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Structural diversity among some dialkyltin(IV) benzoate and related derivatives

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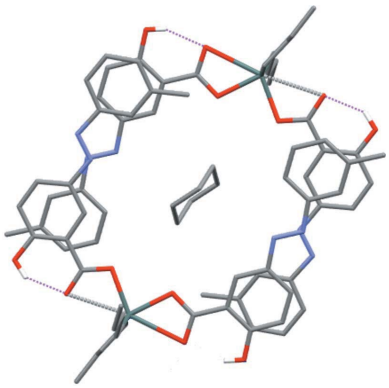
The molecular structures of five diorganotin(IV) carboxylates, (I)–(V), can be categorized into two main well-known structural types for such Sn complexes. One is the mononuclear dialkytin(IV) carboxylates with an $[R_2Sn(LH)_2]$-type skew-trapezoidal bipyramid, where the alkyl ligands are in pseudo-axial positions and the O atoms from two asymmetrically coordinated bidentate carboxylate ligands are in the equatorial plane. This structure type is adopted by dibutylbis{(*E*)-2-hydroxy-5-[(3-methylphenyl)diazenyl]benzoato}tin(IV) cyclohexane hemisolvate, $[Sn(C_4H_9)_2(C_{14}H_{11}N_2O_3)_2]\cdot0.5C_6H_{12}$, (I), dibenzylbis{(*E*)-5-[(4-bromophenyl)diazenyl]-2-hydroxybenzoato}tin(IV), $[Sn(C_7H_7)_2(C_{13}H_8BrN_2O_3)_2]$, (II), and aquadibenzylbis(4-{(*E*)-[(*Z*)-4-hydroxypent-3-en-2-ylidene]amino}benzoato)tin(IV) benzene disolvate, $[Sn(C_7H_7)_2(C_{12}H_{12}NO_3)_2(H_2O)]\cdot2C_6H_6$, (III), although the latter has an additional water ligand to give a distorted pentagonal bipyramidal coordination geometry in which the carboxylate groups are more symmetrically coordinated to the Sn atom than in (I) and (II). The other structure motif is that of the tetranuclear bis(dicarboxylatotetraorganodistannoxanes), $\{[R_2Sn(LH)]_2O\}_2$, which contain an Sn_4O_2 core decorated with four bridging carboxylate ligands, plus two alkyl ligands at each Sn^{IV} centre. The complexes octabutyltetrakis{μ-(*E*)-4-[(4-hydroxy-3,5-dimethylphenyl)diazenyl]benzoato}di-μ_3-oxido-tetratin(IV) ethanol disolvate, $[Sn_4(C_4H_9)_8(C_{15}H_{13}N_2O_3)_4O_2]\cdot2C_2H_6O$, (IV), and octabutyltetrakis{(*E*)-3-[(2-hydroxybenzylidene)amino]propanoato}di-μ_3-oxido-tetratin(IV), $[Sn_4(C_4H_9)_8(C_{10}H_{10}NO_3)_4O_2]$, (V), display this motif. The structures obtained correlate with the 1:1 and 1:2 stoichiometric ratios of the dialkyltin(IV) and carboxylic acid starting materials in the syntheses. The supramolecular structures arising from consideration of secondary Sn$\cdots$O interactions and/or classic hydrogen bonds include discrete molecules for (V), centrosymmetric dimers for (I), extended chains for (II) and (III), and sheets for (IV).

1. Introduction

The structures of organotin(IV) carboxylates are reported frequently and their diverse characteristics include a variety of tin coordination geometries, which manifest themselves in monomeric or discrete *n*-meric species with *n* up to 6, and polymeric extended structures, as well as discrete monomeric, but polynuclear, species (Tiekink, 1991, 1994; Chandrasekhar *et al.*, 2002; Prabusankar & Murugavel, 2004). The range of observed organotin(IV) carboxylate structures has been attributed to the influence of ligand size, shape, steric restrictions, electronic properties, and even to the stoichiometries of the reactants (Buntine *et al.*, 1998; Willem *et al.*, 1998; Dakternieks *et al.*, 2003; Prabusankar & Murugavel, 2004). Some organotin(IV) carboxylates have useful biological properties and, in particular, the cytotoxic potential of triorganotin(IV) and diorganotin(IV) carboxylates has been investigated (Gielen & Tiekink, 2005; Hussain *et al.*, 2015;



Basu Baul, Kehie *et al.*, 2017). A common coordination geometry found for mononuclear dialkytin(IV) carboxylates and, in particular, the subset of benzoates, is the $[R_2Sn(LH)_2]$ (R = alkyl or aryl; L = carboxylate ligand) type skew-trapezoidal bipyramid, with the *R* ligands in pseudo-axial positions and the O atoms from two asymmetrically coordinated bidentate carboxylate ligands in the equatorial plane (Tiekink, 1991, 1994; Basu Baul *et al.*, 2004; Hussain *et al.*, 2015). A second motif is that of the tetranuclear bis(dicarboxylatotetraorganodistannoxanes), $\{[R_2Sn(LH)]_2O\}_2$, which contain an Sn_4O_2 core decorated with four bridging carboxylate ligands, plus two alkyl ligands at each Sn centre (Basu Baul *et al.*, 2006; Basu Baul, Dutta *et al.*, 2017; Debnath *et al.*, 2020). Here we report the molecular and supramolecular structures of five new diorganotin(IV) carboxylates, (I)–(V) (see Scheme 1), which generally fit into one or the other of the above two types, and correlate the structures obtained with the stoichiometry of the reactants. Complexes (I) and (II) are of the $[R_2Sn(LH)_2]$ type (R = ^{n}Bu or Bz), (III) is the similar $[Bz_2Sn(LH)_2(H_2O)]$, while (IV) and (V) are of the $\{[^nBu_2Sn(LH)]_2O\}_2$ type.

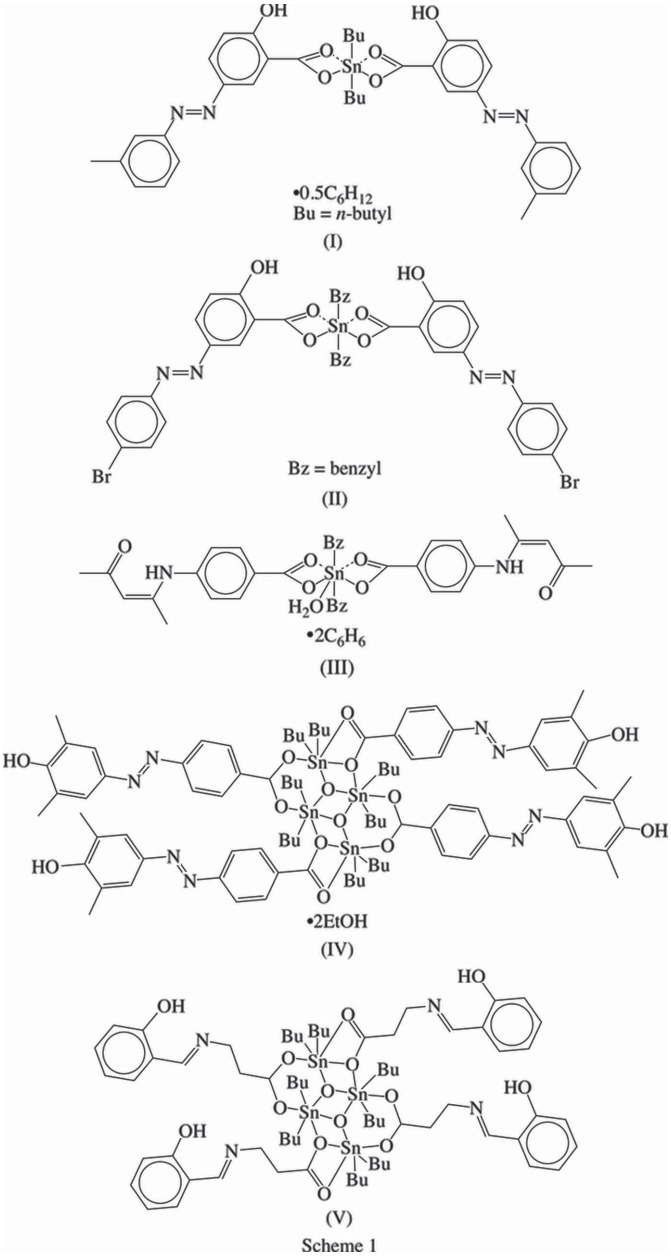
2. Experimental

2.1. Synthesis and crystallization

Dibutyltin(IV) complex (I) was prepared by the reaction of (*E*)-2-hydroxy-5-[(3-methylphenyl)diazenyl]benzoic acid and di-*n*-butyltin(IV) oxide (2:1) in anhydrous benzene under reflux conditions for 8 h. The clear solution was filtered and evaporated to dryness. The dry mass was extracted in a cyclohexane/petroleum ether (60–80 °C) mixture (1:1 *v*/*v*), which, upon slow evaporation, yielded a crystalline material with a yield of 73%. Orange single crystals of the compound were obtained from repeated crystallization from petroleum ether (m.p. 393–394 K). Elemental analysis calculated (%) for $C_{39}H_{46}N_4O_6Sn$: C 59.63, H 5.90, N 7.13; found: C 59.32, H 5.98, N 7.50.

Dibenzyltin(IV) compound (II) was prepared by the reaction of (*E*)-5-[(4-bromophenyl)diazenyl]-2-hydroxybenzoic acid with dibenzyltin(IV) oxide (2:1) in anhydrous toluene under reflux for 6 h using a Dean–Stark water separator and a water-cooled condenser. The orange-coloured reaction mixture was filtered, concentrated to a minimum volume, precipitated with hexane and filtered again. The residue was dissolved in benzene, which, upon slow evaporation, yielded orange crystals (yield 58%; m.p. 448–449 K). Elemental analysis calculated (%) for $C_{40}H_{30}Br_2N_4O_6Sn$: C 51.04, H 3.21, N 5.95; found: C 51.44, H 2.98, N 6.32.

Dibenzyltin(IV) complex (III) was prepared by the reaction of 4-{(*E*)-[(*Z*)-4-hydroxypent-3-en-2-ylidene]amino}benzoic acid and dibenzyltin(IV) dichloride (2:1) in anhydrous benzene. The reaction mixture was refluxed for 1 h; triethylamine (2 mol) was then added dropwise and reflux was continued for an additional 3 h. The reaction mixture was cooled to room temperature and filtered in order to remove triethylammonium chloride. The filtrate was evaporated and the residue dried *in vacuo*. The residue was extracted into benzene and filtered to remove any suspended particles. The filtrate was concentrated and allowed to evaporate slowly at room temperature until the solid material precipitated. The solid material was filtered off, dried *in vacuo* and then recrystallized from benzene, which, upon slow evaporation, afforded colourless crystals (yield 56%; m.p. 359–361 K).



Scheme 1

Tetranuclear Sn complex (IV) was prepared by refluxing equimolar amounts of di-*n*-butyltin(IV) oxide and (*E*)-4-[(4-hydroxy-3,5-dimethylphenyl)diazenyl]benzoic acid in anhydrous toluene for 8 h in a flask equipped with a Dean–Stark water separator and a water-cooled condenser. The clear reaction mixture was filtered and the filtrate was evaporated to dryness. The dried mass was washed with hot hexane and the residue was dissolved in toluene and filtered while hot. A few drops of ethanol were added to facilitate clarification of the

Table 1
Experimental details.

Experiments were carried out at 160 K with Mo $K\alpha$ radiation using a Nonius KappaCCD area-detector diffractometer. Absorption was corrected for by multi-scan methods (*SORTAV*; Blessing, 1995).

	(I)	(II)	(III)
Crystal data			
Chemical formula	$[Sn(C_4H_9)_2(C_{14}H_{11}N_2O_3)_2]\cdot 0.5C_6H_{12}$	$[Sn(C_7H_7)_2(C_{13}H_8BrN_2O_3)_2]$	$[Sn(C_7H_7)_2(C_{12}H_{12}NO_3)_2(H_2O)]\cdot 2C_6H_6$
M_r	785.49	941.19	911.62
Crystal system, space group	Monoclinic, $P2_1/c$	Monoclinic, $P2_1/n$	Monoclinic, $C2/c$
a, b, c (Å)	9.4028 (1), 25.1718 (2), 15.5008 (1)	13.6816 (1), 12.5767 (1), 22.5401 (2)	23.6530 (5), 10.1034 (2), 20.5952 (4)
α, β, γ (°)	90, 93.3046 (3), 90	90, 107.0174 (6), 90	90, 115.0715 (12), 90
V (Å^3)	3662.71 (5)	3708.65 (5)	4458.02 (16)
Z	4	4	4
μ (mm^{-1})	0.75	2.90	0.63
Crystal size (mm)	0.25 × 0.17 × 0.12	0.25 × 0.15 × 0.10	0.25 × 0.22 × 0.10
Data collection			
T_{min}, T_{max}	0.854, 0.917	0.652, 0.843	0.753, 0.943
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	90950, 10708, 7109	107473, 10845, 8598	58583, 6506, 5193
R_{int}	0.066	0.059	0.101
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.704	0.704	0.704
Refinement			
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.040, 0.110, 1.04	0.032, 0.076, 1.04	0.056, 0.148, 1.05
No. of reflections	10702	10845	6506
No. of parameters	623	487	228
No. of restraints	645	0	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.90, −0.63	0.69, −0.87	1.06, −2.17

	(IV)	(V)
Crystal data		
Chemical formula	$[Sn_4(C_4H_9)_8(C_{15}H_{13}N_2O_3)_4O_2]\cdot 2C_2H_6O$	$[Sn_4(C_4H_9)_8(C_{10}H_{10}NO_3)_4O_2]$
M_r	2132.88	1732.41
Crystal system, space group	Monoclinic, $P2_1/c$	Triclinic, $P\overline{1}$
a, b, c (Å)	11.8395 (1), 24.2855 (3), 17.3557 (2)	12.0054 (3), 14.7309 (4), 23.9132 (6)
α, β, γ (°)	90, 93.2962 (7), 90	76.3707 (18), 75.5206 (16), 88.1609 (16)
V (Å^3)	4982.00 (9)	3977.81 (18)
Z	2	2
μ (mm^{-1})	1.06	1.30
Crystal size (mm)	0.35 × 0.20 × 0.15	0.25 × 0.20 × 0.05
Data collection		
T_{min}, T_{max}	0.829, 0.922	0.358, 0.537
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	94026, 11376, 9553	68065, 14030, 8004
R_{int}	0.049	0.107
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.649	0.596
Refinement		
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.077, 1.04	0.046, 0.114, 1.02
No. of reflections	11371	14030
No. of parameters	628	859
No. of restraints	144	0
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.91, −0.93	1.20, −1.11

Computer programs: *COLLECT* (Nonius, 2000), *DENZO-SMN* and *SCALEPACK* (Otwinowski & Minor, 1997), *SIR92* (Altomare *et al.*, 1994), *SHELXS97* (Sheldrick, 2008), *PATTY* and *DIRDIF94* (Beurskens *et al.*, 1992, 1994), *ORTEPII* (Johnson, 1976), *SHELXL2018* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2020) and *PLATON* (Spek, 2020).

solution. An orange microcrystalline material was obtained after standing for a week (yield 63%; m.p. 442–443 K). Elemental analysis calculated (%) for $C_{96}H_{136}N_8O_{14}Sn_4$: C 54.47, H 6.48, N 5.29; found: C 54.54, H 6.82, N 5.70.

Tetranuclear Sn complex (V) was synthesized by reacting equimolar amounts of di-*n*-butyltin(IV) dichloride and potassium (*E*)-3-[(2-hydroxybenzylidene)amino]propanoate, dissolved in anhydrous chloroform and methanol, respectively,

under stirring for 6 h. The reaction mixture was filtered and evaporated to dryness. The dry mass was extracted in chloroform, concentrated and precipitated with hexane. Recrystallization from chloroform/hexane afforded yellow crystals in a yield of 55% (m.p. 644–645 K). Elemental analysis calculated (%) for $C_{72}H_{112}N_4O_{14}Sn_4$: C 49.91, H 6.52, N 3.23; found: C 49.66, H 6.88, N 3.20.

2.2. Refinement

Crystal data, data collection and structure refinement details for (I)–(V) are summarized in Table 1. A correction for secondary extinction was applied only in the case of (II).

The asymmetric unit of (I) contains one molecule of the Sn complex plus one half of a cyclohexane molecule, which sits about a crystallographic centre of inversion. A test refinement of the site-occupation factor of the cyclohexane atoms suggested an occupancy of approximately 86%. Another test refinement, where the SQUEEZE routine (Spek, 2015) of the program *PLATON* (Spek, 2020) was used to account for the solvent molecule, gave an electron count of 52 e per void, whereas cyclohexane has 48 e. There are no voids in the structure when the solvent molecule is included. These tests suggest that the solvent molecule site is essentially fully occupied. The geometry of the cyclohexane molecule is poor because of possible disorder, as indicated by the enlarged atomic displacement parameters, but attempts to model the disorder did not improve the refinement agreement factors significantly and led to unreasonably short intermolecular contacts. The C—C distances within the solvent molecule were restrained to 1.52 (1) Å, while it was preferred not to restrain the atomic displacement parameters of the cyclohexane atoms.

One of the carboxylate ligands in (I) is disordered in its entirety over two conformations, the difference arising from a reversal of the direction of the zigzag at the N═N bond (Fig. 1). Two positions were defined for all the atoms of this ligand, except for the carboxylate O atom bound strongly with the Sn atom, which is not significantly disordered. Refinement of constrained site-occupation factors for the two orientations yielded a value of 0.563 (5) for the major conformation. Similarity restraints were applied to the chemically equivalent bond lengths and angles of all the atoms in the carboxylate ligands, including those of the ordered ligand. Furthermore, neighbouring atoms within and between each conformation of the disordered ligand were restrained to have similar atomic displacement parameters.

The asymmetric unit of (III) contains one half of a molecule of the Sn complex, which sits across a twofold axis, plus a highly disordered benzene molecule. The disordered solvent molecule could not be modelled adequately, so its contribution to the diffraction data was removed using the SQUEEZE routine of *PLATON*. When the solvent molecule is excluded from the model, there are four cavities of 324 Å^3 per unit cell. The total number of electrons contributing to each void was calculated by the SQUEEZE routine to be approximately 85 e. A benzene molecule has 42 e, which suggests that the cavities have two molecules of benzene (one per asymmetric unit) and this approximation was used in the subsequent calculation of the empirical formula, formula weight, density, linear absorption coefficient and $F(000)$. Based on the assumption, the overall ratio of Sn complex molecules to benzene is 1:2.

In (IV), the Sn complex molecule sits across a crystallographic centre of inversion and the asymmetric unit includes a molecule of ethanol. Two butyl ligands at the same Sn atom

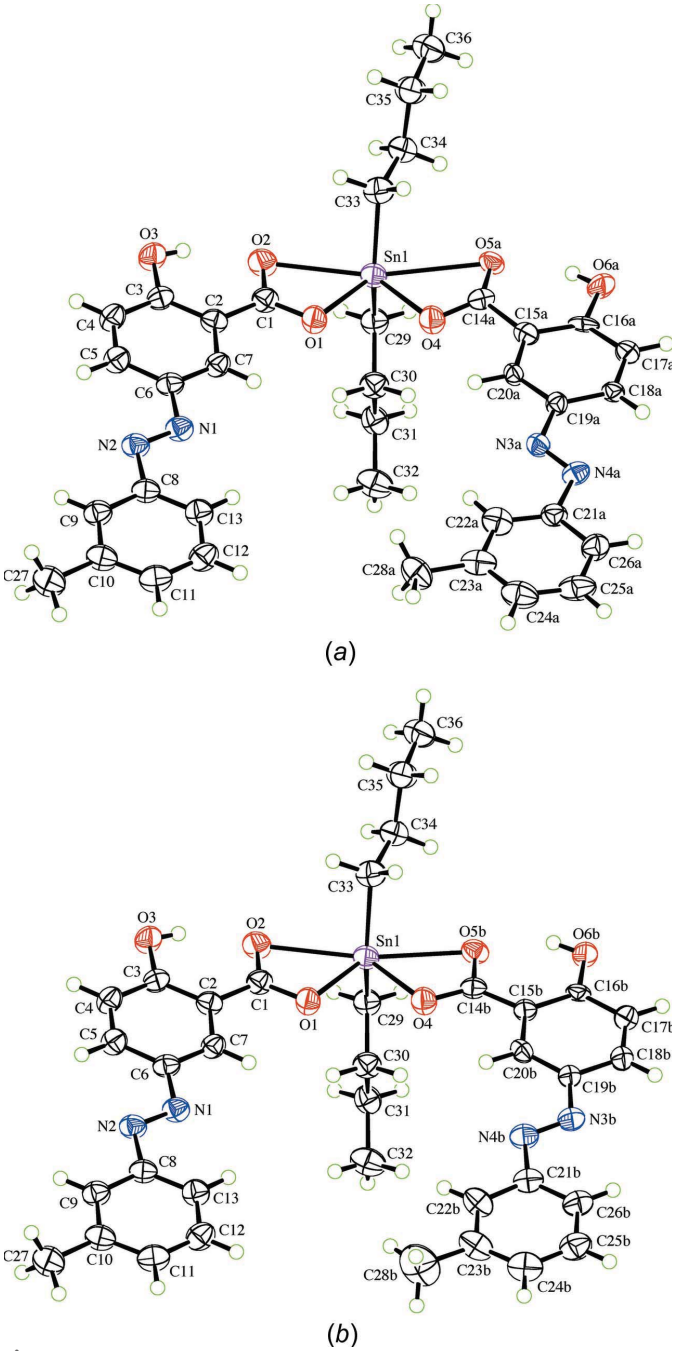


Figure 1
The molecular structure of the Sn^{IV} complex molecule of (I), showing the atom-labelling scheme for (*a*) the minor-disorder conformation of the right-hand benzoate ligand and (*b*) the major-disorder conformation. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

are disordered over two conformations. Two sets of positions were defined for the atoms of one methylene group in one butyl ligand and for all the atoms of the other disordered butyl ligand, and the site-occupation factors of the major conformations of these groups refined to 0.846 (6) and 0.683 (5), respectively. Similarity restraints were applied to the chemically equivalent bond lengths and angles involving all disordered C atoms, while neighbouring atoms within and between each conformation of the disordered butyl groups were restrained to have similar atomic displacement parameters. A pseudo-isotropic restraint was also applied to the atomic displacement parameters of atom O2.

The hydroxy, amine and water H atoms, where present in (I)–(IV), were located in a difference Fourier map and their positions were refined along with individual isotropic displacement parameters. The unique O—H distance in the water ligand of (III) was restrained to 0.84 (1) Å. In (V), the hydroxy H atoms were constrained to an ideal geometry (O—H = 0.84 Å), with U_{iso}(H) = 1.5U_{eq}(O), but were allowed to rotate freely about the O—C bonds. For all structures, the methyl H atoms were constrained to an ideal geometry (C—H = 0.98 Å), with U_{iso}(H) = 1.5U_{eq}(C), but were allowed to rotate freely about the C—C bonds. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic, alkene) or 0.99 Å (methylene) and with U_{iso}(H) = 1.2U_{eq}(C).

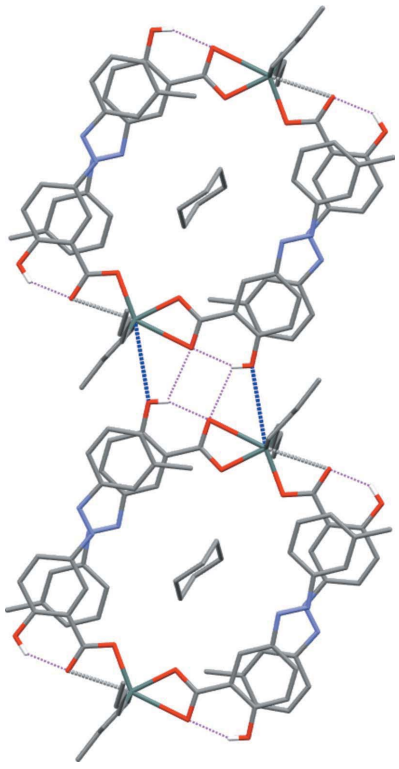


Figure 2
The tetrameric assembly of the Sn^{IV} complex molecules of (I), showing the secondary Sn···O bonds (blue dashed lines), the O—H···O hydrogen bonds (magenta dashed lines), the head-to-tail overlay of the molecules involved in π–π interactions and the cyclohexane molecules in the cavity between the overlaid pairs of molecules. Only one conformation of the disordered benzoate ligand is included. Most H atoms have been omitted for clarity.

Table 2
Selected geometric parameters (Å, °) for (I).

Sn1—O1	2.0961 (16)	Sn1—C29	2.110 (3)
Sn1—O2	2.6252 (18)	Sn1—C33	2.110 (3)
Sn1—O4	2.0954 (17)	Sn1—O3^{i}	3.4786 (17)
Sn1—O5*A*	2.81 (3)	N1—N2	1.250 (3)
Sn1—O5*B*	2.60 (2)		
O1—Sn1—O2	53.93 (5)	O2—Sn1—C33	87.56 (9)
O1—Sn1—O4	82.76 (6)	O4—Sn1—O5*A*	53.3 (3)
O1—Sn1—O5*A*	135.8 (3)	O4—Sn1—O5*B*	52.9 (2)
O1—Sn1—O5*B*	135.6 (2)	O4—Sn1—C29	102.85 (9)
O1—Sn1—C29	103.65 (9)	O4—Sn1—C33	105.25 (9)
O1—Sn1—C33	109.89 (9)	O5*A*—Sn1—C29	91.6 (6)
O2—Sn1—O4	136.44 (6)	O5*A*—Sn1—C33	81.4 (6)
O2—Sn1—O5*A*	167.5 (4)	O5*B*—Sn1—C29	88.7 (5)
O2—Sn1—O5*B*	169.5 (3)	O5*B*—Sn1—C33	84.4 (5)
O2—Sn1—C29	92.83 (8)	C29—Sn1—C33	138.31 (10)

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

3. Results and discussion

3.1. Molecular structures and Sn^{IV} coordination motifs

Dibutylbis{(*E*)-2-hydroxy-5-[(3-methylphenyl)diazenyl]benzoato}tin(IV) cyclohexane hemisolvate, (I), which can be abbreviated as a 3-methylphenylazobenzoate dibutyltin(IV) derivative, is a mononuclear molecule, which crystallizes with the solvent molecule on a crystallographic centre of inversion (Fig. 1). The crystal structure is isostructural with that of the corresponding benzene hemisolvate [compound **3** in Basu Baul *et al.* (2004)]. Even the ratios of site occupation of the disordered conformations of one carboxylate ligand are similar [0.563 (5) in (I) and 0.579 (5) in the benzene hemisolvate]. The disorder results from a reversal of the direction of the zigzag at the azo bond. Nonetheless, the relative orientation of the two coplanar carboxylate ligands in the Sn complex molecule in both structures is the same, even with regard to the directions of the methyl groups, which both point towards the same side of the molecule, regardless of the direction of the azo zigzag. The geometry of the Sn complex molecule in (I) is the same as that described for the benzene hemisolvate, so will not be elaborated in detail here, other than to remind readers that the coordination geometry at the Sn atom is skew-trapezoidal bipyramidal (Table 2), with asymmetrically coordinated carboxylate groups in the equatorial plane and the *n*-butyl ligands extending outwards in slightly bent pseudo-axial positions, as observed for many azocarboxylatodialkyltin(IV) complexes of this type (Tiekink, 1991, 1994). The molecules are linked into centrosymmetric dimers by secondary Sn···O interactions of 3.4786 (17) Å involving the hydroxy O atom of a carboxylate ligand of an adjacent molecule (Fig. 2). This arrangement, with a very similar Sn···O distance of 3.439 (2) Å, was also observed in the structure of the benzene hemisolvate. The structure of the 2-methoxyphenyl analogue shows similar secondary interactions, although a significantly shorter Sn···O distance of 3.192 (4) Å is present (Linden *et al.*, 2007).

The structure of the related 4-bromophenylazobenzoate dibutyltin(IV) derivative dibutylbis{(*E*)-5-[(4-bromophenyl)-diazenyl]-2-hydroxybenzoato}tin(IV) has also been reported

Table 3
Selected geometric parameters (Å, °) for (II).

Sn1—O1	2.1077 (14)	Sn1—C27	2.132 (2)
Sn1—O2	2.5939 (15)	Sn1—C34	2.130 (2)
Sn1—O4	2.1100 (14)	Sn1—O3^{i}	3.0858 (16)
Sn1—O5	2.5426 (16)	N1—N2	1.260 (3)
O1—Sn1—O2	54.69 (5)	O2—Sn1—C34	89.30 (7)
O1—Sn1—O4	81.12 (6)	O4—Sn1—O5	55.27 (5)
O1—Sn1—O5	136.25 (5)	O4—Sn1—C27	106.44 (7)
O1—Sn1—C27	106.31 (8)	O4—Sn1—C34	103.69 (8)
O1—Sn1—C34	102.97 (7)	O5—Sn1—C27	85.08 (8)
O2—Sn1—O4	135.78 (5)	O5—Sn1—C34	91.74 (7)
O2—Sn1—O5	168.06 (5)	C27—Sn1—C34	140.54 (9)
O2—Sn1—C27	86.57 (8)		

Symmetry code: (i) $-x+\frac{5}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

[compound **6** in Basu Baul *et al.* (2004)], but the structure of the corresponding dibenzyltin(IV) derivative, dibenzylbis-{(*E*)-5-[(4-bromophenyl)diazenyl]-2-hydroxybenzoato}tin(IV), (II), is almost unique in that up to now only one other structure of a mononuclear dibenzyltin(IV) derivative with benzoate ligands of any kind has been reported, that being the simple complex bis(4-aminobenzoato)dibenzyltin(IV) (Wang *et al.*, 2005; CSD refcode ACUNIX). Compound (III), described further below, is another new example of a bis(benzoato)dibenzyltin(IV) complex.

In the structure of compound (II), the Sn atom has the usual skew-trapezoidal bipyramidal geometry, with the benzyl ligands in pseudo-axial positions, whereby their phenyl rings fold over and under the carboxylate groups (Fig. 3 and Table 3). Compared with the corresponding dibutyltin(IV) complex, the only significant difference in the geometry of the primary Sn coordination sphere in (II) is a slightly more symmetrical coordination of the carboxylate groups, with the

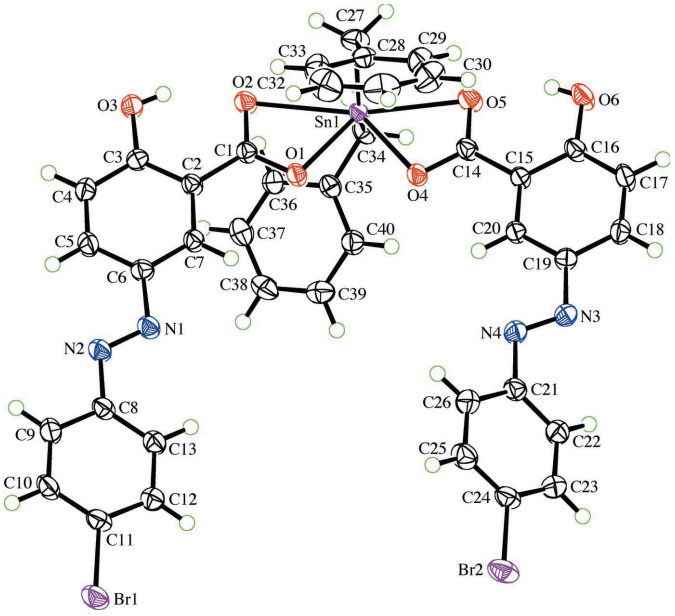


Figure 3
View of the unique molecule of (II), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

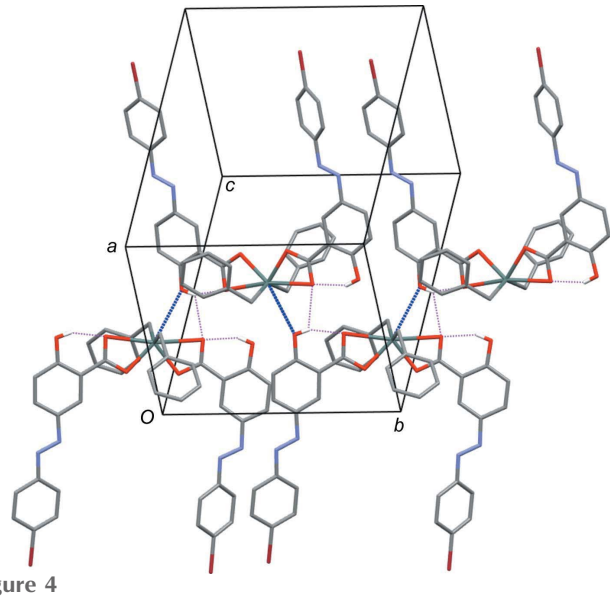


Figure 4
The extended chains of the molecules of (II), showing the secondary Sn···O bonds (blue dashed lines), the O—H···O hydrogen bonds (magenta dashed lines) and the near-overlay of the ring systems of adjacent molecules (such as at the bottom middle of the image). Most H atoms have been omitted for clarity.

longer of the Sn—O distances being about 0.1 Å shorter in (II) than in the dibutyltin(IV) complex. There are no other trends in the geometry of the primary coordination sphere that could be attributed to the replacement of the *n*-butyl ligands with benzyl groups. However, the secondary intermolecular Sn···O contact involving the hydroxy O atom of each carboxylate ligand found in (I) is also present in (II), but is much shorter at 3.0858 (16) Å. In contrast to (I), these interactions do not link the molecules into centrosymmetric dimers, but into extended zigzag chains, which have 2_1-screw symmetry and run parallel to the [010] direction (Fig. 4). Similar chains were also observed for the related phenylazobenzoate dibutyltin(IV) derivative dibutylbis{2-hydroxy-5-[(*E*)-2-phenyl-1-diazenyl]-benzoato}tin(IV) [compound **1** in Basu Baul *et al.* (2004)]. Therefore, the difference in this regard between the structures of (I) and (II) is unlikely to be caused specifically by the change from *n*-butyl to benzyl ligands. While the benzoate ligands in (I) are quite planar and coplanar with one another, those in (II) are only coplanar for the benzoate sections. The planes of the outer bromophenyl rings are twisted by different amounts relative to their parent benzoate planes; the dihedral angles between these planes are 13.09 (11) and 40.63 (11)° for the ligands containing atoms Br1 and Br2, respectively.

Complex (III) crystallized as a benzene disolvate; the asymmetric unit contains a highly disordered molecule of benzene alongside half of a C_2-symmetric molecule of the dibenzyltin(IV) complex, *i.e.* aquadibenzylbis(4-{(*E*)-[(*Z*)-4-hydroxypent-3-en-2-ylidene]amino}benzoato)tin(IV). The coordination sphere of the Sn atom includes a water ligand, which, along with the Sn atom, sits on the twofold axis. The coordination geometry is thus that of a slightly distorted pentagonal bipyramid with the carboxylate and aqua ligands in the equatorial plane and the benzyl ligands occupying axial

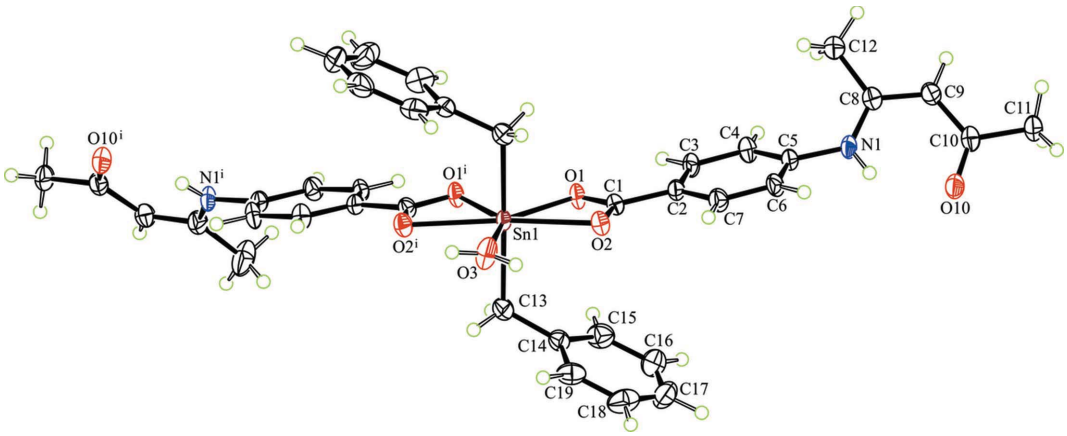


Figure 5
The molecular structure of the Sn^{IV} complex molecule of (III), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size. [Symmetry code: (i) $-x, y, -z+\frac{1}{2}$.]

positions, where the C—Sn—C angle is now much closer to 180° than in complexes (I) and (II) (Fig. 5 and Table 4). In keeping with the symmetry, the benzyl rings now fold sideways and in opposite directions like paddles over the carboxylate groups. As the carboxylate ligands are now 4-substituted benzoates, they extend outwards from the Sn atom almost linearly in a broad V-shaped arrangement, instead of the nearly parallel azophenyl segments of the 2,5-substituted benzoates seen in the structures of (I) and (II). The carboxylate Sn—O distances show that the carboxylate groups coordinate much more symmetrically in (III) than in (I) and (II). The benzoate ligands are not planar along their entirety, but are composed of two distinctly planar segments twisted about the aniline C—N bond. The dihedral angle between the planar fragments is 49.79 (12)°. The hydroxy H atom in each benzoate ligand has migrated to the imino N atom. This zwitterionic nature has caused some delocalization of the bonding electrons in the alkyl chain, as seen by the bond lengths in Table 4.

The molecular structure of the analogous dibutyltin(IV) complex with the same substituted 4-aminobenzoate ligand (Basu Baul *et al.*, 2008) is similar to that of (III), albeit without the additional water ligand. The coordination geometry itself is thus more akin to the skew-trapezoidal bipyramidal arrangement of (I) and (II), with the more asymmetric carboxylate coordination and less linear C—Sn—C angle. The same 4-aminobenzoate ligand also appears in the structures of the trimethyltin(IV) and triphenyltin(IV) complexes. In these structures, as is often observed with this class of trialkyltin(IV) complexes, the benzoate ligand bridges Sn atoms *via* its

Table 4
Selected geometric parameters (Å, °) for (III).

Sn1—O1	2.257 (2)	N1—C5	1.421 (4)
Sn1—O2	2.348 (2)	N1—C8	1.327 (4)
Sn1—O3	2.337 (3)	C8—C9	1.378 (5)
Sn1—C13	2.150 (3)	C9—C10	1.425 (5)
O10—C10	1.248 (4)		
O1—Sn1—O1^{i}	78.94 (11)	O2—Sn1—O2^{i}	166.56 (11)
O1—Sn1—O2	57.26 (8)	O2—Sn1—O3	83.28 (6)
O1—Sn1—O2^{i}	136.18 (8)	O2—Sn1—C13	93.61 (11)
O1—Sn1—O3	140.53 (5)	O2—Sn1—C13^{i}	85.77 (11)
O1—Sn1—C13	93.73 (11)	O3—Sn1—C13	87.35 (10)
O1—Sn1—C13^{i}	90.36 (11)	C13—Sn1—C13^{i}	174.7 (2)

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

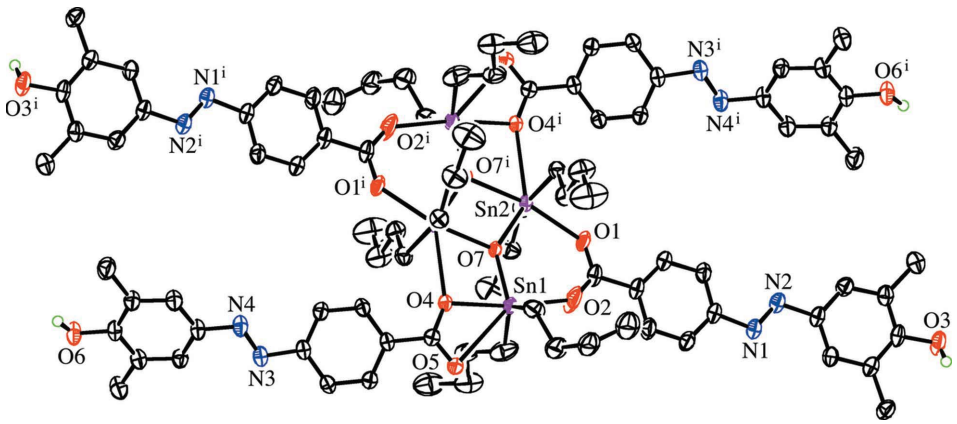


Figure 6
The molecular structure of the Sn^{IV} complex molecule of (IV), showing the atom-labelling scheme for the heteroatoms and the major-disorder conformations of the *n*-butyl ligands. Displacement ellipsoids are drawn at the 50% probability level. Most H atoms have been omitted for clarity. [Symmetry code: (i) $-x, -y+1, -z+1$.]

Table 5
Selected geometric parameters (Å, °) for (IV).

Sn1—O2	2.227 (2)	Sn2—O4^{i}	2.7571 (18)
Sn1—O4	2.1914 (16)	Sn2—O7	2.0418 (16)
Sn1—O5	2.9442 (18)	Sn2—O7^{i}	2.1864 (16)
Sn1—O7	2.0270 (16)	Sn2—C39	2.128 (3)
Sn1—C31	2.094 (3)	Sn2—C43	2.125 (3)
Sn1—C35*A*	2.115 (4)	N1—N2	1.255 (3)
Sn1—C35*B*	2.121 (5)	N3—N4	1.256 (3)
Sn2—O1	2.2736 (18)		
O2—Sn1—O4	170.96 (8)	O1—Sn2—O4^{i}	127.00 (6)
O2—Sn1—O5	140.62 (7)	O1—Sn2—O7	92.10 (7)
O2—Sn1—O7	91.70 (8)	O1—Sn2—O7^{i}	168.16 (7)
O2—Sn1—C31	85.24 (14)	O1—Sn2—C39	85.96 (10)
O2—Sn1—C35*A*	84.4 (2)	O1—Sn2—C43	86.21 (10)
O2—Sn1—C35*B*	91.4 (3)	O4^{i}—Sn2—O7	140.89 (6)
O4—Sn1—O5	48.40 (6)	O4^{i}—Sn2—O7^{i}	64.84 (5)
O4—Sn1—O7	79.26 (6)	O4^{i}—Sn2—C39	76.37 (8)
O4—Sn1—C31	98.12 (12)	O4^{i}—Sn2—C43	79.00 (9)
O4—Sn1—C35*A*	99.5 (2)	O7—Sn2—O7^{i}	76.07 (7)
O4—Sn1—C35*B*	91.8 (3)	O7—Sn2—C39	109.29 (9)
O5—Sn1—O7	127.63 (6)	O7^{i}—Sn2—C39	97.91 (9)
O5—Sn1—C31	77.16 (12)	O7—Sn2—C43	108.14 (9)
O5—Sn1—C35*A*	81.2 (2)	O7^{i}—Sn2—C43	97.29 (9)
O5—Sn1—C35*B*	78.9 (5)	C39—Sn2—C43	141.97 (11)
O7—Sn1—C31	114.14 (11)	Sn1—O4—Sn2^{i}	94.90 (6)
O7—Sn1—C35*A*	114.02 (18)	Sn1—O7—Sn2	135.02 (8)
O7—Sn1—C35*B*	108.7 (4)	Sn1—O7—Sn2^{i}	120.87 (8)
C31—Sn1—C35*A*	130.91 (17)	Sn2—O7—Sn2^{i}	103.93 (7)
C31—Sn1—C35*B*	137.1 (4)		

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

Table 6
Selected geometric parameters (Å, °) for (V).

Sn1—O1	2.157 (4)	Sn3—O1	2.687 (4)
Sn1—O2	2.962 (4)	Sn3—O7	2.185 (4)
Sn1—O4	2.238 (4)	Sn3—O8	2.054 (4)
Sn1—O7	2.021 (4)	Sn3—O13	2.295 (4)
Sn1—C21	2.125 (5)	Sn3—C37	2.130 (5)
Sn1—C25	2.118 (6)	Sn3—C41	2.117 (5)
Sn2—O5	2.289 (4)	Sn4—O8	2.022 (4)
Sn2—O7	2.035 (4)	Sn4—O9	2.170 (4)
Sn2—O8	2.159 (4)	Sn4—O10	2.908 (4)
Sn2—O9	2.749 (4)	Sn4—O12	2.267 (4)
Sn2—C29	2.115 (5)	Sn4—C65	2.125 (6)
Sn2—C33	2.119 (5)	Sn4—C69	2.129 (5)
O1—Sn1—O2	47.92 (13)	O1—Sn3—C41	79.64 (16)
O1—Sn1—O4	168.40 (14)	O7—Sn3—O8	75.04 (13)
O1—Sn1—O7	78.96 (14)	O7—Sn3—O13	164.68 (13)
O1—Sn1—C21	99.87 (19)	O7—Sn3—C37	99.74 (18)
O1—Sn1—C25	95.4 (2)	O7—Sn3—C41	95.43 (18)
O2—Sn1—O4	142.74 (13)	O8—Sn3—O13	90.05 (14)
O2—Sn1—O7	126.82 (14)	O8—Sn3—C37	108.06 (18)
O2—Sn1—C21	80.07 (19)	O8—Sn3—C41	108.35 (18)
O2—Sn1—C25	78.55 (19)	O13—Sn3—C37	88.07 (18)
O4—Sn1—O7	90.39 (14)	O13—Sn3—C41	85.82 (18)
O4—Sn1—C21	88.3 (2)	C37—Sn3—C41	143.0 (2)
O4—Sn1—C25	84.7 (2)	O8—Sn4—O9	78.42 (14)
O7—Sn1—C21	111.7 (2)	O8—Sn4—O10	127.46 (14)
O7—Sn1—C25	114.05 (18)	O8—Sn4—O12	90.96 (14)
C21—Sn1—C25	133.7 (2)	O8—Sn4—C65	113.08 (19)
O5—Sn2—O7	88.76 (14)	O8—Sn4—C69	111.7 (2)
O5—Sn2—O8	164.11 (14)	O9—Sn4—O10	49.09 (13)
O5—Sn2—O9	131.33 (13)	O9—Sn4—O12	168.21 (14)
O5—Sn2—C29	84.77 (19)	O9—Sn4—C65	95.69 (19)
O5—Sn2—C33	88.4 (2)	O9—Sn4—C69	101.3 (2)
O7—Sn2—O8	76.01 (14)	O10—Sn4—O12	141.50 (14)
O7—Sn2—O9	139.90 (13)	O10—Sn4—C65	79.04 (18)
O7—Sn2—C29	107.64 (19)	O10—Sn4—C69	80.90 (19)
O7—Sn2—C33	109.61 (19)	O12—Sn4—C65	83.66 (19)
O8—Sn2—O9	64.10 (12)	O12—Sn4—C69	87.3 (2)
O8—Sn2—C29	95.4 (2)	C65—Sn4—C69	134.4 (2)
O8—Sn2—C33	100.9 (2)	Sn1—O1—Sn3	95.95 (13)
O9—Sn2—C29	81.15 (17)	Sn1—O7—Sn2	136.7 (2)
O9—Sn2—C33	75.58 (18)	Sn1—O7—Sn3	118.47 (17)
C29—Sn2—C33	141.9 (2)	Sn2—O7—Sn3	104.34 (15)
O1—Sn3—O7	65.19 (12)	Sn2—O8—Sn3	104.61 (16)
O1—Sn3—O8	140.08 (13)	Sn2—O8—Sn4	120.77 (17)
O1—Sn3—O13	129.85 (13)	Sn3—O8—Sn4	134.05 (19)
O1—Sn3—C37	76.61 (17)	Sn2—O9—Sn4	94.56 (13)

carboxylate and terminal oxide O atoms (the N atom also becomes protonated in these examples) to give a one-dimensional coordination polymer (Basu Baul *et al.*, 2009).

Complexes (I)–(III) were obtained from syntheses involving a 1:2 stoichiometric ratio of dialkytin(IV) oxide or dichloride and the appropriate benzoic acid. When a 1:1 ratio was used, completely different structures were obtained for compounds (IV) and (V), which contain the familiar bis(dicarboxylatotetraorganodistannoxane) entity (Figs. 6 and 7, respectively). The Sn^{IV} complexes in octabutyltetrakis{μ-(*E*)-4-[(4-hydroxy-3,5-dimethylphenyl)diazenyl]benzoato}di-μ_3-oxido-tetratin(IV) ethanol disolvate, (IV), and octabutyltetrakis{(*E*)-3-[(2-hydroxybenzylidene)amino]propanoato}di-μ_3-oxido-tetratin(IV), (V), are oxo-bridged tetranuclear dibutyltin(IV) complexes with four carboxylate ligands, thus maintaining the 1:1 Sn–carboxylate ligand ratio. The Sn coordination geometry of this class of structures has been described in detail (Basu Baul *et al.*, 2006; Basu Baul, Dutta *et al.*, 2017) and it was pointed out then that the coordination geometry and the distribution of Sn—O distances are quite similar across the 80 structures known at that time (Basu Baul *et al.*, 2006). The Cambridge Structural Database (CSD, Version 5.42, November 2020 update; Groom *et al.*, 2016) now contains 88 entries for this class of bis(dicarboxylatotetraorganodistannoxane) structures with a central Sn_4O_2 core. The molecular structures of compounds (IV) and (V) are no exception to the generally found arrangement (Tables 5 and 6). In the case of complex (IV), the bis(dicarboxylatotetraorganodistannoxane) molecule sits across a crystallographic centre of inversion and the asymmetric unit includes one molecule of ethanol. Complex (V) is a monoclinic packing polymorph of the previously reported triclinic form (Khoo *et al.*, 1993); the molecular conformations, even of the outer ends of the carboxylate ligands, are otherwise very similar. The carboxylate ligand in (V) contains two methylene groups between the imino and carboxylate functions, and neither the imino N atom nor the hydroxy group are involved in coordination with the Sn atoms. In contrast, similar carboxylate ligands containing just one methylene group coordinate in a tridentate fashion with Sn atoms by using the carboxylate, imino and hydroxy donor atoms (Basu Baul *et al.*, 2003; Basu Baul, Kehie *et al.*, 2017; Dakternieks *et al.*, 1998).

It can be speculated that the ratio of reagents is responsible for the quite different classes of complexes. While the carboxylate ligand in (V) is not of the benzoate type, that in (IV) is a 4-azobenzoate derivative, so one might expect a molecular structure not dissimilar to those of (I)–(III) if the nature of the carboxylate ligand was entirely responsible for

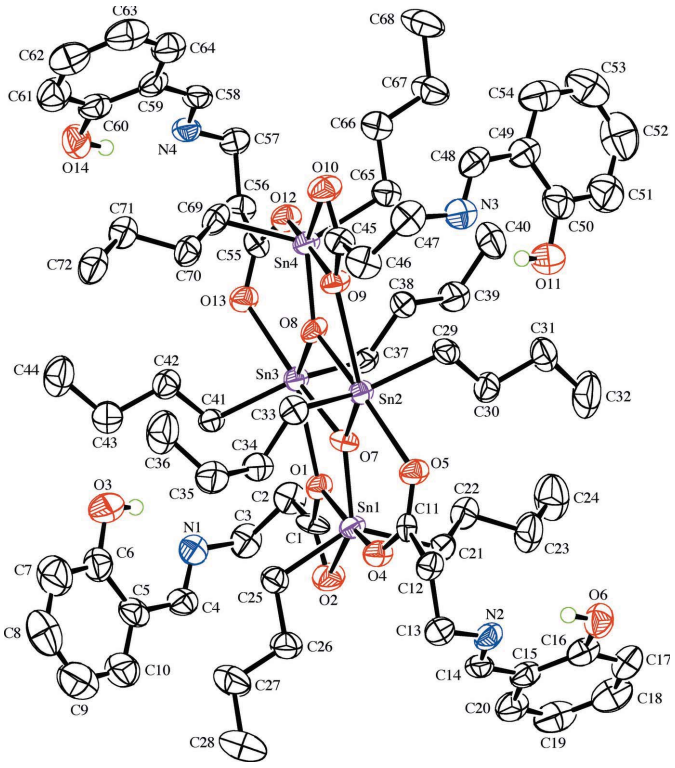


Figure 7
View of the unique molecule of (V), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. Most H atoms have been omitted for clarity.

the resultant structure type. Nonetheless, compounds **5** and **6** in Basu Baul *et al.* (2006) have carboxylate ligands which are very close relatives of that in (V), with just one or two additional methyl substituents within the ligand, yet even a 1:2 ratio of dibutyltin(IV) dichloride to carboxylate in the synthesis reaction led to bis(dicarboxylatotetraorganodistannoxane) structures. In contrast, reaction of the same carboxylate ligand as that present in (V), *i.e.* (*E*)-3-[(2-hydroxybenzylidene)amino]propanoate, with triphenyl- and tributyltin(IV) dichloride in a 1:1 stoichiometric ratio led to one-dimensional coordination polymers, in which the Sn atoms were bridged by the carboxylate groups [structures **1** and **2** in Basu Baul *et al.* (2006)]. There are no structures in the CSD possessing the (*E*)-4-[(4-hydroxy-3,5-dimethylphenyl)-diazenyl]benzoate ligand present in (IV), but the corresponding 2-azobenzoate ligand appears as its trimethyl-, tributyl- and triphenyltin(IV) complexes (Basu Baul *et al.*, 2012). In each structure, the 2-azobenzoate ligand exists in a zwitterionic form, where the hydroxy H atom has transferred to the azo N atom closest to the benzoate group; this transfer has not occurred in the 4-azobenzoate ligands of (IV). In the trimethyl- and tributyltin(IV) structures, the benzoate ligand bridges Sn centres *via* the carboxylate and oxo O atoms to give one-dimensional coordination polymers. The triphenyltin(IV) structure has discrete mononuclear molecules where the benzoate ligand has bidentate coordination to a single Sn atom *via* just its carboxylate group.

Interestingly, the (*E*)-2-hydroxy-5-[(3-methylphenyl)diazenyl]benzoate ligand present in (I) forms a bis(dicarboxylatotetraorganodistannoxane) structure in the presence of dioctyltin(IV) oxide in a 1:1 stoichiometric ratio, as do the corresponding 2-methoxyphenyl- and 4-chlorophenylazobenzoate ligands. However, when dioctyltin(IV) oxide was mixed in a 1:2 ratio with the unsubstituted phenyl- or the 4-methylazobenzoate ligands of this type, the products were mononuclear skew-trapezoidal bipyramidal complexes with a molecular structure akin to that of (I) (Basu Baul *et al.*, 2007). This further supports the hypothesis that the stoichiometric ratio of the regents has a dominant influence on the structure and composition of the resultant Sn complexes.

3.2. Supramolecular interactions

Each hydroxy group in complex (I) forms a strong intramolecular O—H···O hydrogen bond with the immediately adjacent carboxylate O atom, thereby creating six-membered loops with a graph-set motif (Bernstein *et al.*, 1995) of *S*(6) (Table 7). In addition, the O3 hydroxy group forms a weak intermolecular interaction with the corresponding carboxylate

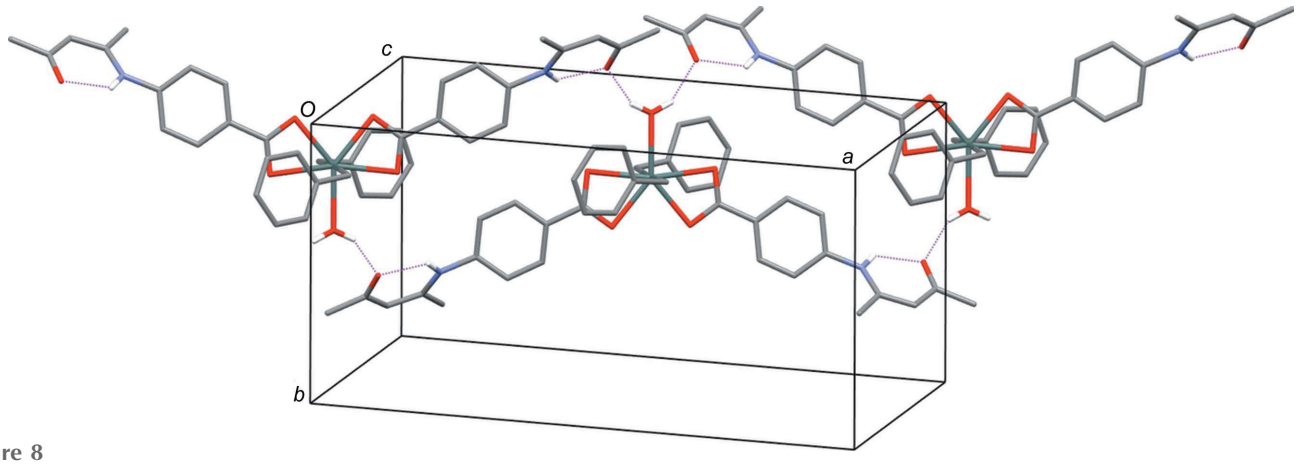


Figure 8
One extended supramolecular chain of the molecules of (III), showing the O—H···O hydrogen bonds (magenta dashed lines). Most H atoms have been omitted for clarity.

Table 7
Hydrogen-bond geometry (Å, °) for (I).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.78 (3)	1.91 (3)	2.623 (3)	153 (3)
O3—H3···O2^{i}	0.78 (3)	2.44 (3)	2.872 (3)	117 (3)
O6*A*—H6*A*···O5*A*	0.84	1.90	2.62 (3)	144
O6*B*—H6*B*···O5*B*	0.84	1.90	2.64 (2)	146

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

Table 8
Hydrogen-bond geometry (Å, °) for (II).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.77 (3)	1.89 (3)	2.586 (2)	152 (3)
O3—H3···O5^{ii}	0.77 (3)	2.42 (3)	2.818 (2)	114 (3)
O6—H6···O5	0.76 (3)	1.89 (3)	2.596 (2)	153 (3)

Symmetry code: (ii) $-x+\frac{5}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

O atom of the centrosymmetrically-disposed neighbouring molecule, although this interaction might merely be a consequence of the bridging secondary Sn···O interaction involving the same carboxylate O atom, as described above (Fig. 2). Complex (II) displays an identical pattern of intra- and intermolecular O—H···O hydrogen-bonding interactions, even though the neighbouring molecules are related by a 2_1-screw axis, instead of a centre of inversion (Table 8 and Fig. 4).

In the structure of complex (III), the protonated imino group forms an intramolecular N—H···O hydrogen bond with the oxide (deprotonated hydroxy) O atom within the same benzoate ligand (Table 9). The intramolecular interactions form closed six-membered loops which can be described by a graph-set motif of $S(6)$. This latter O atom also accepts an intermolecular O—H···O hydrogen bond from the water ligand of a neighbouring molecule. The C_2 symmetry indicates that the water ligand forms two such intermolecular hydrogen bonds with neighbouring Sn complex molecules. The intermolecular interactions link the molecules into extended zigzag chains, which run parallel to the [101] direction and which can be described by a graph-set motif of $C(14)$ (Fig. 8). As a result of the C_2 symmetry, the intermolecular interactions also form a centrosymmetric loop motif with a graph-set descriptor of $R_2^2(28)$ and a chain motif of $C_2^2(26)$, which involves the entire length of one molecule between the two oxide O atoms and just the water ligand of a second molecule bridging across to the next molecule in the chain. The long loop motif involves two water and two benzoate ligands.

In the structure of (IV), intermolecular hydrogen bonds link the hydroxy groups of the bis(dicarboxylatotetraorganodistannoxane) molecules and the ethanol solvent molecules into two-dimensional networks which lie parallel to the (102) plane (Table 10 and Fig. 9). Locally, adjacent Sn complex molecules are linked into chains by a centrosymmetric double bridge, where each bridge consists of an O—H···O interaction between the O3 hydroxy group as donor and the O6 hydroxy group of the next molecule in the chain as acceptor. This repeats in the reverse sense at the other site of the double bridge, as well as at the other end of the bis(dicarboxylatotetraorganodistannoxane) molecule, because the molecule itself is centrosymmetric. The O6 hydroxy group forms an O—H···O hydrogen bond with the O atom of a neighbouring ethanol molecule, which in turn donates a hydrogen bond to a carboxylate O atom in an Sn complex molecule from an adjacent chain of such molecules. In this way, the ethanol molecule crosslinks the chains of bis(dicarboxylatotetraorganodistannoxane) molecules to extend the network into sheets. Within the chains of molecules, the centrosymmetric $R_2^2(56)$ ring motif is discernible and involves four benzoate ligands and one Sn atom from each of two Sn_4O_2 cores. The crosslinking of these chains *via* the ethanol molecules forms additional acentric $R_5^5(38)$ ring motifs.

Table 9
Hydrogen-bond geometry (Å, °) for (III).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O10	0.82 (4)	2.01 (4)	2.631 (3)	132 (4)
O3—H3···O10^{ii}	0.84 (1)	1.95 (2)	2.712 (3)	151 (4)

Symmetry code: (ii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Table 10
Hydrogen-bond geometry (Å, °) for (IV).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O6^{ii}	0.85 (4)	2.05 (4)	2.801 (3)	146 (3)
O6—H6···O8^{iii}	0.93 (4)	1.71 (4)	2.599 (3)	159 (4)
O8—H8···O5	0.91 (5)	1.82 (5)	2.663 (3)	154 (4)

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

Table 11
Hydrogen-bond geometry (Å, °) for (V).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···N1	0.84	1.83	2.575 (7)	147
O6—H6···N2	0.84	1.88	2.616 (6)	146
O11—H11···N3	0.84	1.87	2.602 (7)	145
O14—H14···N4	0.84	1.90	2.637 (6)	147

In the structure of (V), the hydroxy H atom has not migrated to the imino N atom. Each hydroxy group forms an intramolecular hydrogen bond with the adjacent N atom in the same ligand, thereby creating six-membered loops with a graph-set motif of $S(6)$ (Table 11).

In (I), pairs of molecules are aligned head-to-tail across centres of inversion through π–π interactions involving the parallel planar phenylazobenzoate segments. The centroid–centroid distances between the overlaid benzoate–phenyl ring pairs involving one disorder conformation are 3.740 (7) Å for the rings containing atoms C2 and C24*A*, and 3.824 (5) Å for the rings containing atoms C8 and C15*A*, with centroid offsets of 1.33 and 1.65 Å, respectively. The cavity in the centre of this dimeric arrangement is occupied by a cyclohexane molecule (Fig. 2). The fully overlaid dimers resulting from the π–π pairing interactions are extended into tetramers by the secondary Sn···O interactions. These tetramers do not stack further, because the phenyl rings sit above the cyclohexane molecule in the cavity of the next tetramer. The structure of (II) does not display the same type of head-to-tail aggregation.

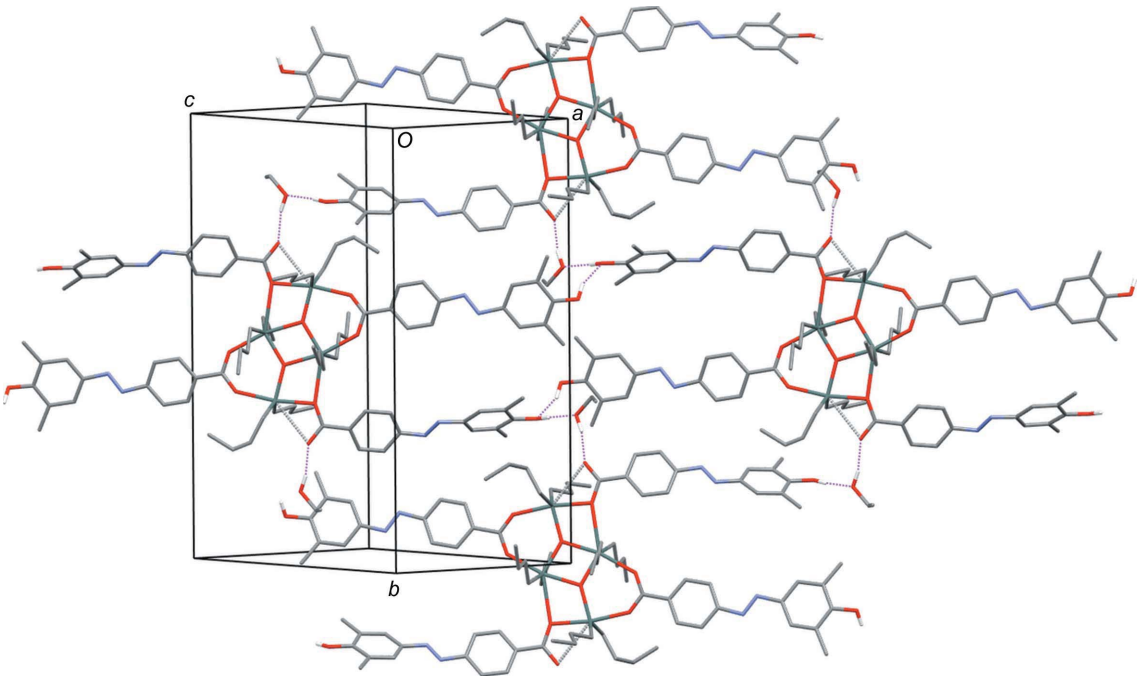


Figure 9
One of the supramolecular sheets present in the structure of (IV), showing the O—H···O hydrogen bonds (magenta dashed lines). One double-bridged chain is visible extending horizontally across the middle of the image, with the ethanol molecules crosslinking adjacent chains. Most H atoms have been omitted for clarity.

Instead, molecules are stacked parallel to one another in a continuous stair-like arrangement, with adjacent members related by a translation of one unit cell parallel to the [010] direction. The less-planar benzoate ligands from adjacent molecules have inter-ligand distances which are suggestive of π–π interactions, but the π-systems are significantly offset, with centroid–centroid distances for the overlaid benzoate rings and overlaid phenyl rings being well in excess of 4.1 Å and the ring-centroid offset for the benzoate rings being 2.93 Å and even more for the phenyl rings (Fig. 4). Both of the above stacking motifs have been discussed by Linden & Basu Baul (2016), being observed in the benzene pseudo-isomorph of (I) and the dibutyltin(IV) analogue of (II), respectively (Basu Baul *et al.*, 2004). However, in the dibutyltin(IV) analogue of (II), the overlay of the benzoate rings indicates much stronger π–π interactions than in (II) [centroid–centroid distance of 3.6310 (13) Å and ring-centroid offset of 1.18 Å]; this could be related to the steric influence of the *n*-butyl *versus* benzyl ligands, respectively. The structures of (III)–(V) do not display significant π–π stacking interactions.

4. Conclusion

The molecular structures of five dialkyltin(IV) carboxylate complexes show two of the main geometric coordination motifs commonly observed for these types of compounds and the results suggest that this diversity may be influenced by the stoichiometric ratio of components in the synthesis. The supramolecular structures arising from consideration of secondary Sn···O interactions and/or classic hydrogen bonds include discrete molecules, centrosymmetric dimers, extended chains and sheets.

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References

Altomare, A., Cascarano, G., Giacovazzo, C., Guagliardi, A., Burla, M. C., Polidori, G. & Camalli, M. (1994). *J. Appl. Cryst.* **27**, 435.
Basu Baul, T. S., Dutta, D., Duthie, A., Guchhait, N., Rocha, B. G. M., Guedes da Silva, M. F. C., Mokhamatam, R. B., Raviprakash, N. & Manna, S. K. (2017). *J. Inorg. Biochem.* **166**, 34–48.
Basu Baul, T. S., Dutta, S., Masharing, C., Rivarola, E. & Englert, U. (2003). *Heteroatom Chem.* **14**, 149–154.
Basu Baul, T. S., Kehie, P., Höpfl, H., Duthie, A., Eng, G. & Linden, A. (2017). *Appl. Organomet. Chem.* **31**, e3547.
Basu Baul, T. S., Masharing, C., Basu, S., Pettinari, C., Rivarola, E., Chantrapromma, S. & Fun, H.-K. (2008). *Appl. Organomet. Chem.* **22**, 114–121.
Basu Baul, T. S., Masharing, C., Basu, S., Rivarola, E., Holčapek, M., Jirásko, R., Lyčka, A., de Vos, D. & Linden, A. (2006). *J. Organomet. Chem.* **691**, 952–965.
Basu Baul, T. S., Masharing, C., Ruisi, G., Pettinari, C. & Linden, A. (2009). *J. Inorg. Organomet. Polym.* **19**, 395–400.
Basu Baul, T. S., Paul, A. & Linden, A. (2012). *J. Organomet. Chem.* **696**, 4229–4235.
Basu Baul, T. S., Rynjah, W., Rivarola, E., Pettinari, C., Holčapek, M., Jirásko, R., Englert, U. & Linden, A. (2007). *J. Organomet. Chem.* **692**, 3625–3635.

Baul, T. S. B., Rynjah, W., Willem, R., Biesemans, M., Verbruggen, I., Holèapek, M., de Vos, D. & Linden, A. (2004). *J. Organomet. Chem.* **689**, 4691–4701.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., de Gelder, R., Israel, R. & Smits, J. M. M. (1994). *DIRDIF94: The DIRDIF program system*. Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., Garcia-Granda, S., Gould, R. O., Smits, J. M. M. & Smykalla, C. (1992). *PATTY: The DIRDIF program system*. Technical Report of the Crystallography Laboratory, University of Nijmegen, The Netherlands.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Buntine, M. A., Hall, V. J., Kosovel, F. J. & Tiekink, E. R. T. (1998). *J. Phys. Chem. A*, **102**, 2472–2482.
Chandrasekhar, V., Nagendran, S. & Baskar, V. (2002). *Coord. Chem. Rev.* **235**, 1–52.
Dakternieks, D., Basu Baul, T. S., Dutta, S. & Tiekink, E. R. T. (1998). *Organometallics*, **17**, 3058–3062.
Dakternieks, D., Duthie, A., Smyth, D. R., Stapleton, C. P. D. & Tiekink, E. R. T. (2003). *Organometallics*, **22**, 4599–4603.
Debnath, P., Singh, K. S., Singh, K. K., Sureshkumar Singh, S., Sieroń, L. & Maniukiewicz, W. (2020). *New J. Chem.* **44**, 5862–5872.
Gielen, M. & Tiekink, E. R. T. (2005). Editors. *Metallotherapeutic drug and metal-based diagnostic agents: ^{50}Sn Tin compounds and their therapeutic potential*, pp. 421–439. Chichester: Wiley.
Groom, C. R., Bruno, I. J., Lightfoot, M. P. & Ward, S. C. (2016). *Acta Cryst.* B**72**, 171–179.
Hussain, S., Ali, S., Shahzadi, S., Tahir, M. N. & Shahid, M. (2015). *J. Coord. Chem.* **68**, 2369–2387.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Khoo, L. E., Zhou, Z.-H. & Mak, T. C. W. (1993). *J. Crystallogr. Spectrosc. Res.* **23**, 153–157.
Linden, A. & Basu Baul, T. S. (2016). *Acta Cryst.* C**72**, 313–325.
Linden, A., Wolstenholme, D., Basu Baul, T. S. & Rynjah, W. (2007). *Acta Cryst.* E**63**, m1547–m1548.
Macrae, C. F., Sovago, I., Cottrell, S. J., Galek, P. T. A., McCabe, P., Pidcock, E., Platings, M., Shields, G. P., Stevens, J. S., Towler, M. & Wood, P. A. (2020). *J. Appl. Cryst.* **53**, 226–235.
Nonius (2000). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography, Part A*, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Prabusankar, G. & Murugavel, R. (2004). *Organometallics*, **23**, 5644–5647.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015). *Acta Cryst.* C**71**, 3–8.
Spek, A. L. (2015). *Acta Cryst.* C**71**, 9–18.
Spek, A. L. (2020). *Acta Cryst.* E**76**, 1–11.
Tiekink, E. R. T. (1991). *Appl. Organomet. Chem.* **5**, 1–23.
Tiekink, E. R. T. (1994). *Trends Organomet. Chem.* **1**, 71–116.
Wang, J.-Q., Kuang, D.-Z., Chen, Z.-M., Feng, Y.-L. & Zhang, F.-X. (2005). *Huaxue Shiji*, **27**, 163.
Willem, R., Verbruggen, I., Gielen, M., Biesemans, M., Mahieu, B., Basu Baul, T. S. & Tiekink, E. R. T. (1998). *Organometallics*, **17**, 5758–5766.

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Structural diversity among some dialkyltin(IV) benzoate and related derivatives

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Computing details

For all structures, 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) for (I); *SHELXS97* (Sheldrick, 2008) for (II), (IV), (V); PATTY and *DIRDIF94* (Beurskens *et al.*, 1992, 1994) for (III). For all structures, program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL2018* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2020) and *PLATON* (Spek, 2020).

Dibutylbis{(*E*)-2-hydroxy-5-[(3-methylphenyl)diazenyl]benzoato}tin(IV) cyclohexane hemisolvate (I)

Crystal data

$[Sn(C_4H_9)_2(C_{14}H_{11}N_2O_3)_2]\cdot 0.5C_6H_{12}$
M_r = 785.49
Monoclinic, $P2_1/c$
a = 9.4028 (1) Å
b = 25.1718 (2) Å
c = 15.5008 (1) Å
β = 93.3046 (3)°
V = 3662.71 (5) Å^3
Z = 4
$F(000)$ = 1624
D_x = 1.424 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 84811 reflections
θ = 2.0–30.0°
μ = 0.75 mm^{-1}
T = 160 K
Prism, orange
0.25 × 0.17 × 0.12 mm

Data collection

Nonius KappaCCD area detector diffractometer
Radiation source: Nonius FR590 sealed tube generator
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
T_{min} = 0.854, T_{max} = 0.917
90950 measured reflections
10708 independent reflections
7109 reflections with $I > 2\sigma(I)$
R_{int} = 0.066
θ_{max} = 30.0°, θ_{min} = 2.6°
h = −13→13
k = −35→35
l = −21→21

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.110
S = 1.04
10702 reflections
623 parameters
645 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 1.0512P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}

Special details

Experimental. Data collection and full structure determination done by Prof. Anthony Linden: anthony.linden@chem.uzh.ch
Solvent used: petrolum ether Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: on a glass fibre Mosaicity (deg.): 0.504 (1) Frames collected: 817 Seconds exposure per frame: 33 Degrees rotation per frame: 1.1 Crystal-detector distance (mm): 39.0 Client: Tushar Basubaul Sample code: TSBB-2 (L0218)

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

Refinement. The asymmetric unit contains one molecule of the Sn-complex, plus one half of a cyclohexane molecule. The cyclohexane molecule sits about a crystallographic centre of inversion. One of the carboxylate ligands is disordered in its entirety over two conformations, the difference arising from a reversal of the direction of the zig-zag at the N=N bond. Two positions were defined for all atoms of this ligand, except for the carboxylate O atom bound strongly with the Sn-atom, which is not significantly disordered. Refinement of constrained site occupation factors for the two orientations yielded a value of 0.563 (5) for the major conformation. Similarity restraints were applied to the chemically equivalent bond lengths and angles of all atoms in the carboxylate ligands, including those of the ordered ligand. Furthermore, neighbouring atoms within and between each conformation of the disordered ligand were restrained to have similar atomic displacement parameters. The geometry of the cyclohexane molecule is poor because of possible disorder, as indicated by the enlarged atomic displacement parameters, but no attempt was made to resolve the disorder; the C-C distances within the solvent molecule were restrained to 1.52 (1) Å.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	1.14355 (2)	0.40458 (2)	0.17524 (2)	0.03777 (7)	
O1	0.99456 (19)	0.45491 (7)	0.22890 (10)	0.0422 (4)	
O2	1.01081 (19)	0.48431 (7)	0.09670 (11)	0.0459 (4)	
O3	0.8742 (2)	0.57069 (8)	0.04591 (11)	0.0452 (4)	
H3	0.922 (4)	0.5455 (14)	0.045 (2)	0.069 (12)*	
N1	0.6414 (2)	0.57079 (8)	0.36788 (13)	0.0389 (5)	
N2	0.5572 (2)	0.60765 (8)	0.38296 (13)	0.0385 (5)	
C1	0.9573 (3)	0.48839 (10)	0.16860 (14)	0.0375 (5)	
C2	0.8560 (2)	0.53078 (9)	0.18696 (14)	0.0354 (5)	
C3	0.8204 (3)	0.56998 (10)	0.12480 (15)	0.0364 (5)	
C4	0.7271 (3)	0.61062 (10)	0.14413 (16)	0.0414 (6)	
H4	0.704542	0.637386	0.102346	0.050*	
C5	0.6672 (3)	0.61257 (10)	0.22263 (16)	0.0401 (6)	
H5	0.604374	0.640728	0.235119	0.048*	
C6	0.6987 (3)	0.57297 (10)	0.28457 (15)	0.0359 (5)	
C7	0.7924 (3)	0.53284 (9)	0.26635 (15)	0.0358 (5)	
H7	0.814077	0.506154	0.308404	0.043*	
C8	0.4993 (3)	0.60429 (9)	0.46625 (15)	0.0370 (5)	
C9	0.3989 (3)	0.64256 (10)	0.48359 (16)	0.0404 (6)	
H9	0.374403	0.668761	0.441186	0.049*	
C10	0.3330 (3)	0.64347 (11)	0.56202 (17)	0.0442 (6)	

C11	0.3726 (3)	0.60474 (11)	0.62258 (17)	0.0475 (7)	
H11	0.330706	0.604756	0.676913	0.057*	
C12	0.4716 (3)	0.56619 (11)	0.60530 (17)	0.0474 (6)	
H12	0.495179	0.539636	0.647273	0.057*	
C13	0.5368 (3)	0.56584 (10)	0.52760 (16)	0.0419 (6)	
H13	0.606252	0.539696	0.516368	0.050*	
C27	0.2235 (3)	0.68518 (13)	0.5788 (2)	0.0584 (8)	
H271	0.184768	0.678779	0.635272	0.088*	
H272	0.146349	0.683583	0.533646	0.088*	
H273	0.268068	0.720375	0.578592	0.088*	
O4	1.16131 (18)	0.37375 (7)	0.30096 (11)	0.0428 (4)	
O5A	1.335 (2)	0.3262 (13)	0.2380 (11)	0.038 (3)	0.437 (5)
O6A	1.4503 (15)	0.2495 (6)	0.3328 (6)	0.0458 (18)	0.437 (5)
H6A	1.426681	0.265078	0.286191	0.069*	0.437 (5)
N3A	1.1171 (13)	0.3174 (6)	0.5944 (7)	0.0364 (18)	0.437 (5)
N4A	1.1244 (5)	0.2927 (2)	0.6633 (3)	0.0403 (12)	0.437 (5)
C14A	1.263 (3)	0.3393 (10)	0.3002 (11)	0.035 (2)	0.437 (5)
C15A	1.276 (2)	0.3105 (7)	0.3838 (9)	0.0336 (17)	0.437 (5)
C16A	1.3711 (14)	0.2678 (5)	0.3955 (6)	0.0361 (17)	0.437 (5)
C17A	1.3879 (9)	0.2418 (3)	0.4754 (5)	0.0358 (15)	0.437 (5)
H171	1.455009	0.213821	0.483992	0.043*	0.437 (5)
C18A	1.3061 (8)	0.2576 (3)	0.5407 (4)	0.0292 (13)	0.437 (5)
H181	1.316526	0.239976	0.594895	0.035*	0.437 (5)
C19A	1.2077 (8)	0.2987 (3)	0.5299 (4)	0.0309 (14)	0.437 (5)
C20A	1.1937 (12)	0.3254 (4)	0.4520 (6)	0.0303 (16)	0.437 (5)
H201	1.128234	0.354046	0.444884	0.036*	0.437 (5)
C21A	1.0284 (8)	0.3130 (3)	0.7254 (5)	0.0394 (15)	0.437 (5)
C22A	0.9380 (17)	0.3551 (7)	0.7085 (9)	0.047 (2)	0.437 (5)
H221	0.938030	0.372809	0.654406	0.057*	0.437 (5)
C23A	0.846 (3)	0.3720 (12)	0.7709 (13)	0.0523 (19)	0.437 (5)
C24A	0.8551 (14)	0.3465 (5)	0.8502 (8)	0.056 (2)	0.437 (5)
H241	0.795821	0.358344	0.893955	0.067*	0.437 (5)
C25A	0.9464 (10)	0.3049 (4)	0.8683 (6)	0.0552 (18)	0.437 (5)
H25A	0.948616	0.288099	0.923288	0.066*	0.437 (5)
C26A	1.0355 (8)	0.2874 (3)	0.8057 (6)	0.0447 (16)	0.437 (5)
H261	1.099738	0.258732	0.817100	0.054*	0.437 (5)
C28A	0.7532 (13)	0.4206 (5)	0.7581 (10)	0.059 (2)	0.437 (5)
H281	0.665835	0.411168	0.724009	0.089*	0.437 (5)
H282	0.804899	0.447936	0.727597	0.089*	0.437 (5)
H283	0.728524	0.434321	0.814542	0.089*	0.437 (5)
O5B	1.3096 (18)	0.3282 (9)	0.2321 (9)	0.038 (2)	0.563 (5)
O6B	1.4630 (12)	0.2517 (4)	0.3081 (5)	0.0430 (13)	0.563 (5)
H6B	1.437641	0.272918	0.268220	0.064*	0.563 (5)
N3B	1.1851 (4)	0.28580 (16)	0.6084 (2)	0.0382 (10)	0.563 (5)
N4B	1.0894 (10)	0.3200 (5)	0.6092 (5)	0.0395 (15)	0.563 (5)
C14B	1.253 (2)	0.3355 (7)	0.3023 (9)	0.034 (2)	0.563 (5)
C15B	1.2916 (16)	0.3040 (5)	0.3807 (7)	0.0325 (14)	0.563 (5)
C16B	1.3935 (10)	0.2631 (4)	0.3785 (5)	0.0335 (14)	0.563 (5)

C17B	1.4235 (7)	0.2322 (3)	0.4516 (4)	0.0376 (13)	0.563 (5)
H172	1.493150	0.204936	0.450500	0.045*	0.563 (5)
C18B	1.3532 (6)	0.2410 (2)	0.5249 (4)	0.0350 (11)	0.563 (5)
H182	1.373890	0.219341	0.574244	0.042*	0.563 (5)
C19B	1.2507 (6)	0.2814 (3)	0.5287 (3)	0.0314 (12)	0.563 (5)
C20B	1.2228 (9)	0.3132 (3)	0.4569 (5)	0.0328 (14)	0.563 (5)
H202	1.156312	0.341497	0.459372	0.039*	0.563 (5)
C21B	1.0245 (7)	0.3227 (3)	0.6912 (4)	0.0404 (13)	0.563 (5)
C22B	0.9174 (13)	0.3598 (5)	0.6964 (7)	0.0474 (17)	0.563 (5)
H222	0.890803	0.380898	0.647321	0.057*	0.563 (5)
C23B	0.847 (3)	0.3667 (9)	0.7726 (10)	0.0531 (17)	0.563 (5)
C24B	0.8824 (11)	0.3341 (4)	0.8423 (6)	0.0554 (18)	0.563 (5)
H242	0.833196	0.337597	0.893834	0.067*	0.563 (5)
C25B	0.9873 (8)	0.2969 (3)	0.8375 (5)	0.0541 (15)	0.563 (5)
H252	1.011694	0.275187	0.886349	0.065*	0.563 (5)
C26B	1.0593 (6)	0.2902 (2)	0.7617 (5)	0.0465 (12)	0.563 (5)
H263	1.131037	0.263793	0.758446	0.056*	0.563 (5)
C28B	0.7288 (11)	0.4068 (4)	0.7728 (8)	0.071 (2)	0.563 (5)
H284	0.754429	0.434989	0.814503	0.107*	0.563 (5)
H285	0.641172	0.389335	0.789138	0.107*	0.563 (5)
H286	0.713613	0.422241	0.714997	0.107*	0.563 (5)
C29	1.0163 (3)	0.34748 (10)	0.10760 (16)	0.0412 (6)	
H291	0.978564	0.362721	0.052015	0.049*	
H292	1.075319	0.316216	0.094748	0.049*	
C30	0.8923 (3)	0.32999 (11)	0.16058 (16)	0.0429 (6)	
H301	0.930799	0.315112	0.216247	0.051*	
H302	0.834154	0.361491	0.173503	0.051*	
C31	0.7970 (3)	0.28867 (11)	0.11466 (17)	0.0444 (6)	
H311	0.757029	0.303476	0.059265	0.053*	
H312	0.854462	0.257036	0.101545	0.053*	
C32	0.6759 (3)	0.27222 (14)	0.1699 (2)	0.0600 (8)	
H321	0.715235	0.256159	0.223728	0.090*	
H322	0.614986	0.246356	0.138249	0.090*	
H323	0.619406	0.303553	0.183397	0.090*	
C33	1.3355 (3)	0.44608 (11)	0.16023 (18)	0.0474 (6)	
H331	1.312307	0.483083	0.142993	0.057*	
H332	1.389692	0.447418	0.216890	0.057*	
C34	1.4310 (3)	0.42214 (11)	0.09390 (18)	0.0450 (6)	
H341	1.447514	0.384176	0.107854	0.054*	
H342	1.380992	0.424035	0.035994	0.054*	
C35	1.5724 (3)	0.44980 (13)	0.0910 (2)	0.0536 (7)	
H351	1.626598	0.444800	0.147116	0.064*	
H352	1.556030	0.488363	0.082824	0.064*	
C36	1.6606 (3)	0.42936 (15)	0.0192 (2)	0.0639 (8)	
H361	1.679330	0.391364	0.027768	0.096*	
H362	1.751182	0.448674	0.020065	0.096*	
H363	1.608370	0.434816	−0.036627	0.096*	
C37	0.9061 (6)	0.5119 (2)	0.5726 (4)	0.149 (3)	

H371	0.948957	0.493958	0.624624	0.179*
H372	0.822029	0.532405	0.589114	0.179*
C38	1.0160 (4)	0.54900 (15)	0.5328 (3)	0.0857 (12)
H381	0.963940	0.572510	0.490655	0.103*
H382	1.057966	0.571923	0.579548	0.103*
C39	1.1321 (5)	0.5243 (2)	0.4897 (3)	0.1039 (15)
H391	1.188027	0.552653	0.463175	0.125*
H392	1.195644	0.506552	0.533944	0.125*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03821 (10)	0.04234 (12)	0.03366 (10)	0.00372 (7)	0.00971 (7)	0.00012 (7)
O1	0.0486 (10)	0.0441 (10)	0.0349 (9)	0.0126 (8)	0.0111 (8)	0.0026 (8)
O2	0.0468 (10)	0.0604 (12)	0.0316 (9)	0.0075 (9)	0.0107 (8)	0.0006 (8)
O3	0.0548 (12)	0.0512 (12)	0.0307 (9)	0.0075 (10)	0.0120 (8)	0.0062 (8)
N1	0.0425 (12)	0.0396 (12)	0.0354 (11)	0.0001 (9)	0.0097 (9)	−0.0034 (9)
N2	0.0390 (11)	0.0406 (12)	0.0368 (11)	−0.0005 (9)	0.0098 (9)	−0.0027 (9)
C1	0.0387 (13)	0.0442 (14)	0.0298 (12)	0.0005 (11)	0.0040 (10)	−0.0001 (10)
C2	0.0351 (12)	0.0407 (13)	0.0305 (12)	−0.0014 (10)	0.0043 (9)	−0.0033 (10)
C3	0.0399 (13)	0.0389 (13)	0.0308 (12)	−0.0033 (10)	0.0055 (10)	0.0015 (10)
C4	0.0506 (15)	0.0387 (13)	0.0352 (13)	0.0013 (11)	0.0045 (11)	0.0046 (10)
C5	0.0462 (15)	0.0353 (13)	0.0393 (14)	0.0013 (11)	0.0069 (11)	−0.0022 (11)
C6	0.0376 (13)	0.0374 (13)	0.0334 (12)	−0.0039 (10)	0.0084 (10)	−0.0028 (10)
C7	0.0405 (13)	0.0358 (13)	0.0314 (12)	−0.0004 (10)	0.0045 (10)	0.0025 (9)
C8	0.0368 (13)	0.0404 (14)	0.0342 (12)	−0.0040 (10)	0.0065 (10)	−0.0051 (10)
C9	0.0427 (14)	0.0412 (14)	0.0380 (13)	−0.0019 (11)	0.0080 (11)	−0.0025 (11)
C10	0.0423 (14)	0.0505 (16)	0.0406 (14)	−0.0029 (12)	0.0087 (11)	−0.0089 (12)
C11	0.0535 (17)	0.0553 (17)	0.0346 (13)	−0.0057 (13)	0.0111 (12)	−0.0065 (12)
C12	0.0578 (17)	0.0490 (16)	0.0360 (14)	−0.0013 (13)	0.0070 (12)	0.0023 (12)
C13	0.0439 (14)	0.0425 (15)	0.0397 (14)	0.0005 (11)	0.0052 (11)	−0.0034 (11)
C27	0.0598 (18)	0.0632 (19)	0.0541 (18)	0.0109 (15)	0.0194 (14)	−0.0048 (15)
O4	0.0445 (10)	0.0474 (11)	0.0369 (9)	0.0082 (8)	0.0057 (8)	0.0012 (8)
O5A	0.031 (6)	0.055 (5)	0.028 (4)	0.010 (4)	0.008 (4)	0.006 (3)
O6A	0.051 (4)	0.051 (3)	0.037 (5)	0.005 (3)	0.017 (4)	0.011 (4)
N3A	0.035 (4)	0.041 (3)	0.033 (3)	0.000 (3)	0.007 (3)	0.001 (3)
N4A	0.044 (2)	0.044 (2)	0.034 (2)	−0.004 (2)	0.009 (2)	0.0025 (19)
C14A	0.036 (4)	0.039 (4)	0.032 (4)	−0.003 (4)	0.006 (3)	0.002 (3)
C15A	0.031 (4)	0.035 (4)	0.035 (3)	−0.001 (3)	0.004 (3)	−0.002 (3)
C16A	0.034 (4)	0.042 (3)	0.033 (3)	−0.004 (3)	0.015 (3)	−0.002 (3)
C17A	0.035 (3)	0.036 (3)	0.037 (4)	0.003 (3)	0.011 (3)	0.002 (3)
C18A	0.029 (3)	0.030 (4)	0.029 (3)	0.000 (3)	0.009 (3)	−0.002 (3)
C19A	0.032 (3)	0.029 (3)	0.032 (2)	0.001 (2)	0.003 (2)	−0.001 (2)
C20A	0.030 (4)	0.033 (4)	0.029 (3)	0.004 (3)	0.005 (2)	0.001 (2)
C21A	0.037 (3)	0.045 (3)	0.037 (4)	−0.002 (3)	0.007 (3)	−0.001 (3)
C22A	0.045 (4)	0.053 (4)	0.043 (4)	−0.003 (3)	0.002 (3)	−0.009 (3)
C23A	0.047 (3)	0.061 (4)	0.050 (3)	−0.005 (3)	0.010 (3)	−0.017 (3)
C24A	0.049 (4)	0.063 (5)	0.057 (4)	−0.006 (3)	0.016 (3)	−0.015 (4)

C25A	0.058 (4)	0.058 (4)	0.052 (4)	−0.008 (3)	0.023 (3)	−0.009 (3)
C26A	0.047 (4)	0.049 (3)	0.039 (4)	0.002 (3)	0.009 (3)	0.000 (3)
C28A	0.050 (4)	0.063 (5)	0.067 (5)	0.007 (4)	0.020 (3)	−0.010 (4)
O5B	0.037 (5)	0.047 (4)	0.031 (3)	0.002 (4)	0.004 (3)	−0.001 (3)
O6B	0.046 (3)	0.050 (2)	0.035 (3)	0.0119 (19)	0.018 (3)	0.009 (3)
N3B	0.039 (2)	0.041 (2)	0.0348 (19)	−0.0003 (16)	0.0087 (15)	0.0036 (16)
N4B	0.043 (4)	0.043 (3)	0.034 (3)	−0.003 (3)	0.006 (2)	0.000 (2)
C14B	0.034 (3)	0.037 (3)	0.033 (3)	−0.005 (3)	0.005 (3)	−0.004 (3)
C15B	0.033 (3)	0.037 (3)	0.028 (2)	−0.001 (2)	0.007 (2)	0.000 (2)
C16B	0.032 (3)	0.038 (3)	0.032 (3)	−0.001 (2)	0.011 (2)	−0.001 (2)
C17B	0.036 (3)	0.036 (3)	0.041 (3)	0.000 (2)	0.005 (2)	0.001 (2)
C18B	0.035 (3)	0.034 (3)	0.037 (3)	0.005 (2)	0.005 (2)	0.003 (2)
C19B	0.030 (3)	0.033 (3)	0.032 (2)	0.001 (2)	0.004 (2)	0.002 (2)
C20B	0.030 (3)	0.033 (3)	0.036 (2)	0.002 (2)	0.003 (2)	−0.004 (2)
C21B	0.042 (2)	0.042 (3)	0.038 (3)	−0.008 (2)	0.007 (2)	−0.007 (2)
C22B	0.044 (4)	0.053 (3)	0.045 (3)	0.002 (3)	0.004 (3)	−0.013 (3)
C23B	0.045 (3)	0.065 (4)	0.050 (3)	−0.002 (3)	0.007 (3)	−0.018 (3)
C24B	0.054 (4)	0.062 (4)	0.052 (3)	−0.007 (3)	0.010 (3)	−0.013 (3)
C25B	0.057 (4)	0.059 (3)	0.048 (4)	−0.002 (3)	0.014 (3)	0.003 (3)
C26B	0.048 (3)	0.051 (3)	0.042 (3)	−0.005 (2)	0.010 (2)	0.002 (3)
C28B	0.066 (4)	0.086 (5)	0.064 (4)	0.007 (4)	0.017 (3)	−0.013 (4)
C29	0.0446 (14)	0.0470 (15)	0.0325 (12)	0.0051 (11)	0.0080 (10)	−0.0024 (11)
C30	0.0454 (15)	0.0493 (15)	0.0345 (13)	0.0006 (12)	0.0077 (11)	−0.0012 (11)
C31	0.0435 (14)	0.0481 (15)	0.0414 (14)	0.0049 (12)	0.0008 (11)	−0.0033 (12)
C32	0.0463 (16)	0.068 (2)	0.066 (2)	−0.0095 (14)	0.0066 (14)	−0.0134 (16)
C33	0.0475 (15)	0.0461 (15)	0.0491 (15)	−0.0055 (12)	0.0080 (12)	−0.0029 (12)
C34	0.0393 (14)	0.0487 (15)	0.0473 (15)	−0.0024 (12)	0.0043 (11)	−0.0005 (12)
C35	0.0438 (15)	0.0635 (19)	0.0539 (17)	−0.0032 (13)	0.0059 (13)	0.0034 (14)
C36	0.0453 (17)	0.081 (2)	0.067 (2)	0.0053 (16)	0.0131 (15)	0.0117 (18)
C37	0.113 (4)	0.210 (7)	0.119 (4)	0.063 (5)	−0.036 (4)	−0.073 (5)
C38	0.081 (3)	0.069 (2)	0.109 (3)	0.007 (2)	0.022 (2)	0.003 (2)
C39	0.098 (3)	0.125 (4)	0.090 (3)	0.032 (3)	0.011 (3)	−0.001 (3)

Geometric parameters (Å, º)

Sn1—O1	2.0961 (16)	C26A—H261	0.9500
Sn1—O2	2.6252 (18)	C28A—H281	0.9800
Sn1—O4	2.0954 (17)	C28A—H282	0.9800
Sn1—O5A	2.81 (3)	C28A—H283	0.9800
Sn1—O5B	2.60 (2)	O5B—C14B	1.253 (4)
Sn1—C29	2.110 (3)	O6B—C16B	1.336 (6)
Sn1—C33	2.110 (3)	O6B—H6B	0.8400
Sn1—O3^{i}	3.4786 (17)	N3B—N4B	1.246 (8)
O1—C1	1.292 (3)	N3B—C19B	1.418 (6)
O2—C1	1.253 (2)	N4B—C21B	1.444 (8)
O3—C3	1.350 (3)	C14B—C15B	1.480 (8)
O3—H3	0.78 (3)	C15B—C20B	1.398 (8)
N1—N2	1.250 (3)	C15B—C16B	1.407 (8)

N1—C6	1.429 (3)	C16B—C17B	1.389 (8)
N2—C8	1.433 (3)	C17B—C18B	1.366 (7)
C1—C2	1.469 (3)	C17B—H172	0.9500
C2—C7	1.400 (3)	C18B—C19B	1.405 (7)
C2—C3	1.406 (3)	C18B—H182	0.9500
C3—C4	1.392 (4)	C19B—C20B	1.383 (7)
C4—C5	1.371 (3)	C20B—H202	0.9500
C4—H4	0.9500	C21B—C22B	1.377 (8)
C5—C6	1.404 (3)	C21B—C26B	1.390 (7)
C5—H5	0.9500	C22B—C23B	1.397 (9)
C6—C7	1.380 (3)	C22B—H222	0.9500
C7—H7	0.9500	C23B—C24B	1.381 (9)
C8—C9	1.386 (3)	C23B—C28B	1.503 (10)
C8—C13	1.388 (3)	C24B—C25B	1.366 (9)
C9—C10	1.396 (3)	C24B—H242	0.9500
C9—H9	0.9500	C25B—C26B	1.401 (8)
C10—C11	1.389 (4)	C25B—H252	0.9500
C10—C27	1.504 (4)	C26B—H263	0.9500
C11—C12	1.382 (4)	C28B—H284	0.9800
C11—H11	0.9500	C28B—H285	0.9800
C12—C13	1.383 (3)	C28B—H286	0.9800
C12—H12	0.9500	C29—C30	1.529 (3)
C13—H13	0.9500	C29—H291	0.9900
C27—H271	0.9800	C29—H292	0.9900
C27—H272	0.9800	C30—C31	1.522 (4)
C27—H273	0.9800	C30—H301	0.9900
O4—C14B	1.291 (4)	C30—H302	0.9900
O4—C14A	1.291 (4)	C31—C32	1.521 (4)
O5A—C14A	1.254 (4)	C31—H311	0.9900
O6A—C16A	1.340 (9)	C31—H312	0.9900
O6A—H6A	0.8400	C32—H321	0.9800
N3A—N4A	1.233 (10)	C32—H322	0.9800
N3A—C19A	1.430 (10)	C32—H323	0.9800
N4A—C21A	1.450 (8)	C33—C34	1.527 (4)
C14A—C15A	1.485 (11)	C33—H331	0.9900
C15A—C20A	1.395 (10)	C33—H332	0.9900
C15A—C16A	1.405 (10)	C34—C35	1.504 (4)
C16A—C17A	1.401 (10)	C34—H341	0.9900
C17A—C18A	1.365 (8)	C34—H342	0.9900
C17A—H171	0.9500	C35—C36	1.516 (4)
C18A—C19A	1.393 (8)	C35—H351	0.9900
C18A—H181	0.9500	C35—H352	0.9900
C19A—C20A	1.382 (9)	C36—H361	0.9800
C20A—H201	0.9500	C36—H362	0.9800
C21A—C22A	1.375 (10)	C36—H363	0.9800
C21A—C26A	1.399 (9)	C37—C39^{ii}	1.360 (5)
C22A—C23A	1.401 (11)	C37—C38	1.546 (6)
C22A—H221	0.9500	C37—H371	0.9900

C23A—C24A	1.386 (11)	C37—H372	0.9900
C23A—C28A	1.508 (11)	C38—C39	1.453 (5)
C24A—C25A	1.374 (11)	C38—H381	0.9900
C24A—H241	0.9500	C38—H382	0.9900
C25A—C26A	1.390 (9)	C39—H391	0.9900
C25A—H25A	0.9500	C39—H392	0.9900

O1—Sn1—O2	53.93 (5)	C23A—C28A—H283	109.5
O1—Sn1—O4	82.76 (6)	H281—C28A—H283	109.5
O1—Sn1—O5A	135.8 (3)	H282—C28A—H283	109.5
O1—Sn1—O5B	135.6 (2)	C14B—O5B—Sn1	84.7 (9)
O1—Sn1—C29	103.65 (9)	C16B—O6B—H6B	109.5
O1—Sn1—C33	109.89 (9)	N4B—N3B—C19B	114.4 (5)
O2—Sn1—O4	136.44 (6)	N3B—N4B—C21B	112.5 (7)
O2—Sn1—O5A	167.5 (4)	O5B—C14B—O4	114.3 (11)
O2—Sn1—O5B	169.5 (3)	O5B—C14B—C15B	122.5 (10)
O2—Sn1—C29	92.83 (8)	O4—C14B—C15B	123.1 (8)
O2—Sn1—C33	87.56 (9)	C20B—C15B—C16B	119.4 (7)
O4—Sn1—O5A	53.3 (3)	C20B—C15B—C14B	120.1 (7)
O4—Sn1—O5B	52.9 (2)	C16B—C15B—C14B	120.5 (6)
O4—Sn1—C29	102.85 (9)	O6B—C16B—C17B	117.4 (6)
O4—Sn1—C33	105.25 (9)	O6B—C16B—C15B	122.8 (7)
O5A—Sn1—C29	91.6 (6)	C17B—C16B—C15B	119.7 (6)
O5A—Sn1—C33	81.4 (6)	C18B—C17B—C16B	120.2 (5)
O5B—Sn1—C29	88.7 (5)	C18B—C17B—H172	119.9
O5B—Sn1—C33	84.4 (5)	C16B—C17B—H172	119.9
C29—Sn1—C33	138.31 (10)	C17B—C18B—C19B	121.2 (5)
C1—O1—Sn1	105.49 (14)	C17B—C18B—H182	119.4
C1—O2—Sn1	81.66 (14)	C19B—C18B—H182	119.4
C3—O3—H3	105 (3)	C20B—C19B—C18B	119.0 (5)
N2—N1—C6	114.6 (2)	C20B—C19B—N3B	125.8 (6)
N1—N2—C8	113.7 (2)	C18B—C19B—N3B	115.3 (5)
O2—C1—O1	118.9 (2)	C19B—C20B—C15B	120.5 (6)
O2—C1—C2	122.0 (2)	C19B—C20B—H202	119.7
O1—C1—C2	119.07 (19)	C15B—C20B—H202	119.7
C7—C2—C3	118.7 (2)	C22B—C21B—C26B	119.6 (6)
C7—C2—C1	120.8 (2)	C22B—C21B—N4B	115.5 (7)
C3—C2—C1	120.6 (2)	C26B—C21B—N4B	124.9 (6)
O3—C3—C4	117.3 (2)	C21B—C22B—C23B	121.1 (8)
O3—C3—C2	122.9 (2)	C21B—C22B—H222	119.5
C4—C3—C2	119.8 (2)	C23B—C22B—H222	119.5
C5—C4—C3	120.9 (2)	C24B—C23B—C22B	118.9 (8)
C5—C4—H4	119.5	C24B—C23B—C28B	122.8 (8)
C3—C4—H4	119.5	C22B—C23B—C28B	118.1 (9)
C4—C5—C6	120.0 (2)	C25B—C24B—C23B	120.4 (8)
C4—C5—H5	120.0	C25B—C24B—H242	119.8
C6—C5—H5	120.0	C23B—C24B—H242	119.8
C7—C6—C5	119.5 (2)	C24B—C25B—C26B	120.9 (7)

C7—C6—N1	115.8 (2)	C24B—C25B—H252	119.6
C5—C6—N1	124.7 (2)	C26B—C25B—H252	119.6
C6—C7—C2	121.1 (2)	C21B—C26B—C25B	119.1 (6)
C6—C7—H7	119.4	C21B—C26B—H263	120.5
C2—C7—H7	119.4	C25B—C26B—H263	120.5
C9—C8—C13	120.1 (2)	C23B—C28B—H284	109.5
C9—C8—N2	115.6 (2)	C23B—C28B—H285	109.5
C13—C8—N2	124.3 (2)	H284—C28B—H285	109.5
C8—C9—C10	121.4 (2)	C23B—C28B—H286	109.5
C8—C9—H9	119.3	H284—C28B—H286	109.5
C10—C9—H9	119.3	H285—C28B—H286	109.5
C11—C10—C9	117.5 (2)	C30—C29—Sn1	110.95 (16)
C11—C10—C27	122.2 (2)	C30—C29—H291	109.4
C9—C10—C27	120.3 (3)	Sn1—C29—H291	109.4
C12—C11—C10	121.3 (2)	C30—C29—H292	109.4
C12—C11—H11	119.4	Sn1—C29—H292	109.4
C10—C11—H11	119.4	H291—C29—H292	108.0
C11—C12—C13	120.7 (3)	C31—C30—C29	113.1 (2)
C11—C12—H12	119.6	C31—C30—H301	109.0
C13—C12—H12	119.6	C29—C30—H301	109.0
C12—C13—C8	119.0 (2)	C31—C30—H302	109.0
C12—C13—H13	120.5	C29—C30—H302	109.0
C8—C13—H13	120.5	H301—C30—H302	107.8
C10—C27—H271	109.5	C32—C31—C30	111.2 (2)
C10—C27—H272	109.5	C32—C31—H311	109.4
H271—C27—H272	109.5	C30—C31—H311	109.4
C10—C27—H273	109.5	C32—C31—H312	109.4
H271—C27—H273	109.5	C30—C31—H312	109.4
H272—C27—H273	109.5	H311—C31—H312	108.0
C14B—O4—Sn1	108.0 (5)	C31—C32—H321	109.5
C14A—O4—Sn1	105.1 (6)	C31—C32—H322	109.5
C14A—O5A—Sn1	73.6 (12)	H321—C32—H322	109.5
C16A—O6A—H6A	109.5	C31—C32—H323	109.5
N4A—N3A—C19A	115.7 (9)	H321—C32—H323	109.5
N3A—N4A—C21A	113.1 (7)	H322—C32—H323	109.5
O5A—C14A—O4	128.0 (15)	C34—C33—Sn1	114.74 (18)
O5A—C14A—C15A	121.5 (13)	C34—C33—H331	108.6
O4—C14A—C15A	110.0 (9)	Sn1—C33—H331	108.6
C20A—C15A—C16A	119.0 (9)	C34—C33—H332	108.6
C20A—C15A—C14A	120.6 (9)	Sn1—C33—H332	108.6
C16A—C15A—C14A	120.3 (8)	H331—C33—H332	107.6
O6A—C16A—C17A	116.3 (8)	C35—C34—C33	113.1 (2)
O6A—C16A—C15A	123.1 (9)	C35—C34—H341	109.0
C17A—C16A—C15A	120.6 (8)	C33—C34—H341	109.0
C18A—C17A—C16A	118.7 (7)	C35—C34—H342	109.0
C18A—C17A—H171	120.6	C33—C34—H342	109.0
C16A—C17A—H171	120.7	H341—C34—H342	107.8
C17A—C18A—C19A	121.8 (6)	C34—C35—C36	112.8 (3)

C17A—C18A—H181	119.1	C34—C35—H351	109.0
C19A—C18A—H181	119.1	C36—C35—H351	109.0
C20A—C19A—C18A	119.7 (6)	C34—C35—H352	109.0
C20A—C19A—N3A	114.9 (7)	C36—C35—H352	109.0
C18A—C19A—N3A	125.4 (7)	H351—C35—H352	107.8
C19A—C20A—C15A	120.1 (8)	C35—C36—H361	109.5
C19A—C20A—H201	119.9	C35—C36—H362	109.5
C15A—C20A—H201	119.9	H361—C36—H362	109.5
C22A—C21A—C26A	121.5 (8)	C35—C36—H363	109.5
C22A—C21A—N4A	123.1 (8)	H361—C36—H363	109.5
C26A—C21A—N4A	115.4 (7)	H362—C36—H363	109.5
C21A—C22A—C23A	120.2 (11)	C39^{ii}—C37—C38	106.1 (5)
C21A—C22A—H221	119.9	C39^{ii}—C37—H371	110.5
C23A—C22A—H221	119.9	C38—C37—H371	110.5
C24A—C23A—C22A	117.5 (10)	C39^{ii}—C37—H372	110.5
C24A—C23A—C28A	119.9 (10)	C38—C37—H372	110.5
C22A—C23A—C28A	122.1 (11)	H371—C37—H372	108.7
C25A—C24A—C23A	122.8 (10)	C39—C38—C37	117.5 (4)
C25A—C24A—H241	118.6	C39—C38—H381	107.9
C23A—C24A—H241	118.6	C37—C38—H381	107.9
C24A—C25A—C26A	119.6 (9)	C39—C38—H382	107.9
C24A—C25A—H25A	120.2	C37—C38—H382	107.9
C26A—C25A—H25A	120.2	H381—C38—H382	107.2
C25A—C26A—C21A	118.4 (8)	C37^{ii}—C39—C38	116.0 (4)
C25A—C26A—H261	120.8	C37^{ii}—C39—H391	108.3
C21A—C26A—H261	120.8	C38—C39—H391	108.3
C23A—C28A—H281	109.5	C37^{ii}—C39—H392	108.3
C23A—C28A—H282	109.5	C38—C39—H392	108.3
H281—C28A—H282	109.5	H391—C39—H392	107.4

C6—N1—N2—C8	179.1 (2)	N3A—C19A—C20A—C15A	−179.4 (15)
Sn1—O2—C1—O1	−0.6 (2)	C16A—C15A—C20A—C19A	1 (2)
Sn1—O2—C1—C2	178.0 (2)	C14A—C15A—C20A—C19A	−179 (2)
Sn1—O1—C1—O2	0.7 (3)	N3A—N4A—C21A—C22A	0.5 (16)
Sn1—O1—C1—C2	−177.90 (18)	N3A—N4A—C21A—C26A	−178.1 (10)
O2—C1—C2—C7	176.8 (2)	C26A—C21A—C22A—C23A	−3 (3)
O1—C1—C2—C7	−4.6 (4)	N4A—C21A—C22A—C23A	179 (2)
O2—C1—C2—C3	−2.9 (4)	C21A—C22A—C23A—C24A	3 (5)
O1—C1—C2—C3	175.7 (2)	C21A—C22A—C23A—C28A	175 (2)
C7—C2—C3—O3	−178.8 (2)	C22A—C23A—C24A—C25A	−2 (4)
C1—C2—C3—O3	0.9 (4)	C28A—C23A—C24A—C25A	−174 (2)
C7—C2—C3—C4	2.0 (4)	C23A—C24A—C25A—C26A	1 (2)
C1—C2—C3—C4	−178.3 (2)	C24A—C25A—C26A—C21A	−0.3 (14)
O3—C3—C4—C5	179.6 (2)	C22A—C21A—C26A—C25A	1.3 (15)
C2—C3—C4—C5	−1.1 (4)	N4A—C21A—C26A—C25A	179.9 (7)
C3—C4—C5—C6	−0.6 (4)	C19B—N3B—N4B—C21B	179.3 (7)
C4—C5—C6—C7	1.3 (4)	Sn1—O5B—C14B—O4	−2.1 (19)
C4—C5—C6—N1	−179.3 (2)	Sn1—O5B—C14B—C15B	−180 (2)

N2—N1—C6—C7	179.8 (2)	Sn1—O4—C14B—O5B	3 (2)
N2—N1—C6—C5	0.4 (4)	Sn1—O4—C14B—C15B	−179.5 (19)
C5—C6—C7—C2	−0.3 (4)	O5B—C14B—C15B—C20B	−179 (2)
N1—C6—C7—C2	−179.8 (2)	O4—C14B—C15B—C20B	4 (3)
C3—C2—C7—C6	−1.3 (4)	O5B—C14B—C15B—C16B	−2 (3)
C1—C2—C7—C6	179.0 (2)	O4—C14B—C15B—C16B	−179.1 (18)
N1—N2—C8—C9	−176.3 (2)	C20B—C15B—C16B—O6B	179.6 (12)
N1—N2—C8—C13	3.3 (4)	C14B—C15B—C16B—O6B	2 (2)
C13—C8—C9—C10	−0.3 (4)	C20B—C15B—C16B—C17B	0.6 (18)
N2—C8—C9—C10	179.3 (2)	C14B—C15B—C16B—C17B	−176.8 (16)
C8—C9—C10—C11	0.5 (4)	O6B—C16B—C17B—C18B	−178.2 (8)
C8—C9—C10—C27	−179.5 (3)	C15B—C16B—C17B—C18B	0.8 (13)
C9—C10—C11—C12	−1.1 (4)	C16B—C17B—C18B—C19B	−0.7 (9)
C27—C10—C11—C12	178.9 (3)	C17B—C18B—C19B—C20B	−0.9 (9)
C10—C11—C12—C13	1.5 (4)	C17B—C18B—C19B—N3B	179.5 (5)
C11—C12—C13—C8	−1.2 (4)	N4B—N3B—C19B—C20B	4.0 (10)
C9—C8—C13—C12	0.6 (4)	N4B—N3B—C19B—C18B	−176.5 (8)
N2—C8—C13—C12	−178.9 (2)	C18B—C19B—C20B—C15B	2.3 (12)
C19A—N3A—N4A—C21A	−179.0 (10)	N3B—C19B—C20B—C15B	−178.1 (9)
Sn1—O5A—C14A—O4	1 (3)	C16B—C15B—C20B—C19B	−2.2 (17)
Sn1—O5A—C14A—C15A	173 (3)	C14B—C15B—C20B—C19B	175.2 (16)
Sn1—O4—C14A—O5A	−1 (4)	N3B—N4B—C21B—C22B	−179.9 (10)
Sn1—O4—C14A—C15A	−174.0 (19)	N3B—N4B—C21B—C26B	−2.0 (14)
O5A—C14A—C15A—C20A	−179 (3)	C26B—C21B—C22B—C23B	3 (2)
O4—C14A—C15A—C20A	−6 (4)	N4B—C21B—C22B—C23B	−179 (2)
O5A—C14A—C15A—C16A	1 (4)	C21B—C22B—C23B—C24B	−3 (4)
O4—C14A—C15A—C16A	174 (2)	C21B—C22B—C23B—C28B	−178.4 (15)
C20A—C15A—C16A—O6A	177.7 (15)	C22B—C23B—C24B—C25B	2 (3)
C14A—C15A—C16A—O6A	−3 (3)	C28B—C23B—C24B—C25B	177.4 (18)
C20A—C15A—C16A—C17A	−2 (2)	C23B—C24B—C25B—C26B	−1.3 (19)
C14A—C15A—C16A—C17A	177 (2)	C22B—C21B—C26B—C25B	−1.8 (11)
O6A—C16A—C17A—C18A	−177.7 (10)	N4B—C21B—C26B—C25B	−179.6 (8)
C15A—C16A—C17A—C18A	2.4 (18)	C24B—C25B—C26B—C21B	1.1 (11)
C16A—C17A—C18A—C19A	−0.4 (12)	Sn1—C29—C30—C31	−179.94 (18)
C17A—C18A—C19A—C20A	−1.4 (11)	C29—C30—C31—C32	179.6 (2)
C17A—C18A—C19A—N3A	179.4 (11)	Sn1—C33—C34—C35	−174.66 (19)
N4A—N3A—C19A—C20A	177.4 (11)	C33—C34—C35—C36	−174.4 (2)
N4A—N3A—C19A—C18A	−3.5 (19)	C39^{ii}—C37—C38—C39	−48.3 (6)
C18A—C19A—C20A—C15A	1.4 (16)	C37—C38—C39—C37^{ii}	53.0 (7)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.78 (3)	1.91 (3)	2.623 (3)	153 (3)
O3—H3···O2^{i}	0.78 (3)	2.44 (3)	2.872 (3)	117 (3)

O6*A*—H6*A*···O5*A*	0.84	1.90	2.62 (3)	144
O6*B*—H6*B*···O5*B*	0.84	1.90	2.64 (2)	146

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.

Dibenzylbis{(*E*)-5-[(4-bromophenyl)diazenyl]-2-hydroxybenzoato}tin(IV) (II)

Crystal data

$[Sn(C_7H_7)_2(C_{13}H_8BrN_2O_3)_2]$
M_r = 941.19
Monoclinic, $P2_1/n$
a = 13.6816 (1) Å
b = 12.5767 (1) Å
c = 22.5401 (2) Å
β = 107.0174 (6)°
V = 3708.65 (5) Å^3
Z = 4
$F(000)$ = 1864
D_x = 1.686 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 89697 reflections
θ = 2.0–30.0°
μ = 2.90 mm^{-1}
T = 160 K
Tablet, orange
0.25 × 0.15 × 0.10 mm

Data collection

Nonius KappaCCD area detector diffractometer
Radiation source: Nonius FR590 sealed tube generator
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
T_{min} = 0.652, T_{max} = 0.843
107473 measured reflections
10845 independent reflections
8598 reflections with $I > 2\sigma(I)$
R_{int} = 0.059
θ_{max} = 30.0°, θ_{min} = 2.0°
h = −19→19
k = −17→16
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.076
S = 1.04
10845 reflections
487 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0342P)^2 + 2.2611P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.87 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick 2015), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00044 (10)

Special details

Experimental. Data collection and full structure determination done by Prof. Anthony Linden: anthony.linden@chem.uzh.ch
Solvent used: benzene Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: on a glass fibre Mosaicity (deg.): 0.497 (1) Frames collected: 621 Seconds exposure per frame: 42 Degrees rotation per frame: 1.4 Crystal-detector distance (mm): 33.0 Client: Tushar Basu Sample code: TSBB-116 (L0503)

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	1.12288 (2)	0.92949 (2)	0.21744 (2)	0.02364 (5)
Br1	0.35337 (2)	0.38616 (2)	−0.16642 (2)	0.04522 (8)
Br2	0.24024 (2)	1.11571 (2)	−0.12676 (2)	0.04297 (7)
O1	1.03424 (11)	0.81362 (11)	0.15792 (7)	0.0267 (3)
O2	1.18264 (11)	0.73803 (12)	0.20301 (7)	0.0295 (3)
O3	1.21624 (12)	0.54381 (14)	0.17681 (8)	0.0341 (4)
H3	1.227 (2)	0.600 (2)	0.1896 (14)	0.043 (9)*
O4	0.99008 (11)	1.02063 (12)	0.17848 (7)	0.0287 (3)
O5	1.10390 (12)	1.12542 (12)	0.23962 (7)	0.0336 (4)
O6	1.06615 (14)	1.32629 (15)	0.24788 (9)	0.0413 (4)
H6	1.095 (2)	1.273 (3)	0.2523 (14)	0.048 (9)*
N1	0.81504 (14)	0.53194 (15)	0.02420 (8)	0.0293 (4)
N2	0.79016 (14)	0.44594 (15)	−0.00499 (9)	0.0312 (4)
N3	0.67967 (13)	1.26118 (15)	0.08248 (8)	0.0290 (4)
N4	0.66500 (14)	1.17649 (15)	0.05176 (9)	0.0304 (4)
C1	1.09302 (15)	0.73155 (16)	0.16653 (9)	0.0241 (4)
C2	1.05433 (16)	0.63236 (16)	0.13312 (9)	0.0246 (4)
C3	1.11879 (16)	0.54387 (17)	0.13959 (10)	0.0275 (4)
C4	1.08292 (18)	0.45075 (18)	0.10642 (11)	0.0336 (5)
H4	1.126847	0.390942	0.110629	0.040*
C5	0.98481 (18)	0.44523 (18)	0.06788 (11)	0.0326 (5)
H5	0.961411	0.381945	0.045143	0.039*
C6	0.91881 (16)	0.53244 (18)	0.06183 (10)	0.0283 (4)
C7	0.95369 (16)	0.62502 (16)	0.09410 (9)	0.0261 (4)
H7	0.909103	0.684281	0.089839	0.031*
C8	0.68605 (16)	0.43989 (17)	−0.04158 (10)	0.0282 (4)
C9	0.66170 (19)	0.35179 (19)	−0.08038 (11)	0.0353 (5)
H9	0.713574	0.302189	−0.081361	0.042*
C10	0.56283 (18)	0.33562 (19)	−0.11754 (11)	0.0347 (5)
H10	0.546201	0.275366	−0.144009	0.042*
C11	0.48879 (17)	0.40869 (18)	−0.11544 (10)	0.0312 (5)
C12	0.51050 (17)	0.49732 (18)	−0.07683 (10)	0.0316 (5)
H12	0.458157	0.546255	−0.075751	0.038*
C13	0.61031 (17)	0.51274 (18)	−0.03988 (10)	0.0313 (5)
H13	0.626884	0.573038	−0.013445	0.038*
C14	1.01655 (16)	1.11307 (17)	0.20191 (10)	0.0270 (4)
C15	0.94456 (15)	1.20272 (16)	0.18346 (9)	0.0246 (4)
C16	0.97321 (17)	1.30496 (17)	0.20791 (10)	0.0295 (4)
C17	0.90408 (19)	1.38837 (18)	0.19048 (11)	0.0348 (5)
H17	0.922534	1.457432	0.207046	0.042*
C18	0.80892 (18)	1.37121 (18)	0.14927 (11)	0.0312 (5)
H18	0.762175	1.428724	0.137696	0.037*
C19	0.78022 (16)	1.27034 (17)	0.12426 (9)	0.0258 (4)
C20	0.84821 (15)	1.18649 (17)	0.14157 (9)	0.0252 (4)
H20	0.829109	1.117652	0.124835	0.030*

C21	0.56306 (16)	1.16501 (18)	0.01224 (10)	0.0289 (4)
C22	0.47863 (17)	1.21300 (19)	0.02333 (11)	0.0338 (5)
H22	0.487192	1.256449	0.058965	0.041*
C23	0.38202 (18)	1.1977 (2)	−0.01744 (12)	0.0371 (5)
H23	0.324028	1.230242	−0.010048	0.045*
C24	0.37124 (17)	1.13422 (18)	−0.06909 (11)	0.0326 (5)
C25	0.45375 (19)	1.0834 (2)	−0.07959 (11)	0.0382 (5)
H25	0.444656	1.038832	−0.114839	0.046*
C26	0.55027 (19)	1.0977 (2)	−0.03824 (12)	0.0364 (5)
H26	0.607427	1.061489	−0.044466	0.044*
C27	1.23394 (17)	0.9824 (2)	0.17457 (11)	0.0345 (5)
H271	1.274498	1.040539	0.199706	0.041*
H272	1.281210	0.923037	0.174009	0.041*
C28	1.18727 (16)	1.02131 (18)	0.10939 (10)	0.0289 (4)
C29	1.15565 (19)	1.1265 (2)	0.09827 (11)	0.0367 (5)
H29	1.163412	1.173705	0.132262	0.044*
C30	1.1131 (2)	1.1634 (2)	0.03845 (12)	0.0470 (7)
H30	1.091423	1.235306	0.031672	0.056*
C31	1.1021 (2)	1.0965 (3)	−0.01115 (13)	0.0511 (7)
H31	1.073282	1.122162	−0.052203	0.061*
C32	1.1324 (2)	0.9933 (3)	−0.00152 (13)	0.0537 (8)
H32	1.124292	0.946947	−0.035900	0.064*
C33	1.1756 (2)	0.9551 (2)	0.05899 (13)	0.0436 (6)
H33	1.197067	0.883071	0.065309	0.052*
C34	1.11013 (17)	0.88479 (18)	0.30603 (10)	0.0295 (5)
H341	1.177731	0.861067	0.332684	0.035*
H342	1.089104	0.947379	0.325971	0.035*
C35	1.03402 (16)	0.79736 (17)	0.30103 (9)	0.0262 (4)
C36	1.06646 (18)	0.69271 (18)	0.31317 (11)	0.0316 (5)
H36	1.137571	0.677401	0.326086	0.038*
C37	0.9968 (2)	0.6103 (2)	0.30672 (12)	0.0387 (5)
H37	1.020131	0.539084	0.314606	0.046*
C38	0.89273 (19)	0.6322 (2)	0.28872 (11)	0.0376 (5)
H38	0.844633	0.576106	0.284560	0.045*
C39	0.85972 (18)	0.7355 (2)	0.27695 (10)	0.0355 (5)
H39	0.788575	0.750619	0.264705	0.043*
C40	0.92922 (17)	0.81773 (19)	0.28278 (10)	0.0308 (5)
H40	0.905311	0.888640	0.274277	0.037*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02239 (7)	0.01846 (7)	0.02550 (7)	−0.00111 (5)	−0.00014 (5)	0.00225 (5)
Br1	0.03174 (13)	0.03595 (14)	0.05510 (16)	−0.00582 (10)	−0.00740 (11)	−0.00544 (11)
Br2	0.03208 (13)	0.04611 (16)	0.04141 (14)	−0.00977 (11)	−0.00380 (10)	0.00158 (11)
O1	0.0273 (7)	0.0195 (7)	0.0282 (7)	0.0003 (6)	0.0004 (6)	−0.0008 (6)
O2	0.0267 (7)	0.0252 (8)	0.0304 (8)	−0.0004 (6)	−0.0010 (6)	−0.0007 (6)
O3	0.0263 (8)	0.0271 (9)	0.0392 (9)	0.0044 (7)	−0.0054 (7)	−0.0047 (7)

O4	0.0254 (7)	0.0202 (7)	0.0346 (8)	0.0010 (6)	−0.0005 (6)	−0.0005 (6)
O5	0.0284 (8)	0.0264 (8)	0.0360 (8)	−0.0014 (6)	−0.0063 (6)	0.0032 (6)
O6	0.0376 (9)	0.0239 (9)	0.0475 (10)	−0.0030 (7)	−0.0112 (8)	−0.0047 (7)
N1	0.0283 (9)	0.0261 (9)	0.0290 (9)	−0.0018 (7)	0.0013 (7)	−0.0022 (7)
N2	0.0278 (9)	0.0276 (10)	0.0329 (10)	−0.0019 (7)	0.0007 (7)	−0.0043 (7)
N3	0.0253 (9)	0.0277 (10)	0.0311 (9)	0.0030 (7)	0.0038 (7)	0.0010 (7)
N4	0.0270 (9)	0.0289 (10)	0.0316 (9)	0.0032 (7)	0.0028 (7)	−0.0013 (7)
C1	0.0254 (10)	0.0224 (10)	0.0225 (9)	0.0000 (8)	0.0041 (7)	−0.0003 (7)
C2	0.0259 (10)	0.0215 (10)	0.0238 (9)	−0.0012 (8)	0.0032 (8)	0.0011 (7)
C3	0.0235 (10)	0.0259 (11)	0.0294 (10)	0.0019 (8)	0.0020 (8)	0.0003 (8)
C4	0.0292 (11)	0.0256 (12)	0.0416 (13)	0.0052 (9)	0.0033 (9)	−0.0048 (9)
C5	0.0322 (11)	0.0255 (11)	0.0355 (12)	0.0004 (9)	0.0028 (9)	−0.0079 (9)
C6	0.0254 (10)	0.0280 (11)	0.0276 (10)	−0.0003 (8)	0.0019 (8)	−0.0004 (8)
C7	0.0265 (10)	0.0214 (10)	0.0270 (10)	0.0012 (8)	0.0024 (8)	0.0013 (8)
C8	0.0276 (10)	0.0247 (11)	0.0280 (10)	−0.0039 (8)	0.0016 (8)	0.0004 (8)
C9	0.0357 (12)	0.0250 (11)	0.0402 (13)	0.0013 (9)	0.0035 (10)	−0.0042 (9)
C10	0.0354 (12)	0.0247 (11)	0.0372 (12)	−0.0061 (9)	0.0000 (10)	−0.0049 (9)
C11	0.0275 (11)	0.0288 (12)	0.0319 (11)	−0.0066 (9)	0.0001 (9)	0.0029 (9)
C12	0.0291 (11)	0.0296 (12)	0.0340 (11)	−0.0008 (9)	0.0059 (9)	−0.0014 (9)
C13	0.0311 (11)	0.0276 (12)	0.0326 (11)	−0.0027 (9)	0.0051 (9)	−0.0046 (9)
C14	0.0276 (10)	0.0213 (10)	0.0282 (10)	−0.0017 (8)	0.0018 (8)	0.0025 (8)
C15	0.0261 (10)	0.0199 (10)	0.0245 (9)	−0.0011 (8)	0.0026 (8)	−0.0001 (7)
C16	0.0304 (11)	0.0244 (11)	0.0284 (10)	−0.0034 (9)	0.0005 (8)	−0.0010 (8)
C17	0.0417 (13)	0.0190 (10)	0.0390 (12)	−0.0016 (9)	0.0044 (10)	−0.0053 (9)
C18	0.0332 (11)	0.0230 (11)	0.0362 (12)	0.0051 (9)	0.0082 (9)	−0.0004 (9)
C19	0.0253 (10)	0.0270 (11)	0.0230 (9)	0.0016 (8)	0.0035 (8)	−0.0001 (8)
C20	0.0262 (10)	0.0209 (10)	0.0261 (10)	0.0000 (8)	0.0039 (8)	−0.0007 (8)
C21	0.0271 (10)	0.0262 (11)	0.0293 (11)	−0.0006 (9)	0.0020 (8)	0.0004 (8)
C22	0.0307 (11)	0.0328 (12)	0.0350 (12)	0.0011 (9)	0.0048 (9)	−0.0064 (9)
C23	0.0265 (11)	0.0364 (13)	0.0451 (14)	0.0014 (10)	0.0051 (10)	−0.0054 (10)
C24	0.0277 (11)	0.0296 (12)	0.0339 (11)	−0.0059 (9)	−0.0010 (9)	0.0026 (9)
C25	0.0392 (13)	0.0402 (14)	0.0330 (12)	−0.0060 (11)	0.0071 (10)	−0.0088 (10)
C26	0.0324 (12)	0.0358 (13)	0.0410 (13)	0.0004 (10)	0.0105 (10)	−0.0084 (10)
C27	0.0256 (11)	0.0349 (13)	0.0386 (12)	−0.0025 (9)	0.0024 (9)	0.0129 (10)
C28	0.0229 (10)	0.0300 (12)	0.0331 (11)	0.0002 (9)	0.0069 (8)	0.0052 (9)
C29	0.0399 (13)	0.0337 (13)	0.0346 (12)	0.0034 (10)	0.0080 (10)	0.0069 (10)
C30	0.0483 (15)	0.0506 (17)	0.0422 (14)	0.0141 (13)	0.0135 (12)	0.0193 (12)
C31	0.0479 (16)	0.070 (2)	0.0322 (13)	0.0005 (14)	0.0074 (11)	0.0115 (13)
C32	0.0634 (19)	0.066 (2)	0.0359 (14)	−0.0111 (16)	0.0215 (13)	−0.0134 (13)
C33	0.0518 (16)	0.0363 (14)	0.0482 (15)	0.0037 (12)	0.0234 (13)	−0.0030 (11)
C34	0.0322 (11)	0.0263 (11)	0.0261 (10)	−0.0051 (9)	0.0024 (8)	−0.0019 (8)
C35	0.0296 (10)	0.0254 (11)	0.0220 (9)	−0.0021 (8)	0.0050 (8)	−0.0015 (8)
C36	0.0305 (11)	0.0281 (11)	0.0357 (12)	0.0009 (9)	0.0090 (9)	0.0041 (9)
C37	0.0447 (14)	0.0257 (12)	0.0461 (14)	−0.0028 (10)	0.0141 (11)	0.0042 (10)
C38	0.0384 (13)	0.0363 (13)	0.0392 (13)	−0.0131 (10)	0.0134 (10)	−0.0024 (10)
C39	0.0275 (11)	0.0452 (15)	0.0329 (12)	−0.0034 (10)	0.0072 (9)	−0.0028 (10)
C40	0.0315 (11)	0.0279 (11)	0.0309 (11)	0.0010 (9)	0.0060 (9)	−0.0006 (9)

Geometric parameters (Å, º)

Sn1—O1	2.1077 (14)	C16—C17	1.390 (3)
Sn1—O2	2.5939 (15)	C17—C18	1.377 (3)
Sn1—O4	2.1100 (14)	C17—H17	0.9500
Sn1—O5	2.5426 (16)	C18—C19	1.397 (3)
Sn1—C27	2.132 (2)	C18—H18	0.9500
Sn1—C34	2.130 (2)	C19—C20	1.385 (3)
Sn1—O3^{i}	3.0858 (16)	C20—H20	0.9500
Br1—C11	1.894 (2)	C21—C26	1.388 (3)
Br2—C24	1.895 (2)	C21—C22	1.389 (3)
O1—C1	1.288 (2)	C22—C23	1.385 (3)
O2—C1	1.263 (2)	C22—H22	0.9500
O3—C3	1.352 (3)	C23—C24	1.383 (3)
O3—H3	0.77 (3)	C23—H23	0.9500
O4—C14	1.284 (3)	C24—C25	1.377 (4)
O5—C14	1.257 (2)	C25—C26	1.387 (3)
O6—C16	1.353 (3)	C25—H25	0.9500
O6—H6	0.76 (3)	C26—H26	0.9500
N1—N2	1.260 (3)	C27—C28	1.502 (3)
N1—C6	1.425 (3)	C27—H271	0.9900
N2—C8	1.424 (3)	C27—H272	0.9900
N3—N4	1.254 (3)	C28—C33	1.379 (3)
N3—C19	1.426 (3)	C28—C29	1.392 (3)
N4—C21	1.425 (3)	C29—C30	1.383 (3)
C1—C2	1.473 (3)	C29—H29	0.9500
C2—C3	1.401 (3)	C30—C31	1.372 (4)
C2—C7	1.403 (3)	C30—H30	0.9500
C3—C4	1.399 (3)	C31—C32	1.360 (5)
C4—C5	1.371 (3)	C31—H31	0.9500
C4—H4	0.9500	C32—C33	1.403 (4)
C5—C6	1.402 (3)	C32—H32	0.9500
C5—H5	0.9500	C33—H33	0.9500
C6—C7	1.382 (3)	C34—C35	1.496 (3)
C7—H7	0.9500	C34—H341	0.9900
C8—C9	1.390 (3)	C34—H342	0.9900
C8—C13	1.392 (3)	C35—C36	1.390 (3)
C9—C10	1.382 (3)	C35—C40	1.395 (3)
C9—H9	0.9500	C36—C37	1.387 (3)
C10—C11	1.379 (3)	C36—H36	0.9500
C10—H10	0.9500	C37—C38	1.389 (4)
C11—C12	1.392 (3)	C37—H37	0.9500
C12—C13	1.389 (3)	C38—C39	1.376 (4)
C12—H12	0.9500	C38—H38	0.9500
C13—H13	0.9500	C39—C40	1.385 (3)
C14—C15	1.475 (3)	C39—H39	0.9500
C15—C20	1.394 (3)	C40—H40	0.9500
C15—C16	1.409 (3)		

O1—Sn1—O2	54.69 (5)	C17—C16—C15	119.34 (19)
O1—Sn1—O4	81.12 (6)	C18—C17—C16	120.2 (2)
O1—Sn1—O5	136.25 (5)	C18—C17—H17	119.9
O1—Sn1—C27	106.31 (8)	C16—C17—H17	119.9
O1—Sn1—C34	102.97 (7)	C17—C18—C19	120.9 (2)
O2—Sn1—O4	135.78 (5)	C17—C18—H18	119.6
O2—Sn1—O5	168.06 (5)	C19—C18—H18	119.6
O2—Sn1—C27	86.57 (8)	C20—C19—C18	119.44 (19)
O2—Sn1—C34	89.30 (7)	C20—C19—N3	124.27 (19)
O4—Sn1—O5	55.27 (5)	C18—C19—N3	116.27 (19)
O4—Sn1—C27	106.44 (7)	C19—C20—C15	120.24 (19)
O4—Sn1—C34	103.69 (8)	C19—C20—H20	119.9
O5—Sn1—C27	85.08 (8)	C15—C20—H20	119.9
O5—Sn1—C34	91.74 (7)	C26—C21—C22	120.0 (2)
C27—Sn1—C34	140.54 (9)	C26—C21—N4	116.1 (2)
O1—Sn1—O3^{i}	164.01 (5)	C22—C21—N4	123.8 (2)
O4—Sn1—O3^{i}	113.64 (5)	C23—C22—C21	120.2 (2)
C34—Sn1—O3^{i}	68.56 (7)	C23—C22—H22	119.9
C27—Sn1—O3^{i}	76.28 (7)	C21—C22—H22	119.9
O5—Sn1—O3^{i}	59.16 (5)	C24—C23—C22	119.0 (2)
O2—Sn1—O3^{i}	110.47 (5)	C24—C23—H23	120.5
C1—O1—Sn1	103.93 (12)	C22—C23—H23	120.5
C1—O2—Sn1	81.95 (12)	C25—C24—C23	121.5 (2)
C3—O3—Sn1^{ii}	146.18 (14)	C25—C24—Br2	118.91 (18)
C3—O3—H3	106 (2)	C23—C24—Br2	119.64 (18)
Sn1^{ii}—O3—H3	97 (2)	C24—C25—C26	119.4 (2)
C14—O4—Sn1	102.46 (12)	C24—C25—H25	120.3
C14—O5—Sn1	83.04 (12)	C26—C25—H25	120.3
C16—O6—H6	105 (2)	C25—C26—C21	119.8 (2)
N2—N1—C6	112.60 (18)	C25—C26—H26	120.1
N1—N2—C8	114.82 (18)	C21—C26—H26	120.1
N4—N3—C19	113.63 (18)	C28—C27—Sn1	112.94 (14)
N3—N4—C21	113.59 (18)	C28—C27—H271	109.0
O2—C1—O1	119.38 (18)	Sn1—C27—H271	109.0
O2—C1—C2	121.50 (18)	C28—C27—H272	109.0
O1—C1—C2	119.12 (17)	Sn1—C27—H272	109.0
C3—C2—C7	119.04 (19)	H271—C27—H272	107.8
C3—C2—C1	119.90 (18)	C33—C28—C29	118.1 (2)
C7—C2—C1	121.06 (19)	C33—C28—C27	121.5 (2)
O3—C3—C4	117.35 (19)	C29—C28—C27	120.4 (2)
O3—C3—C2	122.80 (19)	C30—C29—C28	120.9 (2)
C4—C3—C2	119.85 (19)	C30—C29—H29	119.5
C5—C4—C3	120.4 (2)	C28—C29—H29	119.5
C5—C4—H4	119.8	C31—C30—C29	120.2 (3)
C3—C4—H4	119.8	C31—C30—H30	119.9
C4—C5—C6	120.4 (2)	C29—C30—H30	119.9
C4—C5—H5	119.8	C32—C31—C30	120.0 (3)

C6—C5—H5	119.8	C32—C31—H31	120.0
C7—C6—C5	119.6 (2)	C30—C31—H31	120.0
C7—C6—N1	116.58 (19)	C31—C32—C33	120.3 (3)
C5—C6—N1	123.8 (2)	C31—C32—H32	119.9
C6—C7—C2	120.65 (19)	C33—C32—H32	119.9
C6—C7—H7	119.7	C28—C33—C32	120.5 (3)
C2—C7—H7	119.7	C28—C33—H33	119.7
C9—C8—C13	119.9 (2)	C32—C33—H33	119.7
C9—C8—N2	115.0 (2)	C35—C34—Sn1	111.69 (14)
C13—C8—N2	125.13 (19)	C35—C34—H341	109.3
C10—C9—C8	120.7 (2)	Sn1—C34—H341	109.3
C10—C9—H9	119.7	C35—C34—H342	109.3
C8—C9—H9	119.7	Sn1—C34—H342	109.3
C11—C10—C9	118.7 (2)	H341—C34—H342	107.9
C11—C10—H10	120.7	C36—C35—C40	118.3 (2)
C9—C10—H10	120.7	C36—C35—C34	120.4 (2)
C10—C11—C12	122.1 (2)	C40—C35—C34	121.3 (2)
C10—C11—Br1	118.52 (17)	C37—C36—C35	121.1 (2)
C12—C11—Br1	119.42 (18)	C37—C36—H36	119.4
C13—C12—C11	118.6 (2)	C35—C36—H36	119.4
C13—C12—H12	120.7	C36—C37—C38	119.8 (2)
C11—C12—H12	120.7	C36—C37—H37	120.1
C12—C13—C8	120.0 (2)	C38—C37—H37	120.1
C12—C13—H13	120.0	C39—C38—C37	119.6 (2)
C8—C13—H13	120.0	C39—C38—H38	120.2
O5—C14—O4	119.19 (19)	C37—C38—H38	120.2
O5—C14—C15	121.37 (19)	C38—C39—C40	120.6 (2)
O4—C14—C15	119.44 (18)	C38—C39—H39	119.7
C20—C15—C16	119.90 (19)	C40—C39—H39	119.7
C20—C15—C14	120.02 (18)	C39—C40—C35	120.6 (2)
C16—C15—C14	120.08 (18)	C39—C40—H40	119.7
O6—C16—C17	117.9 (2)	C35—C40—H40	119.7
O6—C16—C15	122.8 (2)		

C6—N1—N2—C8	177.82 (18)	C20—C15—C16—O6	−178.8 (2)
C19—N3—N4—C21	177.10 (18)	C14—C15—C16—O6	0.9 (3)
Sn1—O2—C1—O1	1.81 (17)	C20—C15—C16—C17	0.9 (3)
Sn1—O2—C1—C2	−178.70 (19)	C14—C15—C16—C17	−179.4 (2)
Sn1—O1—C1—O2	−2.3 (2)	O6—C16—C17—C18	179.1 (2)
Sn1—O1—C1—C2	178.23 (15)	C15—C16—C17—C18	−0.6 (4)
O2—C1—C2—C3	−2.6 (3)	C16—C17—C18—C19	−0.1 (4)
O1—C1—C2—C3	176.92 (19)	C17—C18—C19—C20	0.5 (3)
O2—C1—C2—C7	178.11 (19)	C17—C18—C19—N3	179.5 (2)
O1—C1—C2—C7	−2.4 (3)	N4—N3—C19—C20	−15.1 (3)
Sn1^{ii}—O3—C3—C4	−52.7 (3)	N4—N3—C19—C18	166.0 (2)
Sn1^{ii}—O3—C3—C2	127.6 (2)	C18—C19—C20—C15	−0.2 (3)
C7—C2—C3—O3	−179.1 (2)	N3—C19—C20—C15	−179.07 (19)
C1—C2—C3—O3	1.6 (3)	C16—C15—C20—C19	−0.5 (3)

C7—C2—C3—C4	1.2 (3)	C14—C15—C20—C19	179.8 (2)
C1—C2—C3—C4	−178.1 (2)	N3—N4—C21—C26	156.8 (2)
O3—C3—C4—C5	179.9 (2)	N3—N4—C21—C22	−26.1 (3)
C2—C3—C4—C5	−0.4 (4)	C26—C21—C22—C23	−2.9 (4)
C3—C4—C5—C6	−0.8 (4)	N4—C21—C22—C23	−180.0 (2)
C4—C5—C6—C7	1.2 (4)	C21—C22—C23—C24	−0.1 (4)
C4—C5—C6—N1	−178.1 (2)	C22—C23—C24—C25	2.2 (4)
N2—N1—C6—C7	178.1 (2)	C22—C23—C24—Br2	−178.11 (19)
N2—N1—C6—C5	−2.6 (3)	C23—C24—C25—C26	−1.4 (4)
C5—C6—C7—C2	−0.3 (3)	Br2—C24—C25—C26	179.0 (2)
N1—C6—C7—C2	178.98 (19)	C24—C25—C26—C21	−1.6 (4)
C3—C2—C7—C6	−0.8 (3)	C22—C21—C26—C25	3.8 (4)
C1—C2—C7—C6	178.5 (2)	N4—C21—C26—C25	−179.0 (2)
N1—N2—C8—C9	171.5 (2)	Sn1—C27—C28—C33	−94.1 (2)
N1—N2—C8—C13	−9.8 (3)	Sn1—C27—C28—C29	86.8 (2)
C13—C8—C9—C10	0.1 (4)	C33—C28—C29—C30	0.5 (4)
N2—C8—C9—C10	178.9 (2)	C27—C28—C29—C30	179.6 (2)
C8—C9—C10—C11	0.1 (4)	C28—C29—C30—C31	−0.5 (4)
C9—C10—C11—C12	−0.5 (4)	C29—C30—C31—C32	0.5 (4)
C9—C10—C11—Br1	−179.97 (19)	C30—C31—C32—C33	−0.4 (5)
C10—C11—C12—C13	0.7 (4)	C29—C28—C33—C32	−0.5 (4)
Br1—C11—C12—C13	−179.82 (17)	C27—C28—C33—C32	−179.6 (2)
C11—C12—C13—C8	−0.5 (3)	C31—C32—C33—C28	0.4 (4)
C9—C8—C13—C12	0.1 (3)	Sn1—C34—C35—C36	99.9 (2)
N2—C8—C13—C12	−178.5 (2)	Sn1—C34—C35—C40	−78.5 (2)
Sn1—O5—C14—O4	1.63 (19)	C40—C35—C36—C37	0.7 (3)
Sn1—O5—C14—C15	−177.6 (2)	C34—C35—C36—C37	−177.8 (2)
Sn1—O4—C14—O5	−2.0 (2)	C35—C36—C37—C38	−0.9 (4)
Sn1—O4—C14—C15	177.22 (16)	C36—C37—C38—C39	0.5 (4)
O5—C14—C15—C20	−180.0 (2)	C37—C38—C39—C40	0.1 (4)
O4—C14—C15—C20	0.8 (3)	C38—C39—C40—C35	−0.4 (3)
O5—C14—C15—C16	0.3 (3)	C36—C35—C40—C39	0.0 (3)
O4—C14—C15—C16	−178.9 (2)	C34—C35—C40—C39	178.4 (2)

Symmetry codes: (i) −*x*+5/2, *y*+1/2, −*z*+1/2; (ii) −*x*+5/2, *y*−1/2, −*z*+1/2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O2	0.77 (3)	1.89 (3)	2.586 (2)	152 (3)
O3—H3···O5^{ii}	0.77 (3)	2.42 (3)	2.818 (2)	114 (3)
O6—H6···O5	0.76 (3)	1.89 (3)	2.596 (2)	153 (3)

Symmetry code: (ii) −*x*+5/2, *y*−1/2, −*z*+1/2.

Aquadibenzylbis(4-{(*E*)-[(*Z*)-4-hydroxypent-3-en-2-ylidene]amino}benzoato)tin(IV) benzene disolvate (III)

Crystal data

$[Sn(C_7H_7)_2(C_{12}H_{12}NO_3)_2(H_2O)]\cdot 2C_6H_6$
$M_r = 911.62$
Monoclinic, $C2/c$
$a = 23.6530\ (5)$ Å
$b = 10.1034\ (2)$ Å
$c = 20.5952\ (4)$ Å
$\beta = 115.0715\ (12)°$
$V = 4458.02\ (16)$ Å^3
$Z = 4$
$F(000) = 1888$
$D_x = 1.358$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 125492 reflections
$\theta = 2.0–30.0°$
$\mu = 0.63$ mm^{-1}
$T = 160$ K
Tablet, colorless
0.25 × 0.22 × 0.10 mm

Data collection

Nonius KappaCCD area detector diffractometer
Radiation source: Nonius FR590 sealed tube generator
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
$T_{min} = 0.753$, $T_{max} = 0.943$
58583 measured reflections
6506 independent reflections
5193 reflections with $I > 2\sigma(I)$
$R_{int} = 0.101$
$\theta_{max} = 30.0°$, $\theta_{min} = 2.2°$
$h = -32\rightarrow32$
$k = -14\rightarrow14$
$l = -28\rightarrow29$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.148$
$S = 1.05$
6506 reflections
228 parameters
2 restraints
Primary atom site location: heavy-atom method
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0943P)^2 + 4.7027P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.06$ e Å^{-3}
$\Delta\rho_{min} = -2.17$ e Å^{-3}

Special details

Experimental. Data collection and full structure determination done by Prof. Anthony Linden: anthony.linden@chem.uzh.ch
Solvent used: benzene Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: on a glass fibre Mosaicity (deg.): 1.053 (1) Frames collected: 0 Seconds exposure per frame: 33 Degrees rotation per frame: 0.0 Crystal-detector distance (mm): 0.0 Client: Tushar Basu Sample code: TSBB-192 (L0711)

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

Refinement. The asymmetric unit contains one half of a molecule of the Sn-complex, which sits across a two-fold axis, plus a highly disordered benzene molecule. The disordered solvent molecule could not be modelled adequately, so its contribution to the diffraction data was removed using the SQUEEZE routine of the program PLATON. When the solvent molecule is excluded from the model, there are four cavities of 324 Å^3 per unit cell. The total number of electrons contributing to each void was calculated by the SQUEEZE routine to be approximately 85 e. A benzene molecule has 42 e, which suggests that the cavities have two molecules of benzene (one per asymmetric unit) and this approximation was used in the subsequent calculation of the empirical formula, formula weight, density, linear absorption coefficient and F(000). Based on the assumption, the overall ratio of Sn-complex molecules to benzene is 1:2.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.000000	0.20944 (3)	0.250000	0.01902 (10)
O1	−0.06248 (9)	0.0370 (2)	0.19456 (11)	0.0248 (4)
O2	−0.10242 (10)	0.2366 (2)	0.16188 (12)	0.0247 (4)
O3	0.000000	0.4408 (3)	0.250000	0.0353 (8)
H3	0.0301 (14)	0.476 (4)	0.2841 (16)	0.051 (13)*
O10	−0.43538 (10)	−0.1170 (2)	−0.14546 (12)	0.0303 (5)
N1	−0.34338 (12)	−0.1205 (3)	−0.01611 (14)	0.0255 (5)
H1	−0.3581 (18)	−0.084 (4)	−0.055 (2)	0.033 (10)*
C1	−0.10849 (13)	0.1113 (3)	0.15772 (15)	0.0213 (6)
C2	−0.16937 (13)	0.0487 (3)	0.11166 (15)	0.0222 (6)
C3	−0.17658 (13)	−0.0879 (3)	0.11204 (16)	0.0239 (6)
H3A	−0.142047	−0.141854	0.140536	0.029*
C4	−0.23372 (14)	−0.1456 (3)	0.07121 (17)	0.0261 (6)
H4	−0.238480	−0.238854	0.071822	0.031*
C5	−0.28419 (13)	−0.0668 (3)	0.02923 (15)	0.0236 (6)
C6	−0.27703 (14)	0.0703 (3)	0.02811 (17)	0.0268 (6)
H6	−0.311396	0.124213	−0.000880	0.032*
C7	−0.21968 (14)	0.1274 (3)	0.06939 (17)	0.0277 (6)
H7	−0.214750	0.220631	0.068782	0.033*
C8	−0.37763 (15)	−0.2072 (3)	−0.00003 (18)	0.0291 (7)
C9	−0.43476 (15)	−0.2480 (3)	−0.05114 (18)	0.0263 (6)
H9	−0.457607	−0.310895	−0.037549	0.032*
C10	−0.46156 (15)	−0.2012 (3)	−0.12320 (18)	0.0258 (6)
C11	−0.52313 (16)	−0.2589 (4)	−0.17386 (18)	0.0322 (7)
H11A	−0.547018	−0.285054	−0.146995	0.048*
H11B	−0.515815	−0.336583	−0.197729	0.048*
H11C	−0.546698	−0.192478	−0.209889	0.048*
C12	−0.3541 (2)	−0.2594 (6)	0.0753 (2)	0.0541 (12)
H12A	−0.323563	−0.329840	0.082306	0.081*
H12B	−0.389126	−0.294807	0.083429	0.081*
H12C	−0.334203	−0.187465	0.109331	0.081*
C13	0.04032 (16)	0.2193 (4)	0.17412 (18)	0.0316 (7)
H13A	0.069539	0.295146	0.187002	0.038*
H13B	0.065092	0.137904	0.178904	0.038*
C14	−0.00517 (15)	0.2337 (3)	0.09721 (17)	0.0253 (6)
C15	−0.03435 (18)	0.1238 (4)	0.0575 (2)	0.0372 (8)
H15	−0.024141	0.038632	0.078874	0.045*
C16	−0.0783 (2)	0.1349 (5)	−0.0130 (2)	0.0474 (10)
H16	−0.097970	0.058061	−0.039592	0.057*
C17	−0.0931 (2)	0.2581 (6)	−0.0441 (2)	0.0494 (11)
H17	−0.124052	0.267139	−0.091927	0.059*
C18	−0.06295 (19)	0.3685 (4)	−0.0056 (2)	0.0436 (10)
H18	−0.071962	0.453215	−0.027685	0.052*
C19	−0.01989 (18)	0.3569 (4)	0.06461 (19)	0.0346 (8)
H19	−0.000091	0.433880	0.090941	0.042*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01201 (14)	0.02281 (16)	0.01816 (14)	0.000	0.00244 (10)	0.000
O1	0.0133 (10)	0.0248 (11)	0.0282 (10)	−0.0007 (8)	0.0008 (8)	−0.0012 (9)
O2	0.0183 (10)	0.0220 (11)	0.0292 (11)	−0.0009 (8)	0.0057 (9)	−0.0012 (9)
O3	0.039 (2)	0.0160 (15)	0.0325 (18)	0.000	−0.0025 (16)	0.000
O10	0.0229 (11)	0.0344 (13)	0.0259 (11)	−0.0022 (10)	0.0030 (9)	0.0022 (10)
N1	0.0153 (12)	0.0317 (14)	0.0215 (12)	−0.0003 (10)	0.0002 (10)	0.0034 (11)
C1	0.0156 (13)	0.0229 (14)	0.0236 (13)	−0.0010 (11)	0.0067 (11)	−0.0015 (11)
C2	0.0161 (13)	0.0283 (15)	0.0198 (12)	−0.0009 (11)	0.0052 (11)	−0.0017 (11)
C3	0.0141 (13)	0.0286 (15)	0.0240 (13)	0.0037 (11)	0.0033 (11)	−0.0021 (12)
C4	0.0204 (14)	0.0228 (15)	0.0304 (15)	−0.0019 (12)	0.0061 (12)	−0.0057 (13)
C5	0.0158 (13)	0.0309 (16)	0.0211 (13)	−0.0027 (11)	0.0050 (11)	−0.0020 (12)
C6	0.0139 (13)	0.0311 (16)	0.0294 (15)	0.0016 (12)	0.0034 (12)	0.0091 (13)
C7	0.0212 (15)	0.0269 (15)	0.0294 (15)	−0.0012 (12)	0.0055 (12)	0.0051 (13)
C8	0.0205 (15)	0.0376 (18)	0.0271 (15)	−0.0012 (13)	0.0079 (12)	0.0009 (13)
C9	0.0209 (15)	0.0276 (14)	0.0288 (15)	−0.0022 (12)	0.0089 (12)	0.0002 (13)
C10	0.0190 (14)	0.0257 (15)	0.0282 (15)	0.0012 (12)	0.0057 (12)	−0.0040 (12)
C11	0.0206 (16)	0.0419 (19)	0.0277 (16)	−0.0037 (14)	0.0039 (13)	−0.0031 (14)
C12	0.032 (2)	0.091 (3)	0.0306 (19)	−0.021 (2)	0.0044 (16)	0.017 (2)
C13	0.0213 (15)	0.046 (2)	0.0287 (16)	−0.0012 (14)	0.0116 (13)	−0.0015 (14)
C14	0.0218 (15)	0.0290 (17)	0.0265 (15)	0.0010 (12)	0.0118 (12)	−0.0011 (12)
C15	0.045 (2)	0.0318 (18)	0.0383 (18)	−0.0037 (16)	0.0206 (17)	−0.0007 (16)
C16	0.046 (2)	0.062 (3)	0.0314 (18)	−0.016 (2)	0.0139 (17)	−0.0117 (19)
C17	0.034 (2)	0.086 (3)	0.0244 (17)	0.008 (2)	0.0086 (15)	0.003 (2)
C18	0.047 (2)	0.050 (2)	0.042 (2)	0.0243 (19)	0.0264 (18)	0.0200 (19)
C19	0.043 (2)	0.0318 (19)	0.0389 (18)	0.0051 (15)	0.0266 (17)	0.0031 (15)

Geometric parameters (Å, º)

Sn1—O1	2.257 (2)	C9—C10	1.425 (5)
Sn1—O2	2.348 (2)	C9—H9	0.9500
Sn1—O3	2.337 (3)	C10—C11	1.504 (4)
Sn1—C13	2.150 (3)	C11—H11A	0.9800
O1—C1	1.274 (4)	C11—H11B	0.9800
O2—C1	1.273 (4)	C11—H11C	0.9800
O3—H3	0.838 (7)	C12—H12A	0.9800
O10—C10	1.248 (4)	C12—H12B	0.9800
N1—C5	1.421 (4)	C12—H12C	0.9800
N1—C8	1.327 (4)	C13—C14	1.498 (5)
N1—H1	0.82 (4)	C13—H13A	0.9900
C1—C2	1.489 (4)	C13—H13B	0.9900
C2—C7	1.389 (4)	C14—C15	1.378 (5)
C2—C3	1.391 (4)	C14—C19	1.388 (5)
C3—C4	1.382 (4)	C15—C16	1.386 (5)
C3—H3A	0.9500	C15—H15	0.9500
C4—C5	1.390 (4)	C16—C17	1.376 (7)

C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.397 (5)	C17—C18	1.380 (7)
C6—C7	1.385 (4)	C17—H17	0.9500
C6—H6	0.9500	C18—C19	1.376 (5)
C7—H7	0.9500	C18—H18	0.9500
C8—C9	1.378 (5)	C19—H19	0.9500
C8—C12	1.505 (5)		

O1—Sn1—O1^{i}	78.94 (11)	C9—C8—C12	119.9 (3)
O1—Sn1—O2	57.26 (8)	C8—C9—C10	123.8 (3)
O1—Sn1—O2^{i}	136.18 (8)	C8—C9—H9	118.1
O1—Sn1—O3	140.53 (5)	C10—C9—H9	118.1
O1—Sn1—C13	93.73 (11)	O10—C10—C9	122.5 (3)
O1—Sn1—C13^{i}	90.36 (11)	O10—C10—C11	119.6 (3)
O2—Sn1—O2^{i}	166.56 (11)	C9—C10—C11	117.8 (3)
O2—Sn1—O3	83.28 (6)	C10—C11—H11A	109.5
O2—Sn1—C13	93.61 (11)	C10—C11—H11B	109.5
O2—Sn1—C13^{i}	85.77 (11)	H11A—C11—H11B	109.5
O3—Sn1—C13	87.35 (10)	C10—C11—H11C	109.5
C13—Sn1—C13^{i}	174.7 (2)	H11A—C11—H11C	109.5
C1—O1—Sn1	93.31 (18)	H11B—C11—H11C	109.5
C1—O2—Sn1	89.18 (17)	C8—C12—H12A	109.5
Sn1—O3—H3	115 (3)	C8—C12—H12B	109.5
Sn1—O3—H3^{i}	115 (3)	H12A—C12—H12B	109.5
H3—O3—H3^{i}	130 (7)	C8—C12—H12C	109.5
C8—N1—C5	128.6 (3)	H12A—C12—H12C	109.5
C8—N1—H1	120 (3)	H12B—C12—H12C	109.5
C5—N1—H1	111 (3)	C14—C13—Sn1	115.6 (2)
O2—C1—O1	120.1 (3)	C14—C13—H13A	108.4
O2—C1—C2	121.1 (3)	Sn1—C13—H13A	108.4
O1—C1—C2	118.7 (3)	C14—C13—H13B	108.4
C7—C2—C3	119.8 (3)	Sn1—C13—H13B	108.4
C7—C2—C1	119.8 (3)	H13A—C13—H13B	107.4
C3—C2—C1	120.4 (3)	C15—C14—C19	118.4 (3)
C4—C3—C2	120.4 (3)	C15—C14—C13	120.3 (3)
C4—C3—H3A	119.8	C19—C14—C13	121.3 (3)
C2—C3—H3A	119.8	C14—C15—C16	121.4 (4)
C3—C4—C5	119.9 (3)	C14—C15—H15	119.3
C3—C4—H4	120.1	C16—C15—H15	119.3
C5—C4—H4	120.1	C17—C16—C15	119.4 (4)
C4—C5—C6	120.0 (3)	C17—C16—H16	120.3
C4—C5—N1	122.5 (3)	C15—C16—H16	120.3
C6—C5—N1	117.4 (3)	C16—C17—C18	119.7 (4)
C7—C6—C5	119.8 (3)	C16—C17—H17	120.1
C7—C6—H6	120.1	C18—C17—H17	120.1
C5—C6—H6	120.1	C19—C18—C17	120.5 (4)
C6—C7—C2	120.2 (3)	C19—C18—H18	119.7
C6—C7—H7	119.9	C17—C18—H18	119.7

C2—C7—H7	119.9	C18—C19—C14	120.5 (4)
N1—C8—C9	120.8 (3)	C18—C19—H19	119.8
N1—C8—C12	119.4 (3)	C14—C19—H19	119.8
Sn1—O2—C1—O1	−3.3 (3)	C3—C2—C7—C6	0.5 (5)
Sn1—O2—C1—C2	175.1 (2)	C1—C2—C7—C6	−177.9 (3)
Sn1—O1—C1—O2	3.4 (3)	C5—N1—C8—C9	179.5 (3)
Sn1—O1—C1—C2	−175.0 (2)	C5—N1—C8—C12	0.6 (6)
O2—C1—C2—C7	3.5 (4)	N1—C8—C9—C10	−0.6 (5)
O1—C1—C2—C7	−178.1 (3)	C12—C8—C9—C10	178.2 (4)
O2—C1—C2—C3	−174.9 (3)	C8—C9—C10—O10	−1.2 (5)
O1—C1—C2—C3	3.5 (4)	C8—C9—C10—C11	177.5 (3)
C7—C2—C3—C4	−0.7 (5)	Sn1—C13—C14—C15	−83.5 (4)
C1—C2—C3—C4	177.7 (3)	Sn1—C13—C14—C19	95.3 (3)
C2—C3—C4—C5	0.3 (5)	C19—C14—C15—C16	−1.2 (5)
C3—C4—C5—C6	0.3 (5)	C13—C14—C15—C16	177.7 (3)
C3—C4—C5—N1	177.4 (3)	C14—C15—C16—C17	0.0 (6)
C8—N1—C5—C4	51.0 (5)	C15—C16—C17—C18	1.8 (6)
C8—N1—C5—C6	−131.8 (4)	C16—C17—C18—C19	−2.6 (6)
C4—C5—C6—C7	−0.6 (5)	C17—C18—C19—C14	1.4 (5)
N1—C5—C6—C7	−177.8 (3)	C15—C14—C19—C18	0.4 (5)
C5—C6—C7—C2	0.2 (5)	C13—C14—C19—C18	−178.4 (3)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O10	0.82 (4)	2.01 (4)	2.631 (3)	132 (4)
O3—H3···O10^{ii}	0.84 (1)	1.95 (2)	2.712 (3)	151 (4)

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

Octabutyltetrakis{μ-(*E*)-4-[(4-hydroxy-3,5-dimethylphenyl)diazenyl]benzoato}di-μ_3-oxido-tetratin(IV) ethanol disolvate (IV)

Crystal data

$[Sn_4(C_4H_9)_8(C_{15}H_{13}N_2O_3)_4O_2]\cdot 2C_2H_6O$	$F(000) = 2192$
$M_r = 2132.88$	$D_x = 1.422$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$a = 11.8395$ (1) Å	Cell parameters from 171311 reflections
$b = 24.2855$ (3) Å	$\theta = 2.0$–$27.5°$
$c = 17.3557$ (2) Å	$\mu = 1.06$ mm^{-1}
$\beta = 93.2962$ (7)°	$T = 160$ K
$V = 4982.00$ (9) Å^3	Tablet, orange
$Z = 2$	0.35 × 0.20 × 0.15 mm

Data collection

Nonius KappaCCD area detector diffractometer
Radiation source: Nonius FR590 sealed tube generator
Horizontally mounted graphite crystal monochromator
Detector resolution: 9 pixels mm^{-1}
φ and ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995)
T_{min} = 0.829, T_{max} = 0.922
94026 measured reflections
11376 independent reflections
9553 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 2.1°
h = −15→15
k = −31→31
l = −22→22

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.077
S = 1.04
11371 reflections
628 parameters
144 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 6.8029P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}

Special details

Experimental. Data collection and full structure determination done by Prof. Anthony Linden: anthony.linden@chem.uzh.ch
Solvent used: toluene Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: on a glass fibre Mosaicity (deg.): 0.746 (1) Frames collected: 718 Seconds exposure per frame: 60 Degrees rotation per frame: 1.0 Crystal-detector distance (mm): 38.0 Client: Tushar Basu-Baul Sample code: TSBB-304 (L1014)

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

Refinement. The Sn-complex molecule sits across a crystallographic centre of inversion and the asymmetric includes a molecule of EtOH. Two butyl groups at the same Sn atom are disordered over two conformations. Two sets of overlapping positions were defined for the atoms of one methylene group in one ligand and for all atoms of the other disordered butyl group and the site occupation factors of the major conformations of these groups refined to 0.846 (6) and 0.683 (5), respectively. Similarity restraints were applied to the chemically equivalent bond lengths and angles involving all disordered C-atoms, while neighbouring atoms within and between each conformation of the disordered butyl groups were restrained to have similar atomic displacement parameters.

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

	x	y	z	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.05001 (2)	0.37049 (2)	0.45148 (2)	0.03285 (6)	
Sn2	0.08779 (2)	0.52372 (2)	0.43610 (2)	0.02578 (5)	
O1	0.19192 (17)	0.47981 (8)	0.34877 (12)	0.0416 (5)	
O2	0.1733 (3)	0.39106 (10)	0.36369 (17)	0.0832 (10)	
O3	0.86222 (19)	0.39724 (10)	−0.16369 (12)	0.0469 (5)	
H3	0.893 (3)	0.3655 (15)	−0.159 (2)	0.055 (11)*	
O4	−0.07448 (14)	0.36432 (7)	0.53976 (10)	0.0289 (4)	
O5	−0.06043 (16)	0.27469 (8)	0.51891 (12)	0.0375 (4)	

O6	−0.96252 (16)	0.32178 (10)	0.86854 (13)	0.0446 (5)
H6	−0.966 (3)	0.3262 (17)	0.921 (2)	0.076 (13)*
O7	0.02343 (14)	0.45122 (7)	0.47392 (10)	0.0263 (4)
N1	0.49994 (19)	0.38861 (10)	0.08500 (13)	0.0346 (5)
N2	0.5496 (2)	0.42950 (10)	0.05843 (13)	0.0366 (5)
N3	−0.52091 (18)	0.28868 (10)	0.69716 (13)	0.0356 (5)
N4	−0.53547 (19)	0.31997 (11)	0.75336 (13)	0.0377 (5)
C1	0.2124 (2)	0.43154 (13)	0.33106 (16)	0.0367 (6)
C2	0.2894 (2)	0.42124 (12)	0.26719 (15)	0.0342 (6)
C3	0.3003 (3)	0.36865 (13)	0.23750 (18)	0.0438 (7)
H31	0.260555	0.338821	0.258794	0.053*
C4	0.3693 (3)	0.35950 (13)	0.17654 (17)	0.0413 (7)
H4	0.375730	0.323563	0.155619	0.050*
C5	0.4283 (2)	0.40272 (12)	0.14652 (15)	0.0330 (6)
C6	0.4202 (2)	0.45534 (13)	0.17723 (16)	0.0384 (6)
H61	0.462926	0.484808	0.157705	0.046*
C7	0.3490 (2)	0.46434 (12)	0.23667 (16)	0.0375 (6)
H7	0.341064	0.500458	0.256670	0.045*
C8	0.6245 (2)	0.41710 (12)	−0.00080 (15)	0.0335 (6)
C9	0.6373 (2)	0.36544 (12)	−0.03379 (14)	0.0323 (6)
H9	0.591369	0.335693	−0.018730	0.039*
C10	0.7166 (2)	0.35691 (12)	−0.08854 (15)	0.0338 (6)
C11	0.7829 (2)	0.40186 (12)	−0.10944 (15)	0.0347 (6)
C12	0.7715 (2)	0.45410 (12)	−0.07742 (16)	0.0372 (6)
C13	0.6898 (2)	0.46103 (12)	−0.02381 (16)	0.0376 (6)
H13	0.678300	0.496499	−0.002518	0.045*
C14	−0.1081 (2)	0.31416 (11)	0.54896 (14)	0.0290 (5)
C15	−0.2107 (2)	0.30627 (11)	0.59369 (14)	0.0282 (5)
C16	−0.2756 (2)	0.25913 (11)	0.58262 (15)	0.0331 (6)
H16	−0.250333	0.230332	0.550798	0.040*
C17	−0.3774 (2)	0.25384 (12)	0.61792 (16)	0.0353 (6)
H17	−0.423231	0.222120	0.608842	0.042*
C18	−0.4119 (2)	0.29533 (11)	0.66666 (15)	0.0317 (6)
C19	−0.3446 (2)	0.34171 (11)	0.68061 (16)	0.0339 (6)
H19	−0.366960	0.369375	0.715311	0.041*
C20	−0.2452 (2)	0.34710 (12)	0.64359 (16)	0.0335 (6)
H20	−0.199796	0.378994	0.652214	0.040*
C21	−0.6464 (2)	0.31876 (12)	0.78052 (16)	0.0353 (6)
C22	−0.7403 (2)	0.29662 (12)	0.73911 (15)	0.0342 (6)
H22	−0.731344	0.279902	0.690359	0.041*
C23	−0.8464 (2)	0.29884 (12)	0.76852 (15)	0.0341 (6)
C24	−0.8561 (2)	0.32229 (12)	0.84176 (16)	0.0340 (6)
C25	−0.7646 (2)	0.34633 (12)	0.88293 (16)	0.0367 (6)
C26	−0.6596 (2)	0.34449 (13)	0.85090 (16)	0.0384 (6)
H26	−0.595981	0.361054	0.877554	0.046*
C27	0.7332 (3)	0.30115 (12)	−0.12382 (17)	0.0417 (7)
H271	0.805858	0.285805	−0.104178	0.063*
H272	0.732898	0.304692	−0.180080	0.063*

H273	0.671797	0.276597	−0.110190	0.063*	
C28	0.8491 (3)	0.50027 (14)	−0.0985 (2)	0.0493 (8)	
H281	0.925568	0.493058	−0.076133	0.074*	
H282	0.821345	0.535095	−0.078167	0.074*	
H283	0.850778	0.502670	−0.154743	0.074*	
C29	−0.9499 (2)	0.27881 (15)	0.72325 (18)	0.0467 (8)	
H291	−1.002889	0.309436	0.714349	0.070*	
H292	−0.986017	0.249706	0.752224	0.070*	
H293	−0.928331	0.264165	0.673558	0.070*	
C30	−0.7776 (3)	0.37509 (15)	0.95911 (19)	0.0510 (8)	
H301	−0.837317	0.402949	0.952971	0.076*	
H302	−0.706064	0.392894	0.975839	0.076*	
H303	−0.797867	0.348070	0.997917	0.076*	
C31	−0.0504 (3)	0.33948 (15)	0.35816 (19)	0.0621 (10)	
H311	−0.019966	0.354021	0.310265	0.074*	0.846 (6)
H312	−0.040346	0.299023	0.357445	0.074*	0.846 (6)
H313	0.003673	0.319310	0.327125	0.074*	0.154 (6)
H314	−0.097015	0.310760	0.381464	0.074*	0.154 (6)
C32A	−0.1746 (3)	0.35092 (16)	0.35450 (19)	0.0482 (10)	0.846 (6)
H321	−0.186547	0.390964	0.360917	0.058*	0.846 (6)
H322	−0.208716	0.331909	0.397941	0.058*	0.846 (6)
C32B	−0.1307 (9)	0.3665 (5)	0.2985 (9)	0.048 (3)	0.154 (6)
H323	−0.154143	0.402744	0.318202	0.057*	0.154 (6)
H324	−0.090353	0.372993	0.250881	0.057*	0.154 (6)
C33	−0.2352 (3)	0.33224 (16)	0.2787 (2)	0.0650 (10)	
H331	−0.207086	0.353506	0.235028	0.078*	0.846 (6)
H332	−0.220096	0.292717	0.269771	0.078*	0.846 (6)
H333	−0.227730	0.322244	0.223896	0.078*	0.154 (6)
H334	−0.220917	0.297728	0.308001	0.078*	0.154 (6)
C34	−0.3584 (4)	0.34142 (18)	0.2837 (3)	0.0750 (12)	
H341	−0.384999	0.321324	0.328195	0.112*	
H342	−0.398658	0.328149	0.236420	0.112*	
H343	−0.372987	0.380847	0.289956	0.112*	
C35A	0.1923 (5)	0.3365 (3)	0.5137 (3)	0.0520 (11)	0.683 (5)
H351	0.256182	0.362739	0.512478	0.062*	0.683 (5)
H352	0.174183	0.331603	0.568242	0.062*	0.683 (5)
C36A	0.2283 (3)	0.28175 (18)	0.4817 (3)	0.0561 (11)	0.683 (5)
H361	0.215317	0.282017	0.424886	0.067*	0.683 (5)
H362	0.181177	0.252161	0.502419	0.067*	0.683 (5)
C37A	0.3522 (3)	0.2694 (2)	0.5023 (3)	0.0584 (11)	0.683 (5)
H371	0.368956	0.277667	0.557674	0.070*	0.683 (5)
H372	0.366059	0.229671	0.494476	0.070*	0.683 (5)
C38A	0.4320 (5)	0.3023 (3)	0.4547 (4)	0.0740 (14)	0.683 (5)
H381	0.414469	0.295236	0.399770	0.111*	0.683 (5)
H382	0.510245	0.291322	0.468471	0.111*	0.683 (5)
H383	0.422915	0.341678	0.465264	0.111*	0.683 (5)
C35B	0.1813 (8)	0.3411 (7)	0.5291 (5)	0.0499 (18)	0.317 (5)
H353	0.180419	0.365466	0.574715	0.060*	0.317 (5)

H354	0.155412	0.304566	0.546319	0.060*	0.317 (5)
C36B	0.3053 (7)	0.3336 (4)	0.5138 (6)	0.0556 (13)	0.317 (5)
H363	0.335371	0.368597	0.493995	0.067*	0.317 (5)
H364	0.348202	0.324812	0.562901	0.067*	0.317 (5)
C37B	0.3229 (7)	0.2882 (5)	0.4560 (7)	0.0624 (14)	0.317 (5)
H373	0.268332	0.293180	0.411172	0.075*	0.317 (5)
H374	0.306460	0.252346	0.480111	0.075*	0.317 (5)
C38B	0.4416 (9)	0.2867 (6)	0.4277 (9)	0.069 (2)	0.317 (5)
H384	0.455717	0.320455	0.398989	0.104*	0.317 (5)
H385	0.449236	0.254724	0.393922	0.104*	0.317 (5)
H386	0.496459	0.283802	0.472014	0.104*	0.317 (5)
C39	−0.0139 (2)	0.55226 (11)	0.33912 (15)	0.0341 (6)	
H391	−0.063498	0.582067	0.356541	0.041*	
H392	0.036437	0.568497	0.301596	0.041*	
C40	−0.0874 (3)	0.50922 (12)	0.29784 (17)	0.0408 (7)	
H401	−0.136548	0.491785	0.335113	0.049*	
H402	−0.038530	0.480228	0.277378	0.049*	
C41	−0.1604 (3)	0.53376 (16)	0.2320 (2)	0.0556 (9)	
H411	−0.204804	0.564561	0.252264	0.067*	
H412	−0.110612	0.549153	0.193499	0.067*	
C42	−0.2410 (4)	0.4931 (2)	0.1921 (3)	0.0872 (15)	
H421	−0.197718	0.464150	0.167801	0.131*	
H422	−0.288684	0.512244	0.152600	0.131*	
H423	−0.288924	0.476569	0.230118	0.131*	
C43	0.2440 (2)	0.53863 (12)	0.49912 (17)	0.0366 (6)	
H431	0.296430	0.556690	0.464588	0.044*	
H432	0.230664	0.564508	0.541729	0.044*	
C44	0.3002 (2)	0.48697 (13)	0.53277 (18)	0.0417 (7)	
H441	0.244056	0.465861	0.560869	0.050*	
H442	0.324509	0.463603	0.490002	0.050*	
C45	0.4017 (3)	0.49905 (16)	0.5872 (2)	0.0636 (10)	
H451	0.377820	0.522706	0.629762	0.076*	
H452	0.458541	0.519662	0.559023	0.076*	
C46	0.4560 (4)	0.44683 (19)	0.6211 (3)	0.0981 (18)	
H461	0.400622	0.426645	0.649966	0.147*	
H462	0.521129	0.456675	0.655762	0.147*	
H463	0.481311	0.423588	0.579210	0.147*	
O8	−0.0246 (2)	0.16675 (10)	0.50888 (14)	0.0595 (7)	
H8	−0.032 (4)	0.2013 (19)	0.528 (3)	0.084 (14)*	
C47	−0.0545 (3)	0.12520 (15)	0.5618 (2)	0.0549 (9)	
H471	−0.040073	0.088507	0.539589	0.066*	
H472	−0.136335	0.127863	0.570249	0.066*	
C48	0.0098 (4)	0.13068 (18)	0.6355 (2)	0.0752 (12)	
H481	−0.010756	0.165217	0.660340	0.113*	
H482	0.090894	0.130889	0.626875	0.113*	
H483	−0.007377	0.099619	0.668940	0.113*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03794 (11)	0.02823 (10)	0.03422 (10)	0.00428 (8)	0.01800 (8)	0.00162 (7)
Sn2	0.02240 (9)	0.02967 (10)	0.02597 (9)	0.00093 (7)	0.00740 (6)	0.00225 (7)
O1	0.0458 (12)	0.0420 (12)	0.0398 (11)	0.0046 (9)	0.0260 (9)	−0.0031 (9)
O2	0.117 (2)	0.0470 (13)	0.0948 (19)	0.0125 (14)	0.0868 (18)	0.0092 (13)
O3	0.0464 (13)	0.0545 (14)	0.0422 (12)	0.0101 (11)	0.0240 (10)	0.0074 (10)
O4	0.0293 (9)	0.0298 (9)	0.0285 (9)	−0.0024 (7)	0.0102 (7)	−0.0004 (7)
O5	0.0395 (11)	0.0287 (10)	0.0460 (11)	−0.0028 (8)	0.0171 (9)	−0.0038 (8)
O6	0.0283 (10)	0.0646 (14)	0.0419 (12)	0.0000 (9)	0.0122 (9)	−0.0002 (11)
O7	0.0267 (9)	0.0238 (8)	0.0297 (9)	0.0022 (7)	0.0121 (7)	0.0017 (7)
N1	0.0319 (12)	0.0415 (13)	0.0315 (12)	0.0047 (10)	0.0104 (9)	0.0013 (10)
N2	0.0360 (12)	0.0425 (13)	0.0322 (12)	0.0065 (10)	0.0110 (10)	0.0002 (10)
N3	0.0277 (11)	0.0430 (13)	0.0371 (12)	−0.0018 (10)	0.0099 (9)	0.0032 (10)
N4	0.0294 (12)	0.0519 (15)	0.0326 (12)	−0.0011 (10)	0.0089 (9)	0.0018 (11)
C1	0.0348 (14)	0.0470 (17)	0.0294 (14)	0.0086 (13)	0.0121 (11)	0.0071 (12)
C2	0.0327 (14)	0.0431 (16)	0.0277 (13)	0.0094 (12)	0.0105 (11)	0.0047 (11)
C3	0.0462 (17)	0.0426 (17)	0.0451 (17)	0.0056 (14)	0.0238 (14)	0.0059 (13)
C4	0.0438 (16)	0.0405 (16)	0.0413 (16)	0.0053 (13)	0.0180 (13)	−0.0039 (13)
C5	0.0302 (13)	0.0425 (16)	0.0270 (13)	0.0063 (11)	0.0079 (10)	0.0000 (11)
C6	0.0364 (15)	0.0445 (16)	0.0355 (15)	−0.0003 (12)	0.0134 (12)	0.0005 (12)
C7	0.0372 (15)	0.0418 (16)	0.0348 (15)	0.0017 (12)	0.0130 (12)	−0.0048 (12)
C8	0.0327 (14)	0.0411 (15)	0.0276 (13)	0.0075 (12)	0.0092 (10)	0.0024 (11)
C9	0.0327 (14)	0.0401 (15)	0.0245 (12)	0.0025 (11)	0.0046 (10)	0.0043 (11)
C10	0.0334 (14)	0.0407 (15)	0.0275 (13)	0.0070 (12)	0.0045 (11)	0.0003 (11)
C11	0.0314 (13)	0.0490 (17)	0.0246 (13)	0.0082 (12)	0.0089 (10)	0.0057 (11)
C12	0.0353 (15)	0.0427 (16)	0.0344 (15)	0.0014 (12)	0.0088 (12)	0.0054 (12)
C13	0.0429 (16)	0.0367 (15)	0.0340 (15)	0.0050 (12)	0.0100 (12)	0.0006 (12)
C14	0.0286 (13)	0.0303 (14)	0.0281 (13)	0.0011 (10)	0.0027 (10)	0.0004 (10)
C15	0.0235 (12)	0.0332 (13)	0.0282 (12)	−0.0014 (10)	0.0049 (10)	0.0046 (10)
C16	0.0314 (13)	0.0361 (14)	0.0326 (14)	−0.0020 (11)	0.0079 (11)	−0.0030 (11)
C17	0.0290 (13)	0.0386 (15)	0.0391 (15)	−0.0074 (11)	0.0077 (11)	0.0001 (12)
C18	0.0252 (12)	0.0385 (15)	0.0319 (13)	−0.0009 (11)	0.0065 (10)	0.0052 (11)
C19	0.0329 (14)	0.0369 (15)	0.0328 (14)	0.0008 (11)	0.0101 (11)	−0.0012 (11)
C20	0.0295 (13)	0.0356 (14)	0.0361 (14)	−0.0038 (11)	0.0090 (11)	0.0026 (11)
C21	0.0251 (13)	0.0464 (16)	0.0352 (14)	−0.0003 (12)	0.0082 (11)	0.0027 (12)
C22	0.0321 (14)	0.0412 (15)	0.0298 (13)	−0.0002 (12)	0.0060 (11)	0.0004 (11)
C23	0.0284 (13)	0.0419 (15)	0.0320 (14)	−0.0010 (11)	0.0026 (11)	0.0068 (12)
C24	0.0261 (13)	0.0413 (15)	0.0353 (14)	0.0022 (11)	0.0090 (11)	0.0056 (12)
C25	0.0324 (14)	0.0448 (16)	0.0338 (14)	0.0005 (12)	0.0077 (11)	−0.0002 (12)
C26	0.0313 (14)	0.0508 (17)	0.0333 (14)	−0.0026 (12)	0.0044 (11)	0.0001 (13)
C27	0.0492 (17)	0.0429 (16)	0.0339 (15)	0.0047 (13)	0.0108 (13)	−0.0043 (12)
C28	0.0472 (18)	0.0511 (19)	0.0510 (19)	−0.0071 (15)	0.0144 (15)	0.0035 (15)
C29	0.0358 (16)	0.066 (2)	0.0387 (16)	−0.0102 (15)	0.0038 (12)	0.0011 (15)
C30	0.0418 (17)	0.069 (2)	0.0424 (17)	−0.0033 (16)	0.0095 (14)	−0.0133 (16)
C31	0.097 (3)	0.052 (2)	0.0355 (17)	0.006 (2)	−0.0037 (18)	−0.0078 (15)
C32A	0.066 (3)	0.043 (2)	0.0354 (19)	−0.0070 (18)	0.0004 (17)	−0.0079 (16)

C32B	0.064 (5)	0.045 (5)	0.034 (5)	−0.008 (5)	−0.001 (5)	−0.006 (5)
C33	0.077 (3)	0.049 (2)	0.067 (2)	0.0024 (19)	−0.014 (2)	−0.0099 (18)
C34	0.082 (3)	0.066 (3)	0.074 (3)	0.006 (2)	−0.023 (2)	−0.011 (2)
C35A	0.0279 (19)	0.040 (2)	0.089 (3)	0.0098 (17)	0.006 (2)	0.000 (2)
C36A	0.0394 (19)	0.047 (2)	0.082 (3)	0.0142 (17)	0.0011 (19)	−0.007 (2)
C37A	0.043 (2)	0.059 (2)	0.074 (3)	0.0158 (18)	0.0034 (19)	−0.009 (2)
C38A	0.059 (2)	0.078 (3)	0.085 (4)	0.015 (2)	0.003 (3)	−0.002 (3)
C35B	0.027 (3)	0.035 (3)	0.087 (4)	0.009 (3)	0.006 (3)	0.000 (3)
C36B	0.037 (2)	0.048 (3)	0.082 (3)	0.012 (2)	0.004 (2)	−0.003 (2)
C37B	0.048 (2)	0.059 (3)	0.081 (3)	0.016 (2)	0.005 (3)	−0.005 (3)
C38B	0.058 (4)	0.065 (4)	0.085 (5)	0.020 (4)	0.006 (4)	−0.009 (4)
C39	0.0365 (14)	0.0352 (15)	0.0304 (14)	0.0007 (12)	−0.0008 (11)	0.0057 (11)
C40	0.0456 (17)	0.0414 (16)	0.0350 (15)	−0.0039 (13)	−0.0025 (12)	−0.0002 (12)
C41	0.059 (2)	0.065 (2)	0.0413 (18)	−0.0038 (17)	−0.0136 (16)	0.0034 (16)
C42	0.090 (3)	0.102 (4)	0.065 (3)	−0.020 (3)	−0.034 (2)	−0.004 (3)
C43	0.0253 (13)	0.0379 (15)	0.0464 (16)	−0.0003 (11)	0.0001 (11)	−0.0015 (12)
C44	0.0316 (14)	0.0448 (17)	0.0478 (17)	0.0073 (12)	−0.0052 (12)	−0.0026 (13)
C45	0.048 (2)	0.060 (2)	0.080 (3)	0.0170 (17)	−0.0227 (18)	−0.016 (2)
C46	0.089 (3)	0.079 (3)	0.118 (4)	0.034 (3)	−0.063 (3)	−0.017 (3)
O8	0.0842 (18)	0.0429 (13)	0.0552 (15)	0.0171 (12)	0.0370 (13)	0.0126 (11)
C47	0.060 (2)	0.054 (2)	0.051 (2)	0.0039 (17)	0.0091 (16)	0.0125 (16)
C48	0.091 (3)	0.073 (3)	0.062 (3)	−0.001 (2)	0.006 (2)	−0.010 (2)

Geometric parameters (Å, º)

Sn1—O2	2.227 (2)	C30—H302	0.9800
Sn1—O4	2.1914 (16)	C30—H303	0.9800
Sn1—O5	2.9442 (18)	C31—C32A	1.494 (4)
Sn1—O7	2.0270 (16)	C31—C32B	1.515 (5)
Sn1—C31	2.094 (3)	C31—H311	0.9900
Sn1—C35A	2.115 (4)	C31—H312	0.9900
Sn1—C35B	2.121 (5)	C31—H313	0.9900
Sn2—O1	2.2736 (18)	C31—H314	0.9900
Sn2—O4^{i}	2.7571 (18)	C32A—C33	1.531 (3)
Sn2—O7	2.0418 (16)	C32A—H321	0.9900
Sn2—O7^{i}	2.1864 (16)	C32A—H322	0.9900
Sn2—C39	2.128 (3)	C32B—C33	1.514 (5)
Sn2—C43	2.125 (3)	C32B—H323	0.9900
O1—C1	1.239 (3)	C32B—H324	0.9900
O2—C1	1.237 (4)	C33—C34	1.484 (6)
O3—C11	1.372 (3)	C33—H331	0.9900
O3—H3	0.85 (4)	C33—H332	0.9900
O4—C14	1.294 (3)	C33—H333	0.9900
O5—C14	1.243 (3)	C33—H334	0.9900
O6—C24	1.368 (3)	C34—H341	0.9800
O6—H6	0.93 (4)	C34—H342	0.9800
N1—N2	1.255 (3)	C34—H343	0.9800
N1—C5	1.442 (3)	C35A—C36A	1.512 (4)

N2—C8	1.428 (3)	C35A—H351	0.9900
N3—N4	1.256 (3)	C35A—H352	0.9900
N3—C18	1.432 (3)	C36A—C37A	1.519 (4)
N4—C21	1.421 (3)	C36A—H361	0.9900
C1—C2	1.497 (3)	C36A—H362	0.9900
C2—C7	1.385 (4)	C37A—C38A	1.518 (4)
C2—C3	1.386 (4)	C37A—H371	0.9900
C3—C4	1.391 (4)	C37A—H372	0.9900
C3—H31	0.9500	C38A—H381	0.9800
C4—C5	1.380 (4)	C38A—H382	0.9800
C4—H4	0.9500	C38A—H383	0.9800
C5—C6	1.390 (4)	C35B—C36B	1.518 (5)
C6—C7	1.386 (4)	C35B—H353	0.9900
C6—H61	0.9500	C35B—H354	0.9900
C7—H7	0.9500	C36B—C37B	1.513 (4)
C8—C13	1.389 (4)	C36B—H363	0.9900
C8—C9	1.391 (4)	C36B—H364	0.9900
C9—C10	1.389 (4)	C37B—C38B	1.515 (4)
C9—H9	0.9500	C37B—H373	0.9900
C10—C11	1.404 (4)	C37B—H374	0.9900
C10—C27	1.504 (4)	C38B—H384	0.9800
C11—C12	1.395 (4)	C38B—H385	0.9800
C12—C13	1.391 (4)	C38B—H386	0.9800
C12—C28	1.508 (4)	C39—C40	1.513 (4)
C13—H13	0.9500	C39—H391	0.9900
C14—C15	1.491 (3)	C39—H392	0.9900
C15—C16	1.386 (4)	C40—C41	1.514 (4)
C15—C20	1.393 (4)	C40—H401	0.9900
C16—C17	1.390 (4)	C40—H402	0.9900
C16—H16	0.9500	C41—C42	1.513 (5)
C17—C18	1.392 (4)	C41—H411	0.9900
C17—H17	0.9500	C41—H412	0.9900
C18—C19	1.393 (4)	C42—H421	0.9800
C19—C20	1.379 (4)	C42—H422	0.9800
C19—H19	0.9500	C42—H423	0.9800
C20—H20	0.9500	C43—C44	1.521 (4)
C21—C26	1.389 (4)	C43—H431	0.9900
C21—C22	1.397 (4)	C43—H432	0.9900
C22—C23	1.383 (4)	C44—C45	1.514 (4)
C22—H22	0.9500	C44—H441	0.9900
C23—C24	1.404 (4)	C44—H442	0.9900
C23—C29	1.498 (4)	C45—C46	1.524 (5)
C24—C25	1.392 (4)	C45—H451	0.9900
C25—C26	1.392 (4)	C45—H452	0.9900
C25—C30	1.511 (4)	C46—H461	0.9800
C26—H26	0.9500	C46—H462	0.9800
C27—H271	0.9800	C46—H463	0.9800
C27—H272	0.9800	O8—C47	1.423 (4)

C27—H273	0.9800	O8—H8	0.91 (5)
C28—H281	0.9800	C47—C48	1.457 (5)
C28—H282	0.9800	C47—H471	0.9900
C28—H283	0.9800	C47—H472	0.9900
C29—H291	0.9800	C48—H481	0.9800
C29—H292	0.9800	C48—H482	0.9800
C29—H293	0.9800	C48—H483	0.9800
C30—H301	0.9800		

O2—Sn1—O4	170.96 (8)	C32A—C31—Sn1	118.7 (2)
O2—Sn1—O5	140.62 (7)	C32B—C31—Sn1	132.8 (6)
O2—Sn1—O7	91.70 (8)	C32A—C31—H311	107.6
O2—Sn1—C31	85.24 (14)	Sn1—C31—H311	107.6
O2—Sn1—C35A	84.4 (2)	C32A—C31—H312	107.6
O2—Sn1—C35B	91.4 (3)	Sn1—C31—H312	107.6
O4—Sn1—O5	48.40 (6)	H311—C31—H312	107.1
O4—Sn1—O7	79.26 (6)	C32B—C31—H313	104.0
O4—Sn1—C31	98.12 (12)	Sn1—C31—H313	104.0
O4—Sn1—C35A	99.5 (2)	C32B—C31—H314	104.0
O4—Sn1—C35B	91.8 (3)	Sn1—C31—H314	104.0
O5—Sn1—O7	127.63 (6)	H313—C31—H314	105.5
O5—Sn1—C31	77.16 (12)	C31—C32A—C33	113.1 (3)
O5—Sn1—C35A	81.2 (2)	C31—C32A—H321	109.0
O5—Sn1—C35B	78.9 (5)	C33—C32A—H321	109.0
O7—Sn1—C31	114.14 (11)	C31—C32A—H322	109.0
O7—Sn1—C35A	114.02 (18)	C33—C32A—H322	109.0
O7—Sn1—C35B	108.7 (4)	H321—C32A—H322	107.8
C31—Sn1—C35A	130.91 (17)	C33—C32B—C31	112.9 (5)
C31—Sn1—C35B	137.1 (4)	C33—C32B—H323	109.0
O1—Sn2—O4^{i}	127.00 (6)	C31—C32B—H323	109.0
O1—Sn2—O7	92.10 (7)	C33—C32B—H324	109.0
O1—Sn2—O7^{i}	168.16 (7)	C31—C32B—H324	109.0
O1—Sn2—C39	85.96 (10)	H323—C32B—H324	107.8
O1—Sn2—C43	86.21 (10)	C34—C33—C32B	134.2 (8)
O4^{i}—Sn2—O7	140.89 (6)	C34—C33—C32A	108.6 (3)
O4^{i}—Sn2—O7^{i}	64.84 (5)	C34—C33—H331	110.0
O4^{i}—Sn2—C39	76.37 (8)	C32A—C33—H331	110.0
O4^{i}—Sn2—C43	79.00 (9)	C34—C33—H332	110.0
O7—Sn2—O7^{i}	76.07 (7)	C32A—C33—H332	110.0
O7—Sn2—C39	109.29 (9)	H331—C33—H332	108.4
O7^{i}—Sn2—C39	97.91 (9)	C34—C33—H333	103.6
O7—Sn2—C43	108.14 (9)	C32B—C33—H333	103.6
O7^{i}—Sn2—C43	97.29 (9)	C34—C33—H334	103.6
C39—Sn2—C43	141.97 (11)	C32B—C33—H334	103.6
C1—O1—Sn2	136.90 (17)	H333—C33—H334	105.3
C1—O2—Sn1	140.2 (2)	C33—C34—H341	109.5
C11—O3—H3	108 (2)	C33—C34—H342	109.5
C14—O4—Sn1	112.01 (15)	H341—C34—H342	109.5

C14—O4—Sn2^{i}	152.71 (15)	C33—C34—H343	109.5
Sn1—O4—Sn2^{i}	94.90 (6)	H341—C34—H343	109.5
C14—O5—Sn1	77.29 (14)	H342—C34—H343	109.5
C24—O6—H6	116 (2)	C36A—C35A—Sn1	112.9 (3)
Sn1—O7—Sn2	135.02 (8)	C36A—C35A—H351	109.0
Sn1—O7—Sn2^{i}	120.87 (8)	Sn1—C35A—H351	109.0
Sn2—O7—Sn2^{i}	103.93 (7)	C36A—C35A—H352	109.0
N2—N1—C5	113.1 (2)	Sn1—C35A—H352	109.0
N1—N2—C8	114.9 (2)	H351—C35A—H352	107.8
N4—N3—C18	112.7 (2)	C35A—C36A—C37A	112.1 (4)
N3—N4—C21	114.6 (2)	C35A—C36A—H361	109.2
O2—C1—O1	123.7 (2)	C37A—C36A—H361	109.2
O2—C1—C2	117.8 (3)	C35A—C36A—H362	109.2
O1—C1—C2	118.6 (2)	C37A—C36A—H362	109.2
C7—C2—C3	119.6 (2)	H361—C36A—H362	107.9
C7—C2—C1	120.2 (3)	C38A—C37A—C36A	113.0 (5)
C3—C2—C1	120.2 (3)	C38A—C37A—H371	109.0
C2—C3—C4	120.1 (3)	C36A—C37A—H371	109.0
C2—C3—H31	120.0	C38A—C37A—H372	109.0
C4—C3—H31	120.0	C36A—C37A—H372	109.0
C5—C4—C3	119.9 (3)	H371—C37A—H372	107.8
C5—C4—H4	120.1	C37A—C38A—H381	109.5
C3—C4—H4	120.1	C37A—C38A—H382	109.5
C4—C5—C6	120.4 (2)	H381—C38A—H382	109.5
C4—C5—N1	115.5 (2)	C37A—C38A—H383	109.5
C6—C5—N1	124.0 (2)	H381—C38A—H383	109.5
C7—C6—C5	119.3 (3)	H382—C38A—H383	109.5
C7—C6—H61	120.4	C36B—C35B—Sn1	127.6 (7)
C5—C6—H61	120.4	C36B—C35B—H353	105.4
C2—C7—C6	120.7 (3)	Sn1—C35B—H353	105.4
C2—C7—H7	119.7	C36B—C35B—H354	105.4
C6—C7—H7	119.7	Sn1—C35B—H354	105.4
C13—C8—C9	119.9 (2)	H353—C35B—H354	106.0
C13—C8—N2	115.1 (2)	C37B—C36B—C35B	111.9 (5)
C9—C8—N2	125.0 (2)	C37B—C36B—H363	109.2
C10—C9—C8	120.6 (3)	C35B—C36B—H363	109.2
C10—C9—H9	119.7	C37B—C36B—H364	109.2
C8—C9—H9	119.7	C35B—C36B—H364	109.2
C9—C10—C11	118.1 (3)	H363—C36B—H364	107.9
C9—C10—C27	121.5 (3)	C36B—C37B—C38B	113.5 (6)
C11—C10—C27	120.5 (2)	C36B—C37B—H373	108.9
O3—C11—C12	115.7 (3)	C38B—C37B—H373	108.9
O3—C11—C10	121.9 (3)	C36B—C37B—H374	108.9
C12—C11—C10	122.4 (2)	C38B—C37B—H374	108.9
C13—C12—C11	117.6 (3)	H373—C37B—H374	107.7
C13—C12—C28	121.9 (3)	C37B—C38B—H384	109.5
C11—C12—C28	120.4 (3)	C37B—C38B—H385	109.5
C8—C13—C12	121.3 (3)	H384—C38B—H385	109.5

C8—C13—H13	119.4	C37B—C38B—H386	109.5
C12—C13—H13	119.4	H384—C38B—H386	109.5
O5—C14—O4	121.6 (2)	H385—C38B—H386	109.5
O5—C14—C15	121.5 (2)	C40—C39—Sn2	115.66 (19)
O4—C14—C15	116.8 (2)	C40—C39—H391	108.4
C16—C15—C20	119.6 (2)	Sn2—C39—H391	108.4
C16—C15—C14	119.7 (2)	C40—C39—H392	108.4
C20—C15—C14	120.6 (2)	Sn2—C39—H392	108.4
C15—C16—C17	120.2 (3)	H391—C39—H392	107.4
C15—C16—H16	119.9	C39—C40—C41	111.9 (3)
C17—C16—H16	119.9	C39—C40—H401	109.2
C16—C17—C18	119.6 (3)	C41—C40—H401	109.2
C16—C17—H17	120.2	C39—C40—H402	109.2
C18—C17—H17	120.2	C41—C40—H402	109.2
C17—C18—C19	120.4 (2)	H401—C40—H402	107.9
C17—C18—N3	116.4 (2)	C42—C41—C40	114.0 (3)
C19—C18—N3	123.1 (2)	C42—C41—H411	108.8
C20—C19—C18	119.4 (3)	C40—C41—H411	108.8
C20—C19—H19	120.3	C42—C41—H412	108.8
C18—C19—H19	120.3	C40—C41—H412	108.8
C19—C20—C15	120.7 (3)	H411—C41—H412	107.7
C19—C20—H20	119.6	C41—C42—H421	109.5
C15—C20—H20	119.6	C41—C42—H422	109.5
C26—C21—C22	120.0 (2)	H421—C42—H422	109.5
C26—C21—N4	115.8 (2)	C41—C42—H423	109.5
C22—C21—N4	124.1 (2)	H421—C42—H423	109.5
C23—C22—C21	120.5 (3)	H422—C42—H423	109.5
C23—C22—H22	119.7	C44—C43—Sn2	113.95 (19)
C21—C22—H22	119.7	C44—C43—H431	108.8
C22—C23—C24	118.2 (2)	Sn2—C43—H431	108.8
C22—C23—C29	121.7 (3)	C44—C43—H432	108.8
C24—C23—C29	120.0 (2)	Sn2—C43—H432	108.8
O6—C24—C25	122.3 (2)	H431—C43—H432	107.7
O6—C24—C23	115.4 (2)	C45—C44—C43	113.2 (3)
C25—C24—C23	122.2 (2)	C45—C44—H441	108.9
C26—C25—C24	117.9 (3)	C43—C44—H441	108.9
C26—C25—C30	120.2 (3)	C45—C44—H442	108.9
C24—C25—C30	121.8 (2)	C43—C44—H442	108.9
C21—C26—C25	120.9 (3)	H441—C44—H442	107.7
C21—C26—H26	119.5	C44—C45—C46	112.4 (3)
C25—C26—H26	119.5	C44—C45—H451	109.1
C10—C27—H271	109.5	C46—C45—H451	109.1
C10—C27—H272	109.5	C44—C45—H452	109.1
H271—C27—H272	109.5	C46—C45—H452	109.1
C10—C27—H273	109.5	H451—C45—H452	107.8
H271—C27—H273	109.5	C45—C46—H461	109.5
H272—C27—H273	109.5	C45—C46—H462	109.5
C12—C28—H281	109.5	H461—C46—H462	109.5

C12—C28—H282	109.5	C45—C46—H463	109.5
H281—C28—H282	109.5	H461—C46—H463	109.5
C12—C28—H283	109.5	H462—C46—H463	109.5
H281—C28—H283	109.5	C47—O8—H8	113 (3)
H282—C28—H283	109.5	O8—C47—C48	111.4 (3)
C23—C29—H291	109.5	O8—C47—H471	109.3
C23—C29—H292	109.5	C48—C47—H471	109.3
H291—C29—H292	109.5	O8—C47—H472	109.3
C23—C29—H293	109.5	C48—C47—H472	109.3
H291—C29—H293	109.5	H471—C47—H472	108.0
H292—C29—H293	109.5	C47—C48—H481	109.5
C25—C30—H301	109.5	C47—C48—H482	109.5
C25—C30—H302	109.5	H481—C48—H482	109.5
H301—C30—H302	109.5	C47—C48—H483	109.5
C25—C30—H303	109.5	H481—C48—H483	109.5
H301—C30—H303	109.5	H482—C48—H483	109.5
H302—C30—H303	109.5		

C5—N1—N2—C8	177.9 (2)	O5—C14—C15—C16	−20.6 (4)
C18—N3—N4—C21	174.0 (2)	O4—C14—C15—C16	156.1 (2)
Sn1—O2—C1—O1	6.9 (7)	O5—C14—C15—C20	162.7 (3)
Sn1—O2—C1—C2	−173.7 (3)	O4—C14—C15—C20	−20.6 (4)
Sn2—O1—C1—O2	−0.4 (5)	C20—C15—C16—C17	3.3 (4)
Sn2—O1—C1—C2	−179.79 (19)	C14—C15—C16—C17	−173.4 (2)
O2—C1—C2—C7	−170.1 (3)	C15—C16—C17—C18	−2.3 (4)
O1—C1—C2—C7	9.3 (4)	C16—C17—C18—C19	−0.5 (4)
O2—C1—C2—C3	10.8 (5)	C16—C17—C18—N3	176.2 (2)
O1—C1—C2—C3	−169.8 (3)	N4—N3—C18—C17	164.6 (2)
C7—C2—C3—C4	−1.0 (5)	N4—N3—C18—C19	−18.8 (4)
C1—C2—C3—C4	178.0 (3)	C17—C18—C19—C20	2.2 (4)
C2—C3—C4—C5	1.1 (5)	N3—C18—C19—C20	−174.3 (3)
C3—C4—C5—C6	0.6 (5)	C18—C19—C20—C15	−1.2 (4)
C3—C4—C5—N1	178.3 (3)	C16—C15—C20—C19	−1.6 (4)
N2—N1—C5—C4	178.4 (3)	C14—C15—C20—C19	175.1 (2)
N2—N1—C5—C6	−4.0 (4)	N3—N4—C21—C26	168.2 (3)
C4—C5—C6—C7	−2.2 (4)	N3—N4—C21—C22	−15.6 (4)
N1—C5—C6—C7	−179.7 (3)	C26—C21—C22—C23	−1.6 (4)
C3—C2—C7—C6	−0.6 (4)	N4—C21—C22—C23	−177.7 (3)
C1—C2—C7—C6	−179.7 (3)	C21—C22—C23—C24	−2.0 (4)
C5—C6—C7—C2	2.2 (4)	C21—C22—C23—C29	175.9 (3)
N1—N2—C8—C13	−172.6 (2)	C22—C23—C24—O6	−178.1 (2)
N1—N2—C8—C9	5.7 (4)	C29—C23—C24—O6	3.9 (4)
C13—C8—C9—C10	1.4 (4)	C22—C23—C24—C25	4.3 (4)
N2—C8—C9—C10	−176.8 (3)	C29—C23—C24—C25	−173.6 (3)
C8—C9—C10—C11	−0.1 (4)	O6—C24—C25—C26	179.7 (3)
C8—C9—C10—C27	178.9 (3)	C23—C24—C25—C26	−2.9 (4)
C9—C10—C11—O3	−179.2 (2)	O6—C24—C25—C30	−1.9 (5)
C27—C10—C11—O3	1.8 (4)	C23—C24—C25—C30	175.5 (3)

C9—C10—C11—C12	−0.1 (4)	C22—C21—C26—C25	3.1 (4)
C27—C10—C11—C12	−179.1 (3)	N4—C21—C26—C25	179.4 (3)
O3—C11—C12—C13	178.2 (3)	C24—C25—C26—C21	−0.9 (4)
C10—C11—C12—C13	−1.0 (4)	C30—C25—C26—C21	−179.3 (3)
O3—C11—C12—C28	−4.3 (4)	Sn1—C31—C32A—C33	172.7 (3)
C10—C11—C12—C28	176.6 (3)	Sn1—C31—C32B—C33	−141.5 (7)
C9—C8—C13—C12	−2.5 (4)	C31—C32B—C33—C34	120.3 (10)
N2—C8—C13—C12	175.8 (3)	C31—C32A—C33—C34	175.5 (3)
C11—C12—C13—C8	2.3 (4)	Sn1—C35A—C36A—C37A	156.1 (4)
C28—C12—C13—C8	−175.2 (3)	C35A—C36A—C37A—C38A	−75.5 (7)
Sn1—O5—C14—O4	−7.2 (2)	Sn1—C35B—C36B—C37B	−67.6 (15)
Sn1—O5—C14—C15	169.3 (2)	C35B—C36B—C37B—C38B	169.0 (12)
Sn1—O4—C14—O5	10.2 (3)	Sn2—C39—C40—C41	177.4 (2)
Sn2^{i}—O4—C14—O5	−179.9 (2)	C39—C40—C41—C42	−176.2 (3)
Sn1—O4—C14—C15	−166.49 (17)	Sn2—C43—C44—C45	−171.4 (2)
Sn2^{i}—O4—C14—C15	3.5 (5)	C43—C44—C45—C46	179.3 (4)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···O6^{ii}	0.85 (4)	2.05 (4)	2.801 (3)	146 (3)
O6—H6···O8^{iii}	0.93 (4)	1.71 (4)	2.599 (3)	159 (4)
O8—H8···O5	0.91 (5)	1.82 (5)	2.663 (3)	154 (4)

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

Octabutyltetrakis{(*E*)-3-[(2-hydroxybenzylidene)amino]propanoato}di-μ_3-oxido-tetratin(IV) (V)

Crystal data

$[Sn_4(C_4H_9)_8(C_{10}H_{10}NO_3)_4O_2]$	$Z = 2$
$M_r = 1732.41$	$F(000) = 1768$
Triclinic, $P\overline{1}$	$D_x = 1.446$ Mg m^{-3}
$a = 12.0054$ (3) Å	Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
$b = 14.7309$ (4) Å	Cell parameters from 106136 reflections
$c = 23.9132$ (6) Å	$\theta = 2.0$–$25.0°$
$\alpha = 76.3707$ (18)°	$\mu = 1.30$ mm^{-1}
$\beta = 75.5206$ (16)°	$T = 160$ K
$\gamma = 88.1609$ (16)°	Plate, yellow
$V = 3977.81$ (18) Å^3	0.25 × 0.20 × 0.05 mm

Data collection

Nonius KappaCCD area detector diffractometer	$T_{min} = 0.358$, $T_{max} = 0.537$
Radiation source: Nonius FR590 sealed tube generator	68065 measured reflections
Horizontally mounted graphite crystal monochromator	14030 independent reflections
Detector resolution: 9 pixels mm^{-1}	8004 reflections with $I > 2\sigma(I)$
φ and ω scans with κ offsets	$R_{int} = 0.107$
Absorption correction: multi-scan (SORTAV; Blessing, 1995)	$\theta_{max} = 25.0°$, $\theta_{min} = 2.0°$
	$h = -14 \rightarrow 14$
	$k = -17 \rightarrow 17$
	$l = -28 \rightarrow 28$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.046$
$wR(F^2) = 0.114$
$S = 1.02$
14030 reflections
859 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 1.4894P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.20$ e Å^{-3}
$\Delta\rho_{min} = -1.11$ e Å^{-3}

Special details

Experimental. Data collection and full structure determination done by Prof. Anthony Linden: anthony.linden@chem.uzh.ch
Solvent used: hexane / chloroform Cooling Device: Oxford Cryosystems Cryostream 700 Crystal mount: on a glass fibre Mosaicity (deg.): 0.885 (1) Frames collected: 539 Seconds exposure per frame: 16 Degrees rotation per frame: 1.1 Crystal-detector distance (mm): 33.8 Client: Tushar Basu Sample code: TSBB-71 (L0403)

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Sn1	0.38021 (3)	0.02573 (3)	0.23737 (2)	0.03287 (12)
Sn2	0.38814 (3)	0.28443 (3)	0.22852 (2)	0.03121 (12)
Sn3	0.60632 (3)	0.15581 (3)	0.26223 (2)	0.03134 (12)
Sn4	0.61477 (3)	0.41241 (3)	0.25625 (2)	0.03435 (13)
O1	0.5272 (3)	−0.0175 (3)	0.27270 (16)	0.0351 (10)
O2	0.4760 (4)	−0.1604 (3)	0.27374 (19)	0.0491 (12)
O3	0.8718 (4)	−0.0556 (3)	0.1265 (2)	0.0649 (14)
H3	0.845980	−0.084544	0.162059	0.097*
O4	0.2463 (3)	0.0988 (3)	0.19408 (17)	0.0392 (10)
O5	0.2152 (3)	0.2340 (3)	0.22109 (18)	0.0400 (10)
O6	−0.1493 (4)	0.0000 (3)	0.3391 (2)	0.0546 (12)
H6	−0.113764	0.032733	0.305975	0.082*
O7	0.4375 (3)	0.1493 (2)	0.24415 (15)	0.0324 (10)
O8	0.5543 (3)	0.2917 (2)	0.24699 (17)	0.0348 (10)
O9	0.4733 (3)	0.4609 (3)	0.21652 (17)	0.0372 (10)
O10	0.5336 (4)	0.5998 (3)	0.2193 (2)	0.0501 (12)
O11	0.1346 (4)	0.4953 (3)	0.3665 (2)	0.0639 (14)
H11	0.154235	0.528340	0.331607	0.096*
O12	0.7414 (3)	0.3336 (3)	0.30478 (17)	0.0419 (11)
O13	0.7794 (3)	0.2045 (3)	0.27115 (18)	0.0397 (10)
O14	1.1290 (4)	0.4380 (3)	0.1734 (2)	0.0595 (13)
H14	1.097150	0.402687	0.206286	0.089*
N1	0.7526 (4)	−0.1796 (3)	0.2140 (2)	0.0432 (14)
N2	−0.0146 (4)	0.0327 (4)	0.2316 (2)	0.0420 (13)

N3	0.2564 (4)	0.6223 (4)	0.2797 (3)	0.0482 (14)
N4	0.9972 (4)	0.3938 (4)	0.2827 (2)	0.0422 (13)
C1	0.5443 (6)	−0.1067 (4)	0.2818 (3)	0.0371 (15)
C2	0.6454 (5)	−0.1407 (4)	0.3060 (3)	0.0430 (16)
H21	0.619058	−0.165257	0.349583	0.052*
H22	0.700041	−0.087644	0.298497	0.052*
C3	0.7073 (6)	−0.2173 (4)	0.2778 (3)	0.0510 (18)
H31	0.771145	−0.240606	0.296234	0.061*
H32	0.652973	−0.270324	0.284672	0.061*
C4	0.7150 (5)	−0.2121 (4)	0.1774 (3)	0.0442 (17)
H4	0.661028	−0.263207	0.192023	0.053*
C5	0.7517 (6)	−0.1739 (4)	0.1147 (3)	0.0471 (17)
C6	0.8268 (6)	−0.0944 (5)	0.0907 (3)	0.0536 (19)
C7	0.8536 (8)	−0.0556 (6)	0.0308 (4)	0.081 (3)
H7	0.902099	−0.001185	0.015103	0.098*
C8	0.8113 (8)	−0.0944 (7)	−0.0066 (4)	0.087 (3)
H8	0.830824	−0.066773	−0.048047	0.104*
C9	0.7398 (8)	−0.1742 (7)	0.0157 (4)	0.084 (3)
H9	0.711990	−0.201968	−0.010488	0.101*
C10	0.7100 (7)	−0.2121 (6)	0.0756 (4)	0.068 (2)
H10	0.659773	−0.265579	0.090837	0.082*
C11	0.1872 (5)	0.1706 (4)	0.1998 (2)	0.0293 (14)
C12	0.0828 (5)	0.1821 (4)	0.1759 (3)	0.0374 (15)
H121	0.103123	0.223926	0.135549	0.045*
H122	0.023434	0.213047	0.201325	0.045*
C13	0.0318 (5)	0.0912 (4)	0.1724 (3)	0.0447 (17)
H131	−0.030228	0.105022	0.151281	0.054*
H132	0.092047	0.057270	0.149501	0.054*
C14	0.0147 (5)	−0.0521 (4)	0.2431 (3)	0.0417 (16)
H141	0.067197	−0.074667	0.212852	0.050*
C15	−0.0285 (5)	−0.1157 (4)	0.3004 (3)	0.0427 (16)
C16	−0.1085 (5)	−0.0879 (4)	0.3464 (3)	0.0470 (17)
C17	−0.1522 (6)	−0.1512 (5)	0.4001 (3)	0.0556 (19)
H17	−0.208156	−0.133009	0.430990	0.067*
C18	−0.1123 (7)	−0.2420 (5)	0.4079 (4)	0.066 (2)
H18	−0.141016	−0.285644	0.444647	0.079*
C19	−0.0322 (7)	−0.2697 (5)	0.3634 (4)	0.069 (2)
H19	−0.006126	−0.332012	0.369458	0.083*
C20	0.0099 (6)	−0.2069 (5)	0.3103 (3)	0.0523 (18)
H20	0.066025	−0.225865	0.279839	0.063*
C21	0.2455 (5)	−0.0351 (4)	0.3123 (3)	0.0433 (16)
H211	0.181242	0.008841	0.315108	0.052*
H212	0.216866	−0.092719	0.305395	0.052*
C22	0.2778 (5)	−0.0595 (5)	0.3717 (3)	0.0496 (18)
H221	0.303150	−0.001849	0.379999	0.060*
H222	0.343214	−0.102311	0.369154	0.060*
C23	0.1767 (6)	−0.1063 (5)	0.4234 (3)	0.066 (2)
H231	0.111218	−0.063578	0.425921	0.079*

H232	0.151524	−0.164077	0.415209	0.079*
C24	0.2094 (7)	−0.1304 (6)	0.4828 (3)	0.084 (3)
H241	0.279177	−0.167172	0.479287	0.126*
H242	0.146329	−0.166835	0.513454	0.126*
H243	0.223472	−0.072666	0.493938	0.126*
C25	0.4506 (5)	−0.0064 (4)	0.1540 (2)	0.0407 (16)
H251	0.471649	0.052939	0.123549	0.049*
H252	0.522337	−0.040680	0.155886	0.049*
C26	0.3726 (6)	−0.0638 (4)	0.1340 (3)	0.0496 (18)
H261	0.358661	−0.125890	0.162134	0.060*
H262	0.297587	−0.033041	0.136507	0.060*
C27	0.4171 (7)	−0.0777 (6)	0.0726 (3)	0.072 (2)
H271	0.493625	−0.105990	0.069738	0.086*
H272	0.428022	−0.015677	0.044452	0.086*
C28	0.3427 (8)	−0.1376 (5)	0.0534 (3)	0.085 (3)
H281	0.342861	−0.202373	0.075968	0.128*
H282	0.372584	−0.134524	0.010877	0.128*
H283	0.263859	−0.115082	0.060624	0.128*
C29	0.2925 (5)	0.3094 (4)	0.3104 (2)	0.0396 (16)
H291	0.344545	0.336341	0.328884	0.048*
H292	0.233134	0.355677	0.302931	0.048*
C30	0.2344 (5)	0.2202 (4)	0.3532 (3)	0.0448 (17)
H301	0.172808	0.199677	0.337725	0.054*
H302	0.291712	0.170452	0.354718	0.054*
C31	0.1826 (6)	0.2317 (5)	0.4159 (3)	0.0548 (19)
H311	0.131501	0.285862	0.414280	0.066*
H312	0.244997	0.244653	0.433478	0.066*
C32	0.1134 (7)	0.1439 (6)	0.4555 (3)	0.088 (3)
H321	0.056695	0.127225	0.436131	0.132*
H322	0.073700	0.156392	0.493900	0.132*
H323	0.165755	0.092183	0.461656	0.132*
C33	0.4293 (5)	0.3434 (4)	0.1358 (2)	0.0404 (16)
H331	0.365938	0.384474	0.126804	0.048*
H332	0.499367	0.383659	0.125534	0.048*
C34	0.4495 (6)	0.2764 (4)	0.0953 (3)	0.0494 (18)
H341	0.380680	0.234594	0.105779	0.059*
H342	0.515290	0.236991	0.102394	0.059*
C35	0.4742 (6)	0.3249 (5)	0.0293 (3)	0.065 (2)
H351	0.475464	0.277138	0.006190	0.077*
H352	0.410879	0.367490	0.022702	0.077*
C36	0.5858 (6)	0.3796 (6)	0.0066 (3)	0.079 (3)
H361	0.582268	0.431327	0.026348	0.118*
H362	0.599666	0.404677	−0.036349	0.118*
H363	0.648580	0.338785	0.015073	0.118*
C37	0.5619 (5)	0.0987 (4)	0.3557 (2)	0.0356 (15)
H371	0.494429	0.055586	0.365742	0.043*
H372	0.626666	0.061251	0.366409	0.043*
C38	0.5335 (5)	0.1705 (4)	0.3940 (2)	0.0381 (15)

H381	0.602607	0.210739	0.386683	0.046*
H382	0.471993	0.210820	0.381934	0.046*
C39	0.4949 (6)	0.1253 (5)	0.4595 (3)	0.0544 (19)
H391	0.555918	0.084121	0.471401	0.065*
H392	0.425088	0.085813	0.466882	0.065*
C40	0.4685 (6)	0.1967 (5)	0.4977 (3)	0.068 (2)
H401	0.536637	0.237104	0.489802	0.102*
H402	0.447513	0.164027	0.539809	0.102*
H403	0.404351	0.234778	0.488120	0.102*
C41	0.7007 (5)	0.1298 (4)	0.1803 (2)	0.0364 (15)
H411	0.754476	0.078877	0.188434	0.044*
H412	0.646479	0.107701	0.160929	0.044*
C42	0.7696 (5)	0.2149 (4)	0.1371 (3)	0.0433 (16)
H421	0.716977	0.267374	0.130883	0.052*
H422	0.827981	0.234357	0.155086	0.052*
C43	0.8301 (5)	0.1957 (5)	0.0769 (3)	0.0477 (17)
H431	0.868498	0.135001	0.083301	0.057*
H432	0.771960	0.190993	0.054653	0.057*
C44	0.9186 (6)	0.2716 (5)	0.0401 (3)	0.069 (2)
H441	0.879946	0.330760	0.030660	0.104*
H442	0.958892	0.254428	0.003235	0.104*
H443	0.974191	0.278586	0.062772	0.104*
C45	0.4637 (6)	0.5509 (4)	0.2090 (3)	0.0391 (16)
C46	0.3637 (6)	0.5915 (5)	0.1857 (3)	0.0522 (18)
H461	0.307152	0.540893	0.190781	0.063*
H462	0.390804	0.620252	0.142626	0.063*
C47	0.3054 (6)	0.6647 (4)	0.2175 (3)	0.0533 (19)
H471	0.362281	0.714395	0.213773	0.064*
H472	0.243916	0.693754	0.198870	0.064*
C48	0.2906 (5)	0.6530 (4)	0.3187 (3)	0.0477 (18)
H48	0.344980	0.703835	0.305337	0.057*
C49	0.2508 (6)	0.6143 (4)	0.3820 (3)	0.0492 (18)
C50	0.1750 (6)	0.5353 (5)	0.4028 (3)	0.0558 (19)
C51	0.1390 (7)	0.4968 (6)	0.4631 (4)	0.074 (2)
H51	0.089415	0.442877	0.477315	0.089*
C52	0.1745 (8)	0.5359 (7)	0.5027 (4)	0.088 (3)
H52	0.149068	0.508946	0.544147	0.106*
C53	0.2465 (8)	0.6135 (7)	0.4830 (4)	0.086 (3)
H53	0.269119	0.641152	0.510726	0.104*
C54	0.2858 (7)	0.6511 (5)	0.4234 (4)	0.071 (2)
H54	0.337937	0.703355	0.410022	0.086*
C55	0.8014 (5)	0.2636 (4)	0.2982 (2)	0.0320 (14)
C56	0.8970 (5)	0.2426 (4)	0.3284 (3)	0.0416 (16)
H561	0.959387	0.212966	0.303666	0.050*
H562	0.868522	0.197361	0.366945	0.050*
C57	0.9460 (5)	0.3298 (4)	0.3391 (3)	0.0463 (17)
H571	0.883720	0.361065	0.362789	0.056*
H572	1.004904	0.311598	0.361872	0.056*

C58	0.9686 (5)	0.4797 (5)	0.2747 (3)	0.0443 (17)
H58	0.916246	0.498929	0.306425	0.053*
C59	1.0122 (5)	0.5489 (4)	0.2197 (3)	0.0439 (17)
C60	1.0894 (6)	0.5256 (5)	0.1713 (3)	0.0486 (18)
C61	1.1278 (6)	0.5926 (5)	0.1191 (3)	0.061 (2)
H61	1.178796	0.575992	0.085944	0.073*
C62	1.0929 (7)	0.6824 (5)	0.1149 (4)	0.063 (2)
H62	1.120232	0.728209	0.078914	0.076*
C63	1.0179 (7)	0.7071 (5)	0.1628 (4)	0.069 (2)
H63	0.994896	0.770025	0.159890	0.082*
C64	0.9769 (6)	0.6408 (5)	0.2146 (4)	0.0572 (19)
H64	0.924062	0.657759	0.247072	0.069*
C65	0.5379 (5)	0.4422 (4)	0.3400 (2)	0.0388 (15)
H651	0.458205	0.462367	0.340595	0.047*
H652	0.533589	0.384186	0.371469	0.047*
C66	0.6028 (6)	0.5173 (4)	0.3539 (3)	0.0518 (18)
H661	0.685489	0.502701	0.346043	0.062*
H662	0.595041	0.577902	0.326605	0.062*
C67	0.5619 (7)	0.5274 (5)	0.4168 (3)	0.062 (2)
H671	0.578024	0.469346	0.443892	0.074*
H672	0.477484	0.534837	0.426117	0.074*
C68	0.6181 (7)	0.6098 (5)	0.4283 (3)	0.079 (3)
H681	0.701740	0.608241	0.413343	0.118*
H682	0.598895	0.606035	0.471086	0.118*
H683	0.589763	0.668154	0.407839	0.118*
C69	0.7591 (5)	0.4686 (4)	0.1851 (3)	0.0467 (17)
H691	0.788968	0.524488	0.193602	0.056*
H692	0.820284	0.421914	0.184689	0.056*
C70	0.7376 (5)	0.4962 (4)	0.1236 (3)	0.0443 (17)
H701	0.678541	0.544633	0.123013	0.053*
H702	0.706954	0.441030	0.114698	0.053*
C71	0.8458 (6)	0.5334 (5)	0.0757 (3)	0.0531 (19)
H711	0.874022	0.590386	0.083620	0.064*
H712	0.906133	0.486212	0.077909	0.064*
C72	0.8279 (6)	0.5567 (5)	0.0135 (3)	0.066 (2)
H721	0.799710	0.500705	0.005254	0.100*
H722	0.901014	0.578564	−0.015310	0.100*
H723	0.771244	0.605815	0.010237	0.100*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.0271 (2)	0.0292 (2)	0.0445 (3)	0.00029 (18)	−0.0104 (2)	−0.01145 (19)
Sn2	0.0260 (2)	0.0288 (2)	0.0400 (3)	0.00371 (18)	−0.0085 (2)	−0.01030 (19)
Sn3	0.0255 (2)	0.0295 (2)	0.0408 (3)	0.00400 (18)	−0.00891 (19)	−0.01158 (19)
Sn4	0.0289 (2)	0.0294 (2)	0.0472 (3)	0.00047 (19)	−0.0108 (2)	−0.0122 (2)
O1	0.027 (2)	0.038 (3)	0.042 (2)	0.0035 (19)	−0.0121 (19)	−0.0107 (19)
O2	0.049 (3)	0.032 (2)	0.066 (3)	0.000 (2)	−0.012 (2)	−0.015 (2)

O3	0.071 (4)	0.050 (3)	0.071 (3)	−0.016 (3)	−0.011 (3)	−0.015 (3)
O4	0.032 (2)	0.038 (2)	0.054 (3)	0.007 (2)	−0.018 (2)	−0.016 (2)
O5	0.031 (2)	0.038 (3)	0.056 (3)	0.004 (2)	−0.016 (2)	−0.016 (2)
O6	0.047 (3)	0.046 (3)	0.063 (3)	0.003 (2)	−0.001 (2)	−0.010 (2)
O7	0.043 (2)	0.026 (2)	0.033 (2)	0.0025 (18)	−0.0160 (19)	−0.0096 (17)
O8	0.021 (2)	0.031 (2)	0.054 (3)	0.0026 (17)	−0.0106 (19)	−0.0093 (19)
O9	0.035 (2)	0.028 (2)	0.052 (3)	−0.0007 (19)	−0.015 (2)	−0.0107 (19)
O10	0.046 (3)	0.033 (3)	0.074 (3)	0.001 (2)	−0.017 (2)	−0.016 (2)
O11	0.068 (4)	0.053 (3)	0.070 (3)	−0.007 (3)	−0.009 (3)	−0.020 (3)
O12	0.035 (3)	0.041 (3)	0.054 (3)	0.005 (2)	−0.017 (2)	−0.014 (2)
O13	0.030 (2)	0.041 (3)	0.053 (3)	0.0041 (19)	−0.014 (2)	−0.017 (2)
O14	0.052 (3)	0.054 (3)	0.068 (3)	0.005 (2)	0.002 (3)	−0.024 (3)
N1	0.040 (3)	0.028 (3)	0.059 (4)	0.011 (2)	−0.008 (3)	−0.012 (3)
N2	0.028 (3)	0.043 (3)	0.056 (4)	−0.001 (2)	−0.011 (3)	−0.013 (3)
N3	0.041 (3)	0.041 (3)	0.068 (4)	0.013 (3)	−0.020 (3)	−0.018 (3)
N4	0.033 (3)	0.047 (3)	0.055 (4)	0.001 (3)	−0.014 (3)	−0.025 (3)
C1	0.062 (5)	0.015 (3)	0.040 (4)	0.004 (3)	−0.022 (3)	−0.011 (3)
C2	0.040 (4)	0.043 (4)	0.050 (4)	0.017 (3)	−0.024 (3)	−0.007 (3)
C3	0.043 (4)	0.040 (4)	0.065 (5)	0.011 (3)	−0.012 (4)	−0.007 (3)
C4	0.043 (4)	0.030 (4)	0.062 (5)	0.007 (3)	−0.013 (4)	−0.017 (3)
C5	0.048 (4)	0.042 (4)	0.056 (5)	0.014 (3)	−0.014 (4)	−0.024 (4)
C6	0.052 (5)	0.049 (4)	0.053 (5)	0.004 (4)	−0.002 (4)	−0.012 (4)
C7	0.104 (7)	0.068 (6)	0.057 (6)	−0.012 (5)	0.004 (5)	−0.009 (5)
C8	0.101 (8)	0.098 (7)	0.053 (5)	0.017 (6)	−0.006 (5)	−0.019 (5)
C9	0.087 (7)	0.096 (7)	0.087 (7)	0.017 (6)	−0.032 (6)	−0.044 (6)
C10	0.061 (5)	0.071 (5)	0.078 (6)	0.008 (4)	−0.015 (5)	−0.032 (5)
C11	0.025 (3)	0.030 (3)	0.027 (3)	0.005 (3)	−0.001 (3)	−0.002 (3)
C12	0.029 (3)	0.045 (4)	0.038 (4)	0.003 (3)	−0.015 (3)	−0.006 (3)
C13	0.033 (4)	0.059 (4)	0.049 (4)	0.003 (3)	−0.019 (3)	−0.017 (4)
C14	0.033 (4)	0.047 (4)	0.054 (4)	0.000 (3)	−0.013 (3)	−0.026 (3)
C15	0.032 (4)	0.037 (4)	0.062 (5)	0.000 (3)	−0.016 (3)	−0.013 (3)
C16	0.040 (4)	0.037 (4)	0.066 (5)	−0.001 (3)	−0.019 (4)	−0.010 (4)
C17	0.041 (4)	0.059 (5)	0.061 (5)	−0.005 (4)	−0.010 (4)	−0.006 (4)
C18	0.073 (6)	0.042 (4)	0.079 (6)	−0.007 (4)	−0.030 (5)	0.006 (4)
C19	0.058 (5)	0.049 (5)	0.111 (7)	0.005 (4)	−0.039 (5)	−0.022 (5)
C20	0.041 (4)	0.045 (4)	0.074 (5)	0.004 (3)	−0.017 (4)	−0.018 (4)
C21	0.038 (4)	0.044 (4)	0.045 (4)	−0.007 (3)	−0.008 (3)	−0.007 (3)
C22	0.039 (4)	0.053 (4)	0.052 (4)	−0.001 (3)	−0.006 (3)	−0.010 (3)
C23	0.052 (5)	0.090 (6)	0.044 (4)	−0.007 (4)	−0.001 (4)	−0.004 (4)
C24	0.074 (6)	0.114 (7)	0.055 (5)	0.007 (5)	−0.011 (5)	−0.008 (5)
C25	0.045 (4)	0.037 (4)	0.039 (4)	0.000 (3)	−0.007 (3)	−0.011 (3)
C26	0.061 (5)	0.041 (4)	0.047 (4)	−0.009 (3)	−0.011 (4)	−0.013 (3)
C27	0.079 (6)	0.091 (6)	0.061 (5)	0.000 (5)	−0.022 (4)	−0.041 (5)
C28	0.121 (8)	0.072 (6)	0.087 (6)	0.008 (5)	−0.045 (6)	−0.044 (5)
C29	0.035 (4)	0.040 (4)	0.050 (4)	0.009 (3)	−0.011 (3)	−0.023 (3)
C30	0.032 (4)	0.057 (4)	0.045 (4)	−0.001 (3)	−0.006 (3)	−0.014 (3)
C31	0.039 (4)	0.090 (6)	0.042 (4)	0.009 (4)	−0.011 (3)	−0.028 (4)
C32	0.066 (6)	0.128 (8)	0.052 (5)	−0.013 (5)	0.011 (4)	−0.009 (5)

C33	0.045 (4)	0.035 (3)	0.040 (4)	0.004 (3)	−0.012 (3)	−0.005 (3)
C34	0.052 (4)	0.050 (4)	0.047 (4)	−0.006 (3)	−0.011 (3)	−0.014 (3)
C35	0.060 (5)	0.080 (5)	0.057 (5)	−0.011 (4)	−0.013 (4)	−0.022 (4)
C36	0.064 (5)	0.108 (7)	0.052 (5)	−0.007 (5)	−0.006 (4)	−0.006 (5)
C37	0.031 (3)	0.027 (3)	0.046 (4)	−0.004 (3)	−0.007 (3)	−0.006 (3)
C38	0.036 (4)	0.037 (4)	0.041 (4)	0.002 (3)	−0.006 (3)	−0.014 (3)
C39	0.058 (5)	0.054 (4)	0.051 (4)	−0.009 (4)	−0.011 (4)	−0.013 (4)
C40	0.069 (5)	0.086 (6)	0.047 (4)	0.002 (5)	−0.002 (4)	−0.027 (4)
C41	0.024 (3)	0.034 (3)	0.056 (4)	0.005 (3)	−0.009 (3)	−0.024 (3)
C42	0.037 (4)	0.041 (4)	0.050 (4)	0.002 (3)	−0.008 (3)	−0.009 (3)
C43	0.044 (4)	0.059 (4)	0.042 (4)	0.004 (3)	−0.017 (3)	−0.010 (3)
C44	0.054 (5)	0.095 (6)	0.048 (5)	−0.008 (4)	−0.005 (4)	−0.005 (4)
C45	0.049 (4)	0.027 (4)	0.041 (4)	0.006 (3)	−0.014 (3)	−0.005 (3)
C46	0.056 (5)	0.049 (4)	0.058 (4)	0.015 (4)	−0.028 (4)	−0.012 (4)
C47	0.048 (4)	0.042 (4)	0.068 (5)	0.014 (3)	−0.023 (4)	−0.002 (4)
C48	0.032 (4)	0.033 (4)	0.076 (5)	0.005 (3)	−0.013 (4)	−0.010 (4)
C49	0.041 (4)	0.038 (4)	0.070 (5)	0.006 (3)	−0.016 (4)	−0.015 (4)
C50	0.052 (5)	0.052 (5)	0.066 (5)	0.017 (4)	−0.013 (4)	−0.023 (4)
C51	0.073 (6)	0.065 (5)	0.081 (6)	0.008 (4)	−0.012 (5)	−0.020 (5)
C52	0.101 (8)	0.084 (7)	0.067 (6)	0.020 (6)	−0.011 (6)	−0.003 (5)
C53	0.102 (8)	0.093 (7)	0.082 (7)	0.019 (6)	−0.040 (6)	−0.036 (6)
C54	0.068 (6)	0.063 (5)	0.095 (7)	−0.003 (4)	−0.034 (5)	−0.024 (5)
C55	0.032 (4)	0.038 (4)	0.030 (3)	0.013 (3)	−0.013 (3)	−0.010 (3)
C56	0.040 (4)	0.044 (4)	0.047 (4)	0.007 (3)	−0.024 (3)	−0.010 (3)
C57	0.035 (4)	0.065 (5)	0.047 (4)	−0.003 (3)	−0.018 (3)	−0.020 (4)
C58	0.035 (4)	0.052 (4)	0.057 (4)	0.002 (3)	−0.017 (3)	−0.030 (4)
C59	0.028 (4)	0.046 (4)	0.061 (5)	−0.003 (3)	−0.014 (3)	−0.016 (4)
C60	0.038 (4)	0.047 (4)	0.069 (5)	0.000 (3)	−0.023 (4)	−0.021 (4)
C61	0.049 (5)	0.065 (5)	0.069 (5)	0.002 (4)	−0.017 (4)	−0.016 (4)
C62	0.066 (5)	0.057 (5)	0.071 (6)	−0.004 (4)	−0.036 (5)	−0.003 (4)
C63	0.055 (5)	0.054 (5)	0.114 (7)	0.012 (4)	−0.047 (5)	−0.026 (5)
C64	0.041 (4)	0.052 (5)	0.085 (6)	0.006 (4)	−0.018 (4)	−0.027 (4)
C65	0.037 (4)	0.037 (4)	0.047 (4)	0.008 (3)	−0.016 (3)	−0.015 (3)
C66	0.055 (5)	0.049 (4)	0.054 (4)	−0.002 (3)	−0.010 (4)	−0.018 (3)
C67	0.088 (6)	0.057 (5)	0.048 (4)	−0.005 (4)	−0.022 (4)	−0.019 (4)
C68	0.130 (8)	0.058 (5)	0.057 (5)	−0.017 (5)	−0.024 (5)	−0.027 (4)
C69	0.028 (4)	0.050 (4)	0.058 (4)	−0.002 (3)	−0.006 (3)	−0.009 (3)
C70	0.030 (4)	0.047 (4)	0.053 (4)	0.002 (3)	−0.007 (3)	−0.010 (3)
C71	0.046 (4)	0.058 (5)	0.050 (4)	−0.007 (4)	−0.004 (4)	−0.010 (4)
C72	0.053 (5)	0.076 (5)	0.059 (5)	−0.017 (4)	0.002 (4)	−0.008 (4)

Geometric parameters (Å, º)

Sn1—O1	2.157 (4)	C29—C30	1.527 (8)
Sn1—O2	2.962 (4)	C29—H291	0.9900
Sn1—O4	2.238 (4)	C29—H292	0.9900
Sn1—O7	2.021 (4)	C30—C31	1.518 (8)
Sn1—C21	2.125 (5)	C30—H301	0.9900

Sn1—C25	2.118 (6)	C30—H302	0.9900
Sn2—O5	2.289 (4)	C31—C32	1.535 (9)
Sn2—O7	2.035 (4)	C31—H311	0.9900
Sn2—O8	2.159 (4)	C31—H312	0.9900
Sn2—O9	2.749 (4)	C32—H321	0.9800
Sn2—C29	2.115 (5)	C32—H322	0.9800
Sn2—C33	2.119 (5)	C32—H323	0.9800
Sn3—O1	2.687 (4)	C33—C34	1.513 (8)
Sn3—O7	2.185 (4)	C33—H331	0.9900
Sn3—O8	2.054 (4)	C33—H332	0.9900
Sn3—O13	2.295 (4)	C34—C35	1.529 (8)
Sn3—C37	2.130 (5)	C34—H341	0.9900
Sn3—C41	2.117 (5)	C34—H342	0.9900
Sn4—O8	2.022 (4)	C35—C36	1.496 (9)
Sn4—O9	2.170 (4)	C35—H351	0.9900
Sn4—O10	2.908 (4)	C35—H352	0.9900
Sn4—O12	2.267 (4)	C36—H361	0.9800
Sn4—C65	2.125 (6)	C36—H362	0.9800
Sn4—C69	2.129 (5)	C36—H363	0.9800
O1—C1	1.299 (6)	C37—C38	1.532 (7)
O2—C1	1.236 (7)	C37—H371	0.9900
O3—C6	1.355 (8)	C37—H372	0.9900
O3—H3	0.8400	C38—C39	1.509 (8)
O4—C11	1.270 (6)	C38—H381	0.9900
O5—C11	1.254 (6)	C38—H382	0.9900
O6—C16	1.357 (7)	C39—C40	1.526 (9)
O6—H6	0.8400	C39—H391	0.9900
O9—C45	1.299 (7)	C39—H392	0.9900
O10—C45	1.230 (7)	C40—H401	0.9800
O11—C50	1.345 (8)	C40—H402	0.9800
O11—H11	0.8400	C40—H403	0.9800
O12—C55	1.257 (6)	C41—C42	1.535 (7)
O13—C55	1.270 (7)	C41—H411	0.9900
O14—C60	1.355 (7)	C41—H412	0.9900
O14—H14	0.8400	C42—C43	1.528 (8)
N1—C4	1.267 (8)	C42—H421	0.9900
N1—C3	1.463 (8)	C42—H422	0.9900
N2—C14	1.273 (7)	C43—C44	1.516 (8)
N2—C13	1.456 (7)	C43—H431	0.9900
N3—C48	1.283 (8)	C43—H432	0.9900
N3—C47	1.450 (8)	C44—H441	0.9800
N4—C58	1.283 (7)	C44—H442	0.9800
N4—C57	1.453 (7)	C44—H443	0.9800
C1—C2	1.496 (8)	C45—C46	1.498 (8)
C2—C3	1.529 (8)	C46—C47	1.518 (8)
C2—H21	0.9900	C46—H461	0.9900
C2—H22	0.9900	C46—H462	0.9900
C3—H31	0.9900	C47—H471	0.9900

C3—H32	0.9900	C47—H472	0.9900
C4—C5	1.430 (9)	C48—C49	1.446 (9)
C4—H4	0.9500	C48—H48	0.9500
C5—C10	1.395 (9)	C49—C54	1.387 (10)
C5—C6	1.416 (9)	C49—C50	1.414 (9)
C6—C7	1.370 (9)	C50—C51	1.382 (10)
C7—C8	1.368 (11)	C51—C52	1.373 (11)
C7—H7	0.9500	C51—H51	0.9500
C8—C9	1.394 (11)	C52—C53	1.372 (11)
C8—H8	0.9500	C52—H52	0.9500
C9—C10	1.368 (10)	C53—C54	1.368 (11)
C9—H9	0.9500	C53—H53	0.9500
C10—H10	0.9500	C54—H54	0.9500
C11—C12	1.493 (8)	C55—C56	1.489 (8)
C12—C13	1.519 (8)	C56—C57	1.530 (8)
C12—H121	0.9900	C56—H561	0.9900
C12—H122	0.9900	C56—H562	0.9900
C13—H131	0.9900	C57—H571	0.9900
C13—H132	0.9900	C57—H572	0.9900
C14—C15	1.447 (8)	C58—C59	1.449 (8)
C14—H141	0.9500	C58—H58	0.9500
C15—C20	1.392 (8)	C59—C64	1.392 (9)
C15—C16	1.399 (9)	C59—C60	1.395 (9)
C16—C17	1.388 (8)	C60—C61	1.380 (9)
C17—C18	1.392 (9)	C61—C62	1.363 (9)
C17—H17	0.9500	C61—H61	0.9500
C18—C19	1.375 (10)	C62—C63	1.384 (10)
C18—H18	0.9500	C62—H62	0.9500
C19—C20	1.371 (9)	C63—C64	1.373 (10)
C19—H19	0.9500	C63—H63	0.9500
C20—H20	0.9500	C64—H64	0.9500
C21—C22	1.525 (8)	C65—C66	1.517 (8)
C21—H211	0.9900	C65—H651	0.9900
C21—H212	0.9900	C65—H652	0.9900
C22—C23	1.541 (8)	C66—C67	1.502 (8)
C22—H221	0.9900	C66—H661	0.9900
C22—H222	0.9900	C66—H662	0.9900
C23—C24	1.527 (9)	C67—C68	1.518 (9)
C23—H231	0.9900	C67—H671	0.9900
C23—H232	0.9900	C67—H672	0.9900
C24—H241	0.9800	C68—H681	0.9800
C24—H242	0.9800	C68—H682	0.9800
C24—H243	0.9800	C68—H683	0.9800
C25—C26	1.512 (8)	C69—C70	1.516 (8)
C25—H251	0.9900	C69—H691	0.9900
C25—H252	0.9900	C69—H692	0.9900
C26—C27	1.492 (8)	C70—C71	1.519 (8)
C26—H261	0.9900	C70—H701	0.9900

C26—H262	0.9900	C70—H702	0.9900
C27—C28	1.495 (9)	C71—C72	1.514 (9)
C27—H271	0.9900	C71—H711	0.9900
C27—H272	0.9900	C71—H712	0.9900
C28—H281	0.9800	C72—H721	0.9800
C28—H282	0.9800	C72—H722	0.9800
C28—H283	0.9800	C72—H723	0.9800

O1—Sn1—O2	47.92 (13)	H291—C29—H292	107.9
O1—Sn1—O4	168.40 (14)	C31—C30—C29	113.6 (5)
O1—Sn1—O7	78.96 (14)	C31—C30—H301	108.9
O1—Sn1—C21	99.87 (19)	C29—C30—H301	108.9
O1—Sn1—C25	95.4 (2)	C31—C30—H302	108.9
O2—Sn1—O4	142.74 (13)	C29—C30—H302	108.9
O2—Sn1—O7	126.82 (14)	H301—C30—H302	107.7
O2—Sn1—C21	80.07 (19)	C30—C31—C32	111.7 (6)
O2—Sn1—C25	78.55 (19)	C30—C31—H311	109.3
O4—Sn1—O7	90.39 (14)	C32—C31—H311	109.3
O4—Sn1—C21	88.3 (2)	C30—C31—H312	109.3
O4—Sn1—C25	84.7 (2)	C32—C31—H312	109.3
O7—Sn1—C21	111.7 (2)	H311—C31—H312	107.9
O7—Sn1—C25	114.05 (18)	C31—C32—H321	109.5
C21—Sn1—C25	133.7 (2)	C31—C32—H322	109.5
O5—Sn2—O7	88.76 (14)	H321—C32—H322	109.5
O5—Sn2—O8	164.11 (14)	C31—C32—H323	109.5
O5—Sn2—O9	131.33 (13)	H321—C32—H323	109.5
O5—Sn2—C29	84.77 (19)	H322—C32—H323	109.5
O5—Sn2—C33	88.4 (2)	C34—C33—Sn2	117.1 (4)
O7—Sn2—O8	76.01 (14)	C34—C33—H331	108.0
O7—Sn2—O9	139.90 (13)	Sn2—C33—H331	108.0
O7—Sn2—C29	107.64 (19)	C34—C33—H332	108.0
O7—Sn2—C33	109.61 (19)	Sn2—C33—H332	108.0
O8—Sn2—O9	64.10 (12)	H331—C33—H332	107.3
O8—Sn2—C29	95.4 (2)	C33—C34—C35	113.6 (5)
O8—Sn2—C33	100.9 (2)	C33—C34—H341	108.9
O9—Sn2—C29	81.15 (17)	C35—C34—H341	108.9
O9—Sn2—C33	75.58 (18)	C33—C34—H342	108.9
C29—Sn2—C33	141.9 (2)	C35—C34—H342	108.9
O1—Sn3—O7	65.19 (12)	H341—C34—H342	107.7
O1—Sn3—O8	140.08 (13)	C36—C35—C34	113.4 (6)
O1—Sn3—O13	129.85 (13)	C36—C35—H351	108.9
O1—Sn3—C37	76.61 (17)	C34—C35—H351	108.9
O1—Sn3—C41	79.64 (16)	C36—C35—H352	108.9
O7—Sn3—O8	75.04 (13)	C34—C35—H352	108.9
O7—Sn3—O13	164.68 (13)	H351—C35—H352	107.7
O7—Sn3—C37	99.74 (18)	C35—C36—H361	109.5
O7—Sn3—C41	95.43 (18)	C35—C36—H362	109.5
O8—Sn3—O13	90.05 (14)	H361—C36—H362	109.5

O8—Sn3—C37	108.06 (18)	C35—C36—H363	109.5
O8—Sn3—C41	108.35 (18)	H361—C36—H363	109.5
O13—Sn3—C37	88.07 (18)	H362—C36—H363	109.5
O13—Sn3—C41	85.82 (18)	C38—C37—Sn3	115.2 (4)
C37—Sn3—C41	143.0 (2)	C38—C37—H371	108.5
O8—Sn4—O9	78.42 (14)	Sn3—C37—H371	108.5
O8—Sn4—O10	127.46 (14)	C38—C37—H372	108.5
O8—Sn4—O12	90.96 (14)	Sn3—C37—H372	108.5
O8—Sn4—C65	113.08 (19)	H371—C37—H372	107.5
O8—Sn4—C69	111.7 (2)	C39—C38—C37	112.5 (5)
O9—Sn4—O10	49.09 (13)	C39—C38—H381	109.1
O9—Sn4—O12	168.21 (14)	C37—C38—H381	109.1
O9—Sn4—C65	95.69 (19)	C39—C38—H382	109.1
O9—Sn4—C69	101.3 (2)	C37—C38—H382	109.1
O10—Sn4—O12	141.50 (14)	H381—C38—H382	107.8
O10—Sn4—C65	79.04 (18)	C38—C39—C40	112.6 (5)
O10—Sn4—C69	80.90 (19)	C38—C39—H391	109.1
O12—Sn4—C65	83.66 (19)	C40—C39—H391	109.1
O12—Sn4—C69	87.3 (2)	C38—C39—H392	109.1
C65—Sn4—C69	134.4 (2)	C40—C39—H392	109.1
C1—O1—Sn1	114.2 (4)	H391—C39—H392	107.8
C1—O1—Sn3	149.0 (4)	C39—C40—H401	109.5
Sn1—O1—Sn3	95.95 (13)	C39—C40—H402	109.5
C1—O2—Sn1	76.9 (3)	H401—C40—H402	109.5
C6—O3—H3	109.5	C39—C40—H403	109.5
C11—O4—Sn1	133.7 (4)	H401—C40—H403	109.5
C11—O5—Sn2	133.1 (4)	H402—C40—H403	109.5
C16—O6—H6	109.5	C42—C41—Sn3	114.3 (4)
Sn1—O7—Sn2	136.7 (2)	C42—C41—H411	108.7
Sn1—O7—Sn3	118.47 (17)	Sn3—C41—H411	108.7
Sn2—O7—Sn3	104.34 (15)	C42—C41—H412	108.7
Sn2—O8—Sn3	104.61 (16)	Sn3—C41—H412	108.7
Sn2—O8—Sn4	120.77 (17)	H411—C41—H412	107.6
Sn3—O8—Sn4	134.05 (19)	C43—C42—C41	112.9 (5)
Sn2—O9—Sn4	94.56 (13)	C43—C42—H421	109.0
C45—O9—Sn4	111.1 (4)	C41—C42—H421	109.0
C45—O9—Sn2	152.7 (4)	C43—C42—H422	109.0
C45—O10—Sn4	77.5 (3)	C41—C42—H422	109.0
C50—O11—H11	109.5	H421—C42—H422	107.8
C55—O12—Sn4	133.0 (4)	C44—C43—C42	112.2 (6)
C55—O13—Sn3	130.1 (4)	C44—C43—H431	109.2
C60—O14—H14	109.5	C42—C43—H431	109.2
C4—N1—C3	119.7 (6)	C44—C43—H432	109.2
C14—N2—C13	119.0 (5)	C42—C43—H432	109.2
C48—N3—C47	118.3 (6)	H431—C43—H432	107.9
C58—N4—C57	118.7 (5)	C43—C44—H441	109.5
O2—C1—O1	120.9 (6)	C43—C44—H442	109.5
O2—C1—C2	122.5 (5)	H441—C44—H442	109.5

O1—C1—C2	116.6 (5)	C43—C44—H443	109.5
C1—C2—C3	111.7 (5)	H441—C44—H443	109.5
C1—C2—H21	109.3	H442—C44—H443	109.5
C3—C2—H21	109.3	O10—C45—O9	122.1 (6)
C1—C2—H22	109.3	O10—C45—C46	122.0 (5)
C3—C2—H22	109.3	O9—C45—C46	115.9 (6)
H21—C2—H22	107.9	C45—C46—C47	111.8 (6)
N1—C3—C2	109.4 (5)	C45—C46—H461	109.3
N1—C3—H31	109.8	C47—C46—H461	109.3
C2—C3—H31	109.8	C45—C46—H462	109.3
N1—C3—H32	109.8	C47—C46—H462	109.3
C2—C3—H32	109.8	H461—C46—H462	107.9
H31—C3—H32	108.2	N3—C47—C46	110.1 (5)
N1—C4—C5	121.7 (6)	N3—C47—H471	109.6
N1—C4—H4	119.1	C46—C47—H471	109.6
C5—C4—H4	119.1	N3—C47—H472	109.6
C10—C5—C6	118.1 (7)	C46—C47—H472	109.6
C10—C5—C4	120.3 (7)	H471—C47—H472	108.1
C6—C5—C4	121.5 (6)	N3—C48—C49	123.4 (6)
O3—C6—C7	119.5 (7)	N3—C48—H48	118.3
O3—C6—C5	120.6 (6)	C49—C48—H48	118.3
C7—C6—C5	119.9 (7)	C54—C49—C50	118.3 (7)
C8—C7—C6	120.8 (8)	C54—C49—C48	122.3 (7)
C8—C7—H7	119.6	C50—C49—C48	119.3 (7)
C6—C7—H7	119.6	O11—C50—C51	117.5 (7)
C7—C8—C9	120.4 (8)	O11—C50—C49	123.0 (7)
C7—C8—H8	119.8	C51—C50—C49	119.5 (8)
C9—C8—H8	119.8	C52—C51—C50	120.4 (8)
C10—C9—C8	119.3 (8)	C52—C51—H51	119.8
C10—C9—H9	120.4	C50—C51—H51	119.8
C8—C9—H9	120.4	C53—C52—C51	120.5 (9)
C9—C10—C5	121.5 (8)	C53—C52—H52	119.7
C9—C10—H10	119.3	C51—C52—H52	119.7
C5—C10—H10	119.3	C54—C53—C52	119.9 (9)
O5—C11—O4	123.9 (5)	C54—C53—H53	120.1
O5—C11—C12	118.8 (5)	C52—C53—H53	120.1
O4—C11—C12	117.1 (5)	C53—C54—C49	121.3 (8)
C11—C12—C13	114.2 (5)	C53—C54—H54	119.4
C11—C12—H121	108.7	C49—C54—H54	119.4
C13—C12—H121	108.7	O12—C55—O13	123.5 (5)
C11—C12—H122	108.7	O12—C55—C56	119.0 (5)
C13—C12—H122	108.7	O13—C55—C56	117.2 (5)
H121—C12—H122	107.6	C55—C56—C57	112.8 (5)
N2—C13—C12	110.8 (5)	C55—C56—H561	109.0
N2—C13—H131	109.5	C57—C56—H561	109.0
C12—C13—H131	109.5	C55—C56—H562	109.0
N2—C13—H132	109.5	C57—C56—H562	109.0
C12—C13—H132	109.5	H561—C56—H562	107.8

H131—C13—H132	108.1	N4—C57—C56	109.9 (5)
N2—C14—C15	122.8 (6)	N4—C57—H571	109.7
N2—C14—H141	118.6	C56—C57—H571	109.7
C15—C14—H141	118.6	N4—C57—H572	109.7
C20—C15—C16	118.8 (6)	C56—C57—H572	109.7
C20—C15—C14	119.6 (6)	H571—C57—H572	108.2
C16—C15—C14	121.6 (6)	N4—C58—C59	123.3 (6)
O6—C16—C17	118.1 (6)	N4—C58—H58	118.3
O6—C16—C15	121.4 (6)	C59—C58—H58	118.3
C17—C16—C15	120.5 (6)	C64—C59—C60	118.8 (6)
C16—C17—C18	118.7 (7)	C64—C59—C58	119.8 (6)
C16—C17—H17	120.7	C60—C59—C58	121.4 (6)
C18—C17—H17	120.7	O14—C60—C61	117.8 (6)
C19—C18—C17	121.4 (7)	O14—C60—C59	122.1 (6)
C19—C18—H18	119.3	C61—C60—C59	120.1 (7)
C17—C18—H18	119.3	C62—C61—C60	120.4 (7)
C20—C19—C18	119.5 (7)	C62—C61—H61	119.8
C20—C19—H19	120.2	C60—C61—H61	119.8
C18—C19—H19	120.2	C61—C62—C63	120.3 (7)
C19—C20—C15	121.0 (7)	C61—C62—H62	119.9
C19—C20—H20	119.5	C63—C62—H62	119.9
C15—C20—H20	119.5	C64—C63—C62	120.1 (7)
C22—C21—Sn1	115.5 (4)	C64—C63—H63	120.0
C22—C21—H211	108.4	C62—C63—H63	120.0
Sn1—C21—H211	108.4	C63—C64—C59	120.3 (7)
C22—C21—H212	108.4	C63—C64—H64	119.8
Sn1—C21—H212	108.4	C59—C64—H64	119.8
H211—C21—H212	107.5	C66—C65—Sn4	113.4 (4)
C21—C22—C23	112.3 (5)	C66—C65—H651	108.9
C21—C22—H221	109.1	Sn4—C65—H651	108.9
C23—C22—H221	109.1	C66—C65—H652	108.9
C21—C22—H222	109.1	Sn4—C65—H652	108.9
C23—C22—H222	109.1	H651—C65—H652	107.7
H221—C22—H222	107.9	C67—C66—C65	113.9 (5)
C24—C23—C22	112.1 (6)	C67—C66—H661	108.8
C24—C23—H231	109.2	C65—C66—H661	108.8
C22—C23—H231	109.2	C67—C66—H662	108.8
C24—C23—H232	109.2	C65—C66—H662	108.8
C22—C23—H232	109.2	H661—C66—H662	107.7
H231—C23—H232	107.9	C66—C67—C68	113.4 (6)
C23—C24—H241	109.5	C66—C67—H671	108.9
C23—C24—H242	109.5	C68—C67—H671	108.9
H241—C24—H242	109.5	C66—C67—H672	108.9
C23—C24—H243	109.5	C68—C67—H672	108.9
H241—C24—H243	109.5	H671—C67—H672	107.7
H242—C24—H243	109.5	C67—C68—H681	109.5
C26—C25—Sn1	115.3 (4)	C67—C68—H682	109.5
C26—C25—H251	108.4	H681—C68—H682	109.5

Sn1—C25—H251	108.4	C67—C68—H683	109.5
C26—C25—H252	108.4	H681—C68—H683	109.5
Sn1—C25—H252	108.4	H682—C68—H683	109.5
H251—C25—H252	107.5	C70—C69—Sn4	116.3 (4)
C27—C26—C25	115.3 (5)	C70—C69—H691	108.2
C27—C26—H261	108.5	Sn4—C69—H691	108.2
C25—C26—H261	108.5	C70—C69—H692	108.2
C27—C26—H262	108.5	Sn4—C69—H692	108.2
C25—C26—H262	108.5	H691—C69—H692	107.4
H261—C26—H262	107.5	C69—C70—C71	112.5 (5)
C26—C27—C28	115.7 (7)	C69—C70—H701	109.1
C26—C27—H271	108.4	C71—C70—H701	109.1
C28—C27—H271	108.4	C69—C70—H702	109.1
C26—C27—H272	108.4	C71—C70—H702	109.1
C28—C27—H272	108.4	H701—C70—H702	107.8
H271—C27—H272	107.4	C72—C71—C70	113.5 (6)
C27—C28—H281	109.5	C72—C71—H711	108.9
C27—C28—H282	109.5	C70—C71—H711	108.9
H281—C28—H282	109.5	C72—C71—H712	108.9
C27—C28—H283	109.5	C70—C71—H712	108.9
H281—C28—H283	109.5	H711—C71—H712	107.7
H282—C28—H283	109.5	C71—C72—H721	109.5
C30—C29—Sn2	112.0 (4)	C71—C72—H722	109.5
C30—C29—H291	109.2	H721—C72—H722	109.5
Sn2—C29—H291	109.2	C71—C72—H723	109.5
C30—C29—H292	109.2	H721—C72—H723	109.5
Sn2—C29—H292	109.2	H722—C72—H723	109.5

Sn1—O2—C1—O1	2.8 (5)	Sn3—C37—C38—C39	176.0 (4)
Sn1—O2—C1—C2	178.7 (6)	C37—C38—C39—C40	179.1 (6)
Sn1—O1—C1—O2	−4.1 (7)	Sn3—C41—C42—C43	−176.1 (4)
Sn3—O1—C1—O2	−169.8 (4)	C41—C42—C43—C44	−166.9 (5)
Sn1—O1—C1—C2	179.7 (4)	Sn4—O10—C45—O9	−3.7 (5)
Sn3—O1—C1—C2	14.1 (10)	Sn4—O10—C45—C46	177.5 (6)
O2—C1—C2—C3	43.1 (8)	Sn4—O9—C45—O10	5.2 (7)
O1—C1—C2—C3	−140.8 (5)	Sn2—O9—C45—O10	164.3 (5)
C4—N1—C3—C2	−116.4 (6)	Sn4—O9—C45—C46	−175.9 (4)
C1—C2—C3—N1	62.4 (7)	Sn2—O9—C45—C46	−16.9 (11)
C3—N1—C4—C5	176.3 (5)	O10—C45—C46—C47	−43.4 (9)
N1—C4—C5—C10	179.1 (6)	O9—C45—C46—C47	137.8 (6)
N1—C4—C5—C6	−3.7 (10)	C48—N3—C47—C46	121.0 (7)
C10—C5—C6—O3	−178.6 (6)	C45—C46—C47—N3	−63.9 (7)
C4—C5—C6—O3	4.2 (10)	C47—N3—C48—C49	−178.0 (5)
C10—C5—C6—C7	1.9 (10)	N3—C48—C49—C54	−177.5 (7)
C4—C5—C6—C7	−175.3 (7)	N3—C48—C49—C50	3.6 (10)
O3—C6—C7—C8	178.6 (8)	C54—C49—C50—O11	178.9 (7)
C5—C6—C7—C8	−1.9 (12)	C48—C49—C50—O11	−2.0 (10)
C6—C7—C8—C9	0.1 (14)	C54—C49—C50—C51	−0.6 (10)

C7—C8—C9—C10	1.6 (14)	C48—C49—C50—C51	178.4 (6)
C8—C9—C10—C5	−1.5 (13)	O11—C50—C51—C52	−178.2 (7)
C6—C5—C10—C9	−0.2 (11)	C49—C50—C51—C52	1.4 (12)
C4—C5—C10—C9	177.0 (7)	C50—C51—C52—C53	−0.2 (14)
Sn2—O5—C11—O4	24.4 (8)	C51—C52—C53—C54	−1.7 (14)
Sn2—O5—C11—C12	−151.2 (4)	C52—C53—C54—C49	2.4 (13)
Sn1—O4—C11—O5	21.5 (8)	C50—C49—C54—C53	−1.3 (11)
Sn1—O4—C11—C12	−162.8 (3)	C48—C49—C54—C53	179.7 (7)
O5—C11—C12—C13	−158.8 (5)	Sn4—O12—C55—O13	−20.6 (8)
O4—C11—C12—C13	25.3 (7)	Sn4—O12—C55—C56	165.5 (4)
C14—N2—C13—C12	−129.2 (6)	Sn3—O13—C55—O12	−31.0 (8)
C11—C12—C13—N2	66.6 (7)	Sn3—O13—C55—C56	143.1 (4)
C13—N2—C14—C15	−179.0 (5)	O12—C55—C56—C57	−27.0 (8)
N2—C14—C15—C20	−178.2 (6)	O13—C55—C56—C57	158.6 (5)
N2—C14—C15—C16	1.9 (10)	C58—N4—C57—C56	129.5 (6)
C20—C15—C16—O6	−179.7 (6)	C55—C56—C57—N4	−63.6 (7)
C14—C15—C16—O6	0.2 (10)	C57—N4—C58—C59	−178.4 (5)
C20—C15—C16—C17	−2.5 (10)	N4—C58—C59—C64	180.0 (6)
C14—C15—C16—C17	177.4 (6)	N4—C58—C59—C60	−0.1 (10)
O6—C16—C17—C18	179.1 (6)	C64—C59—C60—O14	178.9 (6)
C15—C16—C17—C18	1.8 (10)	C58—C59—C60—O14	−1.0 (10)
C16—C17—C18—C19	−0.7 (11)	C64—C59—C60—C61	−1.3 (10)
C17—C18—C19—C20	0.2 (12)	C58—C59—C60—C61	178.8 (6)
C18—C19—C20—C15	−0.9 (11)	O14—C60—C61—C62	−178.5 (6)
C16—C15—C20—C19	2.0 (10)	C59—C60—C61—C62	1.6 (11)
C14—C15—C20—C19	−177.9 (6)	C60—C61—C62—C63	−0.5 (11)
Sn1—C21—C22—C23	−178.1 (5)	C61—C62—C63—C64	−1.0 (11)
C21—C22—C23—C24	−179.8 (6)	C62—C63—C64—C59	1.4 (11)
Sn1—C25—C26—C27	173.7 (5)	C60—C59—C64—C63	−0.3 (10)
C25—C26—C27—C28	177.7 (7)	C58—C59—C64—C63	179.7 (6)
Sn2—C29—C30—C31	169.9 (4)	Sn4—C65—C66—C67	−169.9 (5)
C29—C30—C31—C32	173.5 (6)	C65—C66—C67—C68	−173.5 (6)
Sn2—C33—C34—C35	177.9 (4)	Sn4—C69—C70—C71	−178.7 (4)
C33—C34—C35—C36	66.6 (9)	C69—C70—C71—C72	177.0 (6)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3···N1	0.84	1.83	2.575 (7)	147
O6—H6···N2	0.84	1.88	2.616 (6)	146
O11—H11···N3	0.84	1.87	2.602 (7)	145
O14—H14···N4	0.84	1.90	2.637 (6)	147