C33B—H334	106.4
C16—C15—C14	121.5 (5)	Sn1—C33B—H334	106.4
C20—C15—C14	119.6 (4)	H333—C33B—H334	106.4
O7—C16—C15	123.0 (5)	C33B—C34B—C35B	105.6 (12)
O7—C16—C17	117.2 (5)	C33B—C34B—H343	110.6
C15—C16—C17	119.8 (5)	C35B—C34B—H343	110.6
C18—C17—C16	120.5 (5)	C33B—C34B—H344	110.6
C18—C17—H17	119.7	C35B—C34B—H344	110.6
C16—C17—H17	119.7	H343—C34B—H344	108.8
C17—C18—C19	120.5 (5)	C36B—C35B—C34B	109.5 (12)
C17—C18—H18	119.8	C36B—C35B—H353	109.8

C19—C18—H18	119.8	C34B—C35B—H353	109.8
C20—C19—C18	119.3 (5)	C36B—C35B—H354	109.8
C20—C19—N3	115.9 (4)	C34B—C35B—H354	109.8
C18—C19—N3	124.7 (5)	H353—C35B—H354	108.2
C19—C20—C15	120.9 (5)	C35B—C36B—H364	109.5
C19—C20—H20	119.5	C35B—C36B—H365	109.5
C15—C20—H20	119.5	H364—C36B—H365	109.5
C22—C21—C26	119.7 (5)	C35B—C36B—H366	109.5
C22—C21—N4	124.0 (5)	H364—C36B—H366	109.5
C26—C21—N4	116.3 (5)	H365—C36B—H366	109.5
C23—C22—C21	120.8 (5)		
C29A—Sn1—O1—C1	67.4 (7)	N2—C8—C13—C12	178.6 (5)
O5—Sn1—O1—C1	179.1 (4)	Sn1—O6—C14—O5	2.5 (5)
C33B—Sn1—O1—C1	−83.3 (7)	Sn1—O6—C14—C15	−176.0 (6)
C33A—Sn1—O1—C1	−74.4 (7)	Sn1—O5—C14—O6	−3.0 (7)
C29B—Sn1—O1—C1	80.0 (6)	Sn1—O5—C14—C15	175.5 (5)
O6—Sn1—O1—C1	176.2 (4)	O6—C14—C15—C16	−3.0 (10)
O2—Sn1—O1—C1	−0.3 (4)	O5—C14—C15—C16	178.6 (6)
O1—Sn1—O2—C1	0.3 (4)	O6—C14—C15—C20	176.3 (6)
C29A—Sn1—O2—C1	−115.5 (8)	O5—C14—C15—C20	−2.1 (9)
O5—Sn1—O2—C1	−0.6 (5)	C20—C15—C16—O7	−179.5 (6)
C33B—Sn1—O2—C1	105.4 (9)	C14—C15—C16—O7	−0.2 (11)
C33A—Sn1—O2—C1	110.0 (10)	C20—C15—C16—C17	0.2 (10)
C29B—Sn1—O2—C1	−102.5 (6)	C14—C15—C16—C17	179.4 (6)
O6—Sn1—O2—C1	−167.8 (8)	O7—C16—C17—C18	178.5 (7)
O1—Sn1—O5—C14	−176.0 (4)	C15—C16—C17—C18	−1.3 (11)
C29A—Sn1—O5—C14	−72.5 (11)	C16—C17—C18—C19	1.0 (11)
C33B—Sn1—O5—C14	81.4 (9)	C17—C18—C19—C20	0.4 (9)
C33A—Sn1—O5—C14	83.0 (9)	C17—C18—C19—N3	−178.0 (6)
C29B—Sn1—O5—C14	−78.5 (7)	N4—N3—C19—C20	−162.8 (5)
O6—Sn1—O5—C14	1.6 (4)	N4—N3—C19—C18	15.6 (7)
O2—Sn1—O5—C14	−175.3 (3)	C18—C19—C20—C15	−1.5 (8)
O1—Sn1—O6—C14	1.9 (5)	N3—C19—C20—C15	177.0 (5)
C29A—Sn1—O6—C14	116.1 (7)	C16—C15—C20—C19	1.2 (9)
O5—Sn1—O6—C14	−1.6 (4)	C14—C15—C20—C19	−178.1 (5)
C33B—Sn1—O6—C14	−105.0 (9)	N3—N4—C21—C22	−10.1 (7)
C33A—Sn1—O6—C14	−111.0 (10)	N3—N4—C21—C26	173.3 (4)
C29B—Sn1—O6—C14	102.4 (6)	C26—C21—C22—C23	−2.8 (8)
O2—Sn1—O6—C14	167.6 (7)	N4—C21—C22—C23	−179.3 (5)
C6—N1—N2—C8	175.3 (4)	C21—C22—C23—C24	1.1 (8)
C19—N3—N4—C21	177.3 (4)	C22—C23—C24—C25	0.9 (9)
Sn1—O2—C1—O1	−0.4 (6)	C23—C24—C25—C26	−1.0 (10)
Sn1—O2—C1—C2	179.9 (6)	C28—O8—C26—C25	−6.1 (8)
Sn1—O1—C1—O2	0.5 (7)	C28—O8—C26—C21	174.2 (5)
Sn1—O1—C1—C2	−179.8 (5)	C24—C25—C26—O8	179.6 (6)
O2—C1—C2—C7	−176.9 (6)	C24—C25—C26—C21	−0.7 (9)
O1—C1—C2—C7	3.4 (9)	C22—C21—C26—O8	−177.7 (5)
O2—C1—C2—C3	1.9 (10)	N4—C21—C26—O8	−0.9 (7)
O1—C1—C2—C3	−177.7 (6)	C22—C21—C26—C25	2.5 (8)

C7—C2—C3—O3	177.9 (6)	N4—C21—C26—C25	179.3 (5)
C1—C2—C3—O3	−1.0 (9)	O1—Sn1—C29A—C30A	92.9 (18)
C7—C2—C3—C4	−0.9 (9)	O5—Sn1—C29A—C30A	5(2)
C1—C2—C3—C4	−179.8 (5)	C33A—Sn1—C29A—C30A	−142.2 (13)
O3—C3—C4—C5	−178.1 (6)	O6—Sn1—C29A—C30A	−46.9 (18)
C2—C3—C4—C5	0.7 (9)	O2—Sn1—C29A—C30A	142.3 (18)
C3—C4—C5—C6	0.0 (9)	Sn1—C29A—C30A—C31A	−60 (3)
N2—N1—C6—C7	−24.0 (7)	C29A—C30A—C31A—C32A	−179 (2)
N2—N1—C6—C5	157.5 (5)	O1—Sn1—C29B—C30B	42.7 (14)
C4—C5—C6—C7	−0.5 (8)	O5—Sn1—C29B—C30B	−40.5 (14)
C4—C5—C6—N1	178.0 (5)	C33B—Sn1—C29B—C30B	−174.0 (13)
C3—C2—C7—C6	0.3 (8)	O6—Sn1—C29B—C30B	−94.6 (13)
C1—C2—C7—C6	179.2 (5)	O2—Sn1—C29B—C30B	96.1 (14)
N1—C6—C7—C2	−178.1 (5)	Sn1—C29B—C30B—C31B	−173.6 (15)
C5—C6—C7—C2	0.4 (8)	C29B—C30B—C31B—C32B	178.5 (18)
N1—N2—C8—C9	−28.8 (7)	O1—Sn1—C33A—C34A	−123.3 (19)
N1—N2—C8—C13	154.5 (5)	C29A—Sn1—C33A—C34A	111 (2)
C13—C8—C9—C10	−1.1 (8)	O5—Sn1—C33A—C34A	−38 (2)
N2—C8—C9—C10	−177.8 (5)	O6—Sn1—C33A—C34A	17 (2)
C8—C9—C10—C11	0.1 (9)	O2—Sn1—C33A—C34A	−175 (2)
C9—C10—C11—C12	0.3 (10)	Sn1—C33A—C34A—C35A	−178.5 (15)
C10—C11—C12—C13	0.3 (9)	C33A—C34A—C35A—C36A	−179 (2)
C27—O4—C13—C12	−6.8 (8)	O1—Sn1—C33B—C34B	47.2 (19)
C27—O4—C13—C8	174.7 (5)	O5—Sn1—C33B—C34B	131.0 (17)
C11—C12—C13—O4	−179.7 (5)	C29B—Sn1—C33B—C34B	−95 (3)
C11—C12—C13—C8	−1.3 (8)	O6—Sn1—C33B—C34B	−175.0 (19)
C9—C8—C13—O4	−179.7 (5)	O2—Sn1—C33B—C34B	−6.7 (19)
N2—C8—C13—O4	−2.9 (7)	Sn1—C33B—C34B—C35B	78 (2)
C9—C8—C13—C12	1.7 (8)	C33B—C34B—C35B—C36B	−172.0 (17)

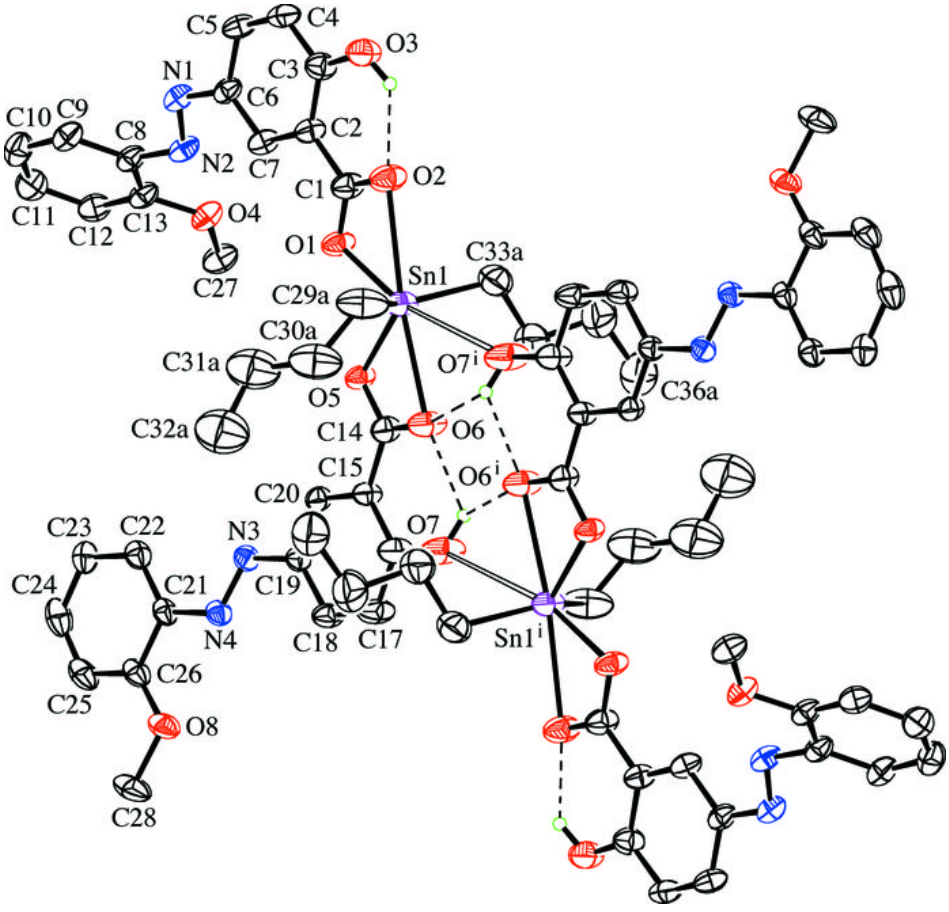
Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.84	1.93	2.613 (6)	138
O7—H7···O6	0.84	2.01	2.603 (6)	127
O7—H7···O6^{i}	0.84	2.39	2.871 (6)	117
C22—H22···O8^{ii}	0.95	2.62	3.334 (7)	134
C27—H271···O8^{ii}	0.98	2.62	3.449 (8)	142
C27—H272···O4^{iii}	0.98	2.67	3.434 (8)	136
C32B—H326···O3^{iv}	0.98	2.69	3.67 (2)	170
C33B—H333···O7^{i}	0.99	2.64	3.33 (3)	127

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

Fig. 1


C5
C4
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C13
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C33a
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C32a
C14
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C15
O6i
C20
O7
C23
C22
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C24
C21
C19
N4
C18
C17
Sn1i
C26
C25
O8
C28