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Octabenzyldichlorodi-μ_2-hydroxo-di-μ_3-oxo-tetratin toluene disolvate

E. Mothi Mohamed,[a] Krishnaswamy Panchanatheswaran,[a] John N. Low[b]‡ and Christopher Glidewell[c]*

[a]Department of Chemistry, Bharathidasan University, Tiruchirappalli, Tamil Nadu 620 024, India, [b]Department of Chemistry, University of Aberdeen, Meston Walk, Old Aberdeen AB24 3UE, Scotland, and [c]School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland

‡ Postal address: Department of Electrical Engineering and Physics, University of Dundee, Dundee DD1 4HN, Scotland

Correspondence e-mail: cg@st-andrews.ac.uk

Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.007 Å
R factor = 0.038
wR factor = 0.088
Data-to-parameter ratio = 20.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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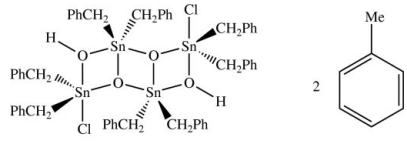
The title tin complex crystallizes as a stoichiometric toluene-solvated dimer of 1,1,3,3-tetrabenzyl-1-chloro-3-hydroxydistannoxane, $[Sn_4(C_7H_7)_8Cl_2O_2(OH)_2]\cdot 2C_7H_8$. The tetranuclear molecule lies across a centre of inversion in space group $P2_1/n$; the Sn_4O_4 framework, in which the two independent Sn centres both have distorted trigonal bipyramidal coordination, is essentially planar.

Comment

The organotin component of the title compound, (I), was obtained as an adventitious product of the partial hydrolysis of dibenzyldichlorotin(IV) during the attempted preparation of adducts of this tin precursor complex with amines. It crystallizes from toluene as the stoichiometric disolvate 1,1,3,3-tetrabenzyl-1-chloro-3-hydroxydistannoxane–toluene (1/2).



(I)

The tetranuclear molecule is a dimeric form of the simple distannoxane $ClSn(CH_2Ph)_2OSn(CH_2Ph)_2OH$. The dimer lies across a centre of inversion and the Sn_4O_4 framework, which is essentially planar, takes the form of three edge-fused Sn_2O_2 rings (Fig. 1 and Table 1). Each of the two independent Sn atoms is five-coordinate, adopting approximate trigonal

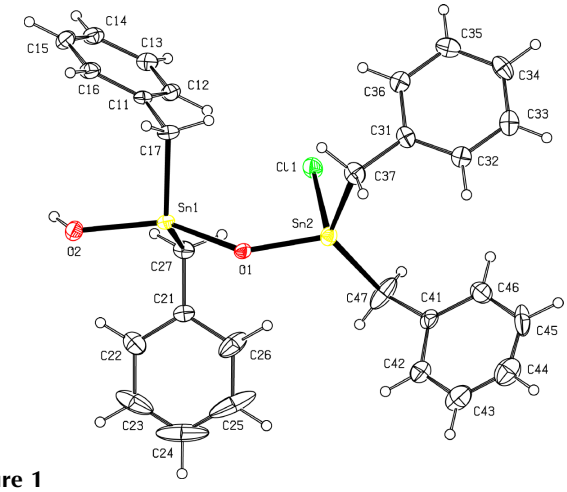


Figure 1
The asymmetric unit of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level. For the sake of clarity, the toluene solvent molecule has been omitted.

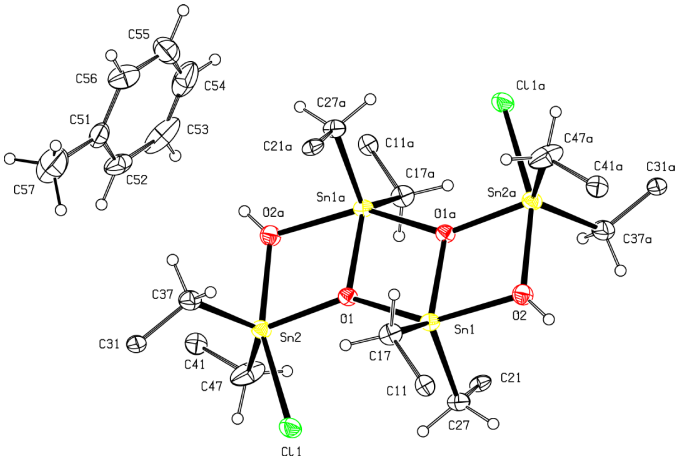


Figure 2
The centrosymmetric distannoxane dimer and the unique toluene solvent molecule. Displacement ellipsoids are drawn at the 30% probability level. For the sake of clarity, the phenyl ring atoms C*n*2–C*n*6 (n = 1–4) and the associated H atoms have been omitted. The atoms with the suffix a are at the symmetry position $(1-x, 1-y, 1-z)$.

bipyramidal coordination, as demonstrated by the bond angles (Table 1): the benzyl groups occupy equatorial sites and the unique Cl bonded to Sn2 occupies an axial site.

This type of molecular architecture appears to be rather characteristic of functionalized distannoxanes $X\mathrm{Sn}R_2\mathrm{OSn}R_2Y$, where X and Y are electron-rich substituents, such as OH, Cl, I or NCS, all of which are capable of coordinating to a second Sn atom (Chow, 1971; Puff *et al.*, 1981; Graziani *et al.*, 1983; Blair *et al.*, 1997; Dakternieks *et al.*, 1997; Lu *et al.*, 2001). The present example is unusual only inasmuch as the two electron-rich substituents X and Y are different, here Cl and OH; in most previously reported examples, these two substituents are the same, although an example with X = I and Y = OEt has been reported by Blair *et al.* (1997).

The Sn—O distances for the equatorial sites are slightly shorter than those for the axial sites (Table 1) and the Sn—C distances lie in the rather narrow range 2.144 (3)–2.156 (4) Å. There are no direction-specific interactions between the dimeric tin units. In particular, the hydroxyl group acts neither as a donor nor as an acceptor of hydrogen bonds: there are no O or C atoms within 3.6 Å of atom O2 other than those in the same dimer unit, and none of these is appropriately positioned to act as a hydrogen-bond donor or acceptor. It is likely that the hydroxyl group at (x, y, z) is effectively shielded by the adjacent benzyl substituents, especially by the phenyl rings C11–C16 and C21–C26 at (x, y, z) and C41–C46 at $(1-x, 1-y, 1-z)$ (Figs. 1 and 2).

Experimental

The title distannoxane was obtained as an adventitious product from the attempted reaction of dibenzyldichlorotin(IV) with either 2-(dimethylamino)pyridine or *N,N,N′,N′*-tetramethylethylenediamine. Crystallization from toluene solution gave the stoichiometric disolvate (I) in each case. Crystals of both were examined, and they proved to have identical cell dimensions; data sets were collected for both and they gave essentially identical refinements.

Crystal data

$[Sn_4(C_7H_7)Cl_2O_2(OH)_2]\cdot 2C_7H_8$	D_x = 1.594 Mg m^{-3}
M_r = 1525.03	Mo Kα radiation
Monoclinic, $P2_1/n$	Cell parameters from 7235 reflections
a = 10.0738 (2) Å	θ = 3.3–27.5°
b = 15.5680 (3) Å	μ = 1.69 mm^{-1}
c = 20.3943 (3) Å	T = 120 (2) K
β = 96.6730 (10)°	Block, colourless
V = 3176.75 (10) Å^3	0.40 × 0.20 × 0.10 mm
Z = 2	

Data collection

Nonius KappaCCD diffractometer	5628 reflections with $I > 2\sigma(I)$
φ scans, and ω scans with κ offsets	R_{int} = 0.074
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995, 1997)	θ_{max} = 27.5°
T_{min} = 0.552, T_{max} = 0.850	$h = -13 \rightarrow 13$
38321 measured reflections	$k = -20 \rightarrow 20$
7235 independent reflections	$l = -26 \rightarrow 26$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 3.0069P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$(\Delta/\sigma)_{max}$ = 0.002
$wR(F^2)$ = 0.088	$\Delta\rho_{max}$ = 1.03 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −1.08 e Å^{-3}
7235 reflections	
361 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.132 (2)	Sn2—O1	2.024 (2)
Sn1—O2	2.147 (2)	Sn2—Cl1	2.4819 (10)
Sn1—C17	2.143 (3)	Sn2—C37	2.145 (4)
Sn1—C27	2.146 (3)	Sn2—C47	2.156 (4)
Sn1—O1^{i}	2.051 (2)	Sn2—O2^{i}	2.197 (3)
O1—Sn1—O2	146.07 (9)	Cl1—Sn2—O2^{i}	159.64 (7)
O1—Sn1—O1^{i}	73.34 (10)	Cl1—Sn2—O1	87.55 (7)
O1—Sn1—C17	100.30 (12)	Cl1—Sn2—C37	96.70 (12)
O1—Sn1—C27	99.02 (12)	Cl1—Sn2—C47	95.02 (13)
O2—Sn1—C17	97.73 (13)	O2^{i}—Sn2—O1	72.21 (10)
O2—Sn1—C27	96.07 (13)	O2^{i}—Sn2—C37	93.47 (13)
O2—Sn1—O1^{i}	72.76 (10)	O2^{i}—Sn2—C47	92.76 (15)
O1^{i}—Sn1—C17	120.11 (12)	O1—Sn2—C37	113.48 (13)
O1^{i}—Sn1—C27	119.09 (11)	O1—Sn2—C47	118.24 (18)
C17—Sn1—C27	120.70 (14)	C37—Sn2—C47	127.27 (19)
Sn1—O1—Sn2	140.75 (11)	Sn1^{i}—O1—Sn2	112.52 (11)
Sn1^{i}—O1—Sn1	106.66 (10)	Sn1—O2—Sn2^{i}	102.50 (11)
O2—Sn1—C17—C11	−62.5 (3)	O1—Sn2—C37—C31	−148.5 (3)
Sn1—C17—C11—C12	−69.0 (4)	Sn2—C37—C31—C32	−84.2 (4)
O2—Sn1—C27—C21	−81.4 (3)	O1—Sn2—C47—C41	−124.5 (3)
Sn1—C27—C21—C22	93.1 (4)	Sn2—C47—C41—C42	93.2 (4)

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

All H atoms were located from difference maps and then treated as riding atoms. H atoms bonded to C atoms were assigned C—H distances of 0.95 (aromatic) or 0.99 Å (CH_2), with U_{iso}(H) = 1.2U_{eq}(C); the H atom bonded to O2 was assigned an O—H distance of 0.84 Å and a U_{iso}(H) value of 1.2U_{eq}(O). The anisotropic displacement parameter values gave some indication of libration about Sn—C bonds in several of the benzyl groups: however, it did not prove possible to account for this using a static disorder model. The highest maximum is the diference map is adjacemt to the C45—C46 bond, 1.15 Å from C45 and 1.00 Å from C46; the deepest hole is 0.85 Å from Sn2.

Data collection: *KappaCCD Server Software* (Nonius, 1997); cell refinement: *DENZO–SMN* (Otwinowski & Minor, 1997); data

reduction: *DENZO–SMN*; program(s) used to solve structure: *OSCAIL* (McArdle, 2003) and *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *OSCAIL* and *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL*97 and *PRPKAPPA* (Ferguson, 1999).

X-ray data were collected at the EPSRC X-ray Crystallographic Service, University of Southampton, England; the authors thank the staff for all their help and advice. JNL thanks NCR Self-Service, Dundee, for grants which have provided computing facilities for this work.

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supporting information

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(I)

Crystal data

$[Sn_4(C_7H_7)Cl_2O_2(OH)_2]\cdot 2C_7H_8$
$M_r = 1525.03$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 10.0738$ (2) Å
$b = 15.5680$ (3) Å
$c = 20.3943$ (3) Å
$\beta = 96.673$ (1)°
$V = 3176.75$ (10) Å^3
$Z = 2$
$F(000) = 1520$
$D_x = 1.594$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7235 reflections
$\theta = 3.3$–27.5°
$\mu = 1.69$ mm^{-1}
$T = 120$ K
Block, colourless
0.40 × 0.20 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: rotating anode
Graphite monochromator
φ scans, and ω scans with κ offsets
Absorption correction: multi-scan (SORTAV; Blessing, 1995, 1997)
$T_{min} = 0.552$, $T_{max} = 0.850$
38321 measured reflections
7235 independent reflections
5628 reflections with $I > 2\sigma(I)$
$R_{int} = 0.074$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -13\rightarrow13$
$k = -20\rightarrow20$
$l = -26\rightarrow26$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.039$
$wR(F^2) = 0.088$
$S = 1.04$
7235 reflections
361 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
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 3.0069P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 1.03$ e Å^{-3}
$\Delta\rho_{min} = -1.08$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.47186 (2)	0.400543 (15)	0.526877 (11)	0.02463 (8)	
Sn2	0.38725 (2)	0.613123 (16)	0.615749 (12)	0.02976 (8)	

Cl1	0.31601 (10)	0.48300 (6)	0.67267 (5)	0.0391 (2)
O1	0.4503 (2)	0.53387 (15)	0.54706 (11)	0.0257 (5)
O2	0.5363 (2)	0.30670 (17)	0.46019 (12)	0.0338 (6)
C11	0.5656 (3)	0.2717 (2)	0.63170 (16)	0.0280 (8)
C12	0.4452 (4)	0.2526 (2)	0.65557 (18)	0.0330 (8)
C13	0.4112 (4)	0.1698 (2)	0.67068 (18)	0.0358 (9)
C14	0.4984 (4)	0.1025 (2)	0.66102 (19)	0.0359 (9)
C15	0.6181 (4)	0.1201 (2)	0.6384 (2)	0.0386 (9)
C16	0.6522 (4)	0.2042 (3)	0.62379 (18)	0.0356 (9)
C17	0.5992 (4)	0.3619 (2)	0.61338 (18)	0.0338 (8)
C21	0.1925 (3)	0.4032 (2)	0.45308 (18)	0.0284 (8)
C22	0.1784 (4)	0.3588 (3)	0.3935 (2)	0.0465 (11)
C23	0.1146 (5)	0.3957 (6)	0.3372 (3)	0.084 (2)
C24	0.0619 (6)	0.4748 (6)	0.3382 (4)	0.111 (3)
C25	0.0737 (6)	0.5207 (4)	0.3969 (5)	0.105 (3)
C26	0.1393 (4)	0.4847 (3)	0.4539 (3)	0.0618 (14)
C27	0.2647 (3)	0.3649 (3)	0.51373 (18)	0.0327 (8)
C31	0.5053 (3)	0.6673 (2)	0.75837 (18)	0.0322 (8)
C32	0.4554 (4)	0.7470 (2)	0.77449 (19)	0.0350 (9)
C33	0.4260 (4)	0.7653 (3)	0.8375 (2)	0.0409 (10)
C34	0.4463 (4)	0.7043 (3)	0.8862 (2)	0.0430 (10)
C35	0.4933 (4)	0.6240 (3)	0.8716 (2)	0.0415 (10)
C36	0.5223 (4)	0.6056 (3)	0.8078 (2)	0.0367 (9)
C37	0.5432 (4)	0.6508 (3)	0.69090 (19)	0.0396 (9)
C41	0.1906 (3)	0.7620 (2)	0.60061 (19)	0.0336 (9)
C42	0.1958 (4)	0.8100 (3)	0.5442 (2)	0.0479 (11)
C43	0.2033 (5)	0.8968 (3)	0.5428 (3)	0.0645 (14)
C44	0.2060 (5)	0.9399 (4)	0.5986 (3)	0.0645 (14)
C45	0.1993 (5)	0.9013 (4)	0.6576 (3)	0.0660 (17)
C46	0.1896 (4)	0.8070 (4)	0.6590 (2)	0.0608 (14)
C47	0.1893 (4)	0.6669 (3)	0.5971 (3)	0.0643 (15)
C51	0.7260 (5)	0.8822 (3)	0.6469 (2)	0.0468 (11)
C52	0.5969 (5)	0.8867 (3)	0.6167 (3)	0.0600 (15)
C53	0.5732 (6)	0.8918 (3)	0.5481 (4)	0.078 (2)
C54	0.6756 (9)	0.8928 (3)	0.5118 (3)	0.084 (2)
C55	0.8000 (7)	0.8893 (3)	0.5407 (3)	0.0664 (15)
C56	0.8286 (5)	0.8841 (3)	0.6077 (3)	0.0544 (12)
C57	0.7563 (9)	0.8762 (5)	0.7207 (3)	0.122 (3)
H2	0.5182	0.2541	0.4618	0.041*
H12	0.3847	0.2979	0.6616	0.040*
H13	0.3290	0.1586	0.6876	0.043*
H14	0.4748	0.0450	0.6701	0.043*
H15	0.6786	0.0746	0.6325	0.046*
H16	0.7359	0.2154	0.6082	0.043*
H17A	0.6938	0.3650	0.6048	0.041*
H17B	0.5869	0.4013	0.6503	0.041*
H22	0.2132	0.3023	0.3917	0.056*
H23	0.1079	0.3647	0.2968	0.101*

H24	0.0168	0.4991	0.2991	0.133*	
H25	0.0369	0.5768	0.3981	0.127*	
H26	0.1476	0.5165	0.4939	0.074*	
H27A	0.2575	0.3015	0.5111	0.039*	
H27B	0.2220	0.3840	0.5526	0.039*	
H32	0.4413	0.7899	0.7413	0.042*	
H33	0.3917	0.8202	0.8471	0.049*	
H34	0.4280	0.7172	0.9297	0.052*	
H35	0.5060	0.5813	0.9050	0.050*	
H36	0.5540	0.5501	0.7980	0.044*	
H37A	0.6124	0.6053	0.6945	0.048*	
H37B	0.5851	0.7037	0.6758	0.048*	
H42	0.1938	0.7801	0.5035	0.057*	
H43	0.2067	0.9262	0.5022	0.077*	
H44	0.2130	1.0007	0.5973	0.077*	
H45	0.2009	0.9341	0.6970	0.079*	
H46	0.1827	0.7776	0.6992	0.073*	
H47A	0.1484	0.6488	0.5528	0.077*	
H47B	0.1334	0.6441	0.6300	0.077*	
H52	0.5241	0.8863	0.6424	0.072*	
H53	0.4841	0.8945	0.5270	0.094*	
H54	0.6589	0.8961	0.4651	0.101*	
H55	0.8714	0.8904	0.5141	0.080*	
H56	0.9189	0.8817	0.6272	0.065*	
H57A	0.8468	0.8535	0.7320	0.183*	0.50
H57B	0.6917	0.8377	0.7381	0.183*	0.50
H57C	0.7502	0.9334	0.7402	0.183*	0.50
H57D	0.6790	0.8963	0.7415	0.183*	0.50
H57E	0.8341	0.9120	0.7354	0.183*	0.50
H57F	0.7756	0.8164	0.7334	0.183*	0.50

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02328 (13)	0.02541 (13)	0.02479 (13)	0.00154 (9)	0.00109 (9)	0.00599 (10)
Sn2	0.02910 (14)	0.02791 (15)	0.03366 (15)	0.00235 (10)	0.00955 (11)	0.00097 (10)
Cl1	0.0486 (6)	0.0358 (5)	0.0352 (5)	−0.0013 (4)	0.0148 (4)	0.0039 (4)
O1	0.0289 (13)	0.0233 (13)	0.0253 (12)	0.0027 (9)	0.0044 (10)	0.0051 (10)
O2	0.0361 (14)	0.0292 (14)	0.0371 (14)	0.0033 (11)	0.0081 (12)	0.0004 (11)
C11	0.0285 (19)	0.033 (2)	0.0205 (17)	0.0049 (15)	−0.0045 (14)	0.0040 (15)
C12	0.033 (2)	0.033 (2)	0.033 (2)	0.0057 (16)	0.0023 (16)	0.0053 (16)
C13	0.034 (2)	0.040 (2)	0.033 (2)	−0.0006 (17)	0.0016 (16)	0.0058 (17)
C14	0.044 (2)	0.027 (2)	0.034 (2)	−0.0016 (17)	−0.0068 (17)	0.0031 (16)
C15	0.041 (2)	0.032 (2)	0.042 (2)	0.0094 (17)	−0.0018 (18)	0.0014 (17)
C16	0.031 (2)	0.042 (2)	0.033 (2)	0.0062 (17)	−0.0005 (16)	0.0078 (17)
C17	0.032 (2)	0.037 (2)	0.0306 (19)	0.0026 (16)	−0.0055 (16)	0.0099 (17)
C21	0.0207 (17)	0.031 (2)	0.0326 (19)	−0.0069 (14)	−0.0015 (14)	0.0056 (15)
C22	0.024 (2)	0.078 (3)	0.038 (2)	0.000 (2)	0.0022 (17)	−0.008 (2)

C23	0.029 (3)	0.190 (8)	0.033 (3)	−0.013 (4)	0.000 (2)	0.014 (4)
C24	0.037 (3)	0.183 (9)	0.102 (5)	−0.041 (4)	−0.033 (3)	0.101 (6)
C25	0.052 (3)	0.059 (4)	0.189 (8)	−0.015 (3)	−0.058 (4)	0.062 (5)
C26	0.042 (3)	0.035 (3)	0.100 (4)	0.001 (2)	−0.028 (3)	−0.003 (2)
C27	0.0278 (19)	0.039 (2)	0.032 (2)	−0.0045 (16)	0.0036 (16)	0.0058 (17)
C31	0.0242 (18)	0.039 (2)	0.034 (2)	−0.0081 (16)	0.0074 (15)	−0.0056 (17)
C32	0.031 (2)	0.035 (2)	0.040 (2)	−0.0055 (16)	0.0082 (17)	0.0010 (17)
C33	0.031 (2)	0.040 (2)	0.053 (3)	−0.0071 (17)	0.0098 (18)	−0.011 (2)
C34	0.038 (2)	0.059 (3)	0.033 (2)	−0.014 (2)	0.0116 (18)	−0.010 (2)
C35	0.039 (2)	0.047 (3)	0.038 (2)	−0.0115 (19)	0.0019 (18)	0.0078 (19)
C36	0.031 (2)	0.036 (2)	0.043 (2)	−0.0024 (16)	0.0039 (17)	−0.0016 (18)
C37	0.032 (2)	0.047 (3)	0.040 (2)	−0.0056 (18)	0.0085 (17)	−0.0023 (19)
C41	0.0215 (18)	0.038 (2)	0.041 (2)	0.0083 (15)	0.0025 (16)	−0.0013 (18)
C42	0.047 (3)	0.048 (3)	0.049 (3)	0.013 (2)	0.006 (2)	0.002 (2)
C43	0.060 (3)	0.055 (3)	0.080 (4)	0.014 (2)	0.014 (3)	0.014 (3)
C44	0.050 (3)	0.055 (3)	0.086 (4)	0.002 (2)	0.000 (3)	−0.003 (3)
C45	0.042 (3)	0.085 (4)	0.068 (4)	0.019 (2)	−0.008 (2)	−0.053 (3)
C46	0.044 (3)	0.100 (4)	0.037 (2)	0.034 (3)	0.001 (2)	−0.005 (3)
C47	0.028 (2)	0.035 (3)	0.132 (5)	0.0054 (18)	0.018 (3)	0.011 (3)
C51	0.069 (3)	0.034 (2)	0.036 (2)	−0.016 (2)	0.000 (2)	−0.0021 (18)
C52	0.048 (3)	0.027 (2)	0.112 (5)	−0.0037 (19)	0.040 (3)	−0.009 (3)
C53	0.063 (4)	0.039 (3)	0.119 (6)	−0.013 (2)	−0.050 (4)	0.024 (3)
C54	0.148 (7)	0.054 (4)	0.044 (3)	−0.039 (4)	−0.021 (4)	0.007 (2)
C55	0.093 (4)	0.051 (3)	0.062 (4)	0.003 (3)	0.037 (3)	−0.002 (3)
C56	0.037 (2)	0.050 (3)	0.075 (4)	0.001 (2)	0.001 (2)	0.017 (2)
C57	0.213 (9)	0.109 (6)	0.041 (3)	−0.086 (6)	−0.003 (4)	0.007 (3)

Geometric parameters (Å, º)

Sn1—O1	2.132 (2)	C31—C32	1.392 (5)
Sn1—O2	2.147 (2)	C32—C33	1.382 (6)
Sn1—C17	2.143 (3)	C32—H32	0.95
Sn1—C27	2.146 (3)	C33—C34	1.372 (6)
Sn1—O1^{i}	2.051 (2)	C33—H33	0.95
Sn2—O1	2.024 (2)	C34—C35	1.381 (6)
Sn2—Cl1	2.4819 (10)	C34—H34	0.95
Sn2—C37	2.145 (4)	C35—C36	1.396 (6)
Sn2—C47	2.156 (4)	C35—H35	0.95
Sn2—O2^{i}	2.197 (3)	C36—H36	0.95
O2—H2	0.84	C47—C41	1.482 (6)
C17—C11	1.502 (5)	C47—H47A	0.99
C17—H17A	0.99	C47—H47B	0.99
C17—H17B	0.99	C41—C42	1.377 (6)
C11—C16	1.387 (5)	C41—C46	1.382 (6)
C11—C12	1.391 (5)	C42—C43	1.354 (6)
C12—C13	1.378 (5)	C42—H42	0.95
C12—H12	0.95	C43—C44	1.318 (7)
C13—C14	1.395 (5)	C43—H43	0.95

C13—H13	0.95	C44—C45	1.354 (8)
C14—C15	1.369 (6)	C44—H44	0.95
C14—H14	0.95	C45—C46	1.472 (8)
C15—C16	1.394 (5)	C45—H45	0.95
C15—H15	0.95	C46—H46	0.95
C16—H16	0.95	C51—C52	1.374 (7)
C27—C21	1.486 (5)	C51—C56	1.380 (7)
C27—H27A	0.99	C51—C57	1.503 (7)
C27—H27B	0.99	C52—C53	1.394 (9)
C21—C26	1.377 (5)	C52—H52	0.95
C21—C22	1.391 (5)	C53—C54	1.338 (10)
C22—C23	1.376 (7)	C53—H53	0.95
C22—H22	0.95	C54—C55	1.322 (9)
C23—C24	1.341 (10)	C54—H54	0.95
C23—H23	0.95	C55—C56	1.366 (7)
C24—C25	1.387 (11)	C55—H55	0.95
C24—H24	0.95	C56—H56	0.95
C25—C26	1.387 (8)	C57—H57A	0.98
C25—H25	0.95	C57—H57B	0.98
C26—H26	0.95	C57—H57C	0.98
C37—C31	1.492 (5)	C57—H57D	0.98
C37—H37A	0.99	C57—H57E	0.98
C37—H37B	0.99	C57—H57F	0.98
C31—C36	1.388 (5)		

O1—Sn1—O2	146.07 (9)	C36—C31—C37	121.8 (4)
O1—Sn1—O1^{i}	73.34 (10)	C32—C31—C37	120.6 (4)
O1—Sn1—C17	100.30 (12)	C33—C32—C31	121.7 (4)
O1—Sn1—C27	99.02 (12)	C33—C32—H32	119.1
O2—Sn1—C17	97.73 (13)	C31—C32—H32	119.1
O2—Sn1—C27	96.07 (13)	C34—C33—C32	119.9 (4)
O2—Sn1—O1^{i}	72.76 (10)	C34—C33—H33	120.0
O1^{i}—Sn1—C17	120.11 (12)	C32—C33—H33	120.0
O1^{i}—Sn1—C27	119.09 (11)	C33—C34—C35	119.8 (4)
C17—Sn1—C27	120.70 (14)	C33—C34—H34	120.1
Sn1—O1—Sn2	140.75 (11)	C35—C34—H34	120.1
Sn1^{i}—O1—Sn1	106.66 (10)	C34—C35—C36	120.0 (4)
Cl1—Sn2—O2^{i}	159.64 (7)	C34—C35—H35	120.0
Cl1—Sn2—O1	87.55 (7)	C36—C35—H35	120.0
Cl1—Sn2—C37	96.70 (12)	C31—C36—C35	120.9 (4)
Cl1—Sn2—C47	95.02 (13)	C31—C36—H36	119.5
O2^{i}—Sn2—O1	72.21 (10)	C35—C36—H36	119.5
O2^{i}—Sn2—C37	93.47 (13)	C41—C47—Sn2	112.1 (3)
O2^{i}—Sn2—C47	92.76 (15)	C41—C47—H47A	109.2
O1—Sn2—C37	113.48 (13)	Sn2—C47—H47A	109.2
O1—Sn2—C47	118.24 (18)	C41—C47—H47B	109.2
C37—Sn2—C47	127.27 (19)	Sn2—C47—H47B	109.2
Sn1^{i}—O1—Sn2	112.52 (11)	H47A—C47—H47B	107.9

Sn1—O2—Sn2^{i}	102.50 (11)	C42—C41—C46	116.7 (4)
Sn1—O2—H2	123.7	C42—C41—C47	120.2 (4)
Sn2^{i}—O2—H2	132.7	C46—C41—C47	123.1 (4)
C11—C17—Sn1	109.7 (2)	C43—C42—C41	124.5 (5)
C11—C17—H17A	109.7	C43—C42—H42	117.8
Sn1—C17—H17A	109.7	C41—C42—H42	117.8
C11—C17—H17B	109.7	C44—C43—C42	119.1 (5)
Sn1—C17—H17B	109.7	C44—C43—H43	120.5
H17A—C17—H17B	108.2	C42—C43—H43	120.5
C16—C11—C12	117.7 (3)	C43—C44—C45	122.9 (5)
C16—C11—C17	121.1 (3)	C43—C44—H44	118.6
C12—C11—C17	121.2 (3)	C45—C44—H44	118.6
C13—C12—C11	121.9 (3)	C44—C45—C46	118.0 (4)
C13—C12—H12	119.1	C44—C45—H45	121.0
C11—C12—H12	119.1	C46—C45—H45	121.0
C12—C13—C14	119.6 (4)	C41—C46—C45	118.8 (5)
C12—C13—H13	120.2	C41—C46—H46	120.6
C14—C13—H13	120.2	C45—C46—H46	120.6
C15—C14—C13	119.4 (4)	C52—C51—C56	118.1 (4)
C15—C14—H14	120.3	C52—C51—C57	121.6 (6)
C13—C14—H14	120.3	C56—C51—C57	120.2 (5)
C14—C15—C16	120.6 (4)	C51—C52—C53	119.7 (5)
C14—C15—H15	119.7	C51—C52—H52	120.1
C16—C15—H15	119.7	C53—C52—H52	120.1
C11—C16—C15	120.8 (4)	C54—C53—C52	120.2 (5)
C11—C16—H16	119.6	C54—C53—H53	119.9
C15—C16—H16	119.6	C52—C53—H53	119.9
C21—C27—Sn1	112.0 (2)	C55—C54—C53	120.3 (5)
C21—C27—H27A	109.2	C55—C54—H54	119.8
Sn1—C27—H27A	109.2	C53—C54—H54	119.8
C21—C27—H27B	109.2	C54—C55—C56	121.8 (5)
Sn1—C27—H27B	109.2	C54—C55—H55	119.1
H27A—C27—H27B	107.9	C56—C55—H55	119.1
C26—C21—C22	117.9 (4)	C55—C56—C51	119.8 (5)
C26—C21—C27	120.9 (4)	C55—C56—H56	120.1
C22—C21—C27	121.2 (4)	C51—C56—H56	120.1
C23—C22—C21	120.8 (5)	C51—C57—H57A	109.5
C23—C22—H22	119.6	C51—C57—H57B	109.5
C21—C22—H22	119.6	H57A—C57—H57B	109.5
C24—C23—C22	121.1 (6)	C51—C57—H57C	109.5
C24—C23—H23	119.4	H57A—C57—H57C	109.5
C22—C23—H23	119.4	H57B—C57—H57C	109.5
C23—C24—C25	119.5 (5)	C51—C57—H57D	109.5
C23—C24—H24	120.3	H57A—C57—H57D	141.1
C25—C24—H24	120.3	H57B—C57—H57D	56.3
C26—C25—C24	120.0 (6)	H57C—C57—H57D	56.3
C26—C25—H25	120.0	C51—C57—H57E	109.5
C24—C25—H25	120.0	H57A—C57—H57E	56.3

C21—C26—C25	120.7 (6)	H57B—C57—H57E	141.1
C21—C26—H26	119.7	H57C—C57—H57E	56.3
C25—C26—H26	119.7	H57D—C57—H57E	109.5
C31—C37—Sn2	117.5 (2)	C51—C57—H57F	109.5
C31—C37—H37A	107.9	H57A—C57—H57F	56.3
Sn2—C37—H37A	107.9	H57B—C57—H57F	56.3
C31—C37—H37B	107.9	H57C—C57—H57F	141.1
Sn2—C37—H37B	107.9	H57D—C57—H57F	109.5
H37A—C37—H37B	107.2	H57E—C57—H57F	109.5
C36—C31—C32	117.6 (3)		

C37—Sn2—O1—Sn1^{i}	−84.97 (16)	C22—C23—C24—C25	1.1 (9)
C47—Sn2—O1—Sn1^{i}	84.40 (17)	C23—C24—C25—C26	−0.2 (9)
O2^{i}—Sn2—O1—Sn1^{i}	1.01 (10)	C22—C21—C26—C25	0.1 (7)
Cl1—Sn2—O1—Sn1^{i}	178.79 (10)	C27—C21—C26—C25	179.0 (4)
C37—Sn2—O1—Sn1	91.3 (2)	C24—C25—C26—C21	−0.4 (9)
C47—Sn2—O1—Sn1	−99.3 (2)	O1—Sn2—C37—C31	−148.5 (3)
O2^{i}—Sn2—O1—Sn1	177.3 (2)	C47—Sn2—C37—C31	43.3 (4)
Cl1—Sn2—O1—Sn1	−4.95 (17)	O2^{i}—Sn2—C37—C31	139.4 (3)
O1^{i}—Sn1—O1—Sn2	−176.4 (2)	Cl1—Sn2—C37—C31	−58.3 (3)
C17—Sn1—O1—Sn2	−57.9 (2)	Sn2—C37—C31—C36	98.0 (4)
C27—Sn1—O1—Sn2	65.8 (2)	Sn2—C37—C31—C32	−84.2 (4)
O2—Sn1—O1—Sn2	−178.86 (14)	C36—C31—C32—C33	1.2 (5)
C17—Sn1—O1—Sn1^{i}	118.54 (13)	C37—C31—C32—C33	−176.7 (3)
C27—Sn1—O1—Sn1^{i}	−117.80 (12)	C31—C32—C33—C34	0.2 (6)
O2—Sn1—O1—Sn1^{i}	−2.5 (2)	C32—C33—C34—C35	−1.4 (6)
O1^{i}—Sn1—O2—Sn2^{i}	−0.90 (8)	C33—C34—C35—C36	1.1 (6)
O1—Sn1—O2—Sn2^{i}	1.6 (2)	C32—C31—C36—C35	−1.6 (5)
C17—Sn1—O2—Sn2^{i}	−120.10 (13)	C37—C31—C36—C35	176.3 (3)
C27—Sn1—O2—Sn2^{i}	117.72 (12)	C34—C35—C36—C31	0.4 (6)
O1^{i}—Sn1—C17—C11	−137.0 (2)	O1—Sn2—C47—C41	−124.5 (3)
O1—Sn1—C17—C11	146.4 (2)	C37—Sn2—C47—C41	43.2 (5)
C27—Sn1—C17—C11	39.3 (3)	O2^{i}—Sn2—C47—C41	−53.3 (4)
O2—Sn1—C17—C11	−62.5 (3)	Cl1—Sn2—C47—C41	145.6 (4)
Sn1—C17—C11—C16	109.4 (3)	Sn2—C47—C41—C42	93.2 (4)
Sn1—C17—C11—C12	−69.0 (4)	Sn2—C47—C41—C46	−85.5 (4)
C16—C11—C12—C13	−0.4 (5)	C46—C41—C42—C43	1.8 (6)
C17—C11—C12—C13	178.0 (3)	C47—C41—C42—C43	−176.9 (4)
C11—C12—C13—C14	−1.0 (6)	C41—C42—C43—C44	−0.1 (8)
C12—C13—C14—C15	1.8 (6)	C42—C43—C44—C45	−1.1 (8)
C13—C14—C15—C16	−1.2 (6)	C43—C44—C45—C46	0.4 (8)
C12—C11—C16—C15	1.0 (5)	C42—C41—C46—C45	−2.4 (6)
C17—C11—C16—C15	−177.4 (3)	C47—C41—C46—C45	176.3 (4)
C14—C15—C16—C11	−0.2 (6)	C44—C45—C46—C41	1.4 (6)
O1^{i}—Sn1—C27—C21	−7.7 (3)	C56—C51—C52—C53	0.9 (6)
O1—Sn1—C27—C21	68.2 (3)	C57—C51—C52—C53	−179.7 (5)
C17—Sn1—C27—C21	175.9 (2)	C51—C52—C53—C54	−0.4 (7)
O2—Sn1—C27—C21	−81.4 (3)	C52—C53—C54—C55	−0.2 (8)

Sn1—C27—C21—C26	−85.8 (4)	C53—C54—C55—C56	0.4 (8)
Sn1—C27—C21—C22	93.1 (4)	C54—C55—C56—C51	0.1 (8)
C26—C21—C22—C23	0.8 (6)	C52—C51—C56—C55	−0.7 (7)
C27—C21—C22—C23	−178.2 (4)	C57—C51—C56—C55	179.8 (5)
C21—C22—C23—C24	−1.4 (7)		

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