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Octa-*n*-butylbis(μ_2-4-chloro-3,5-dinitrobenzoato-κ^2O:O')bis(4-chloro-3,5-dinitrobenzoato-κO)di-μ_3-oxo-tetratin(IV)

Aziz-ur-Rehman,[a] Saira Shahzadi,[a] Saqib Ali[a]* and Madeleine Helliwell[b]

[a]Department of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan, and [b]School of Chemistry, University of Manchester, Manchester M13 9PL, England

Correspondence e-mail: drsa54@yahoo.com

Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.005 Å
Disorder in main residue
R factor = 0.032
wR factor = 0.086
Data-to-parameter ratio = 15.3

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

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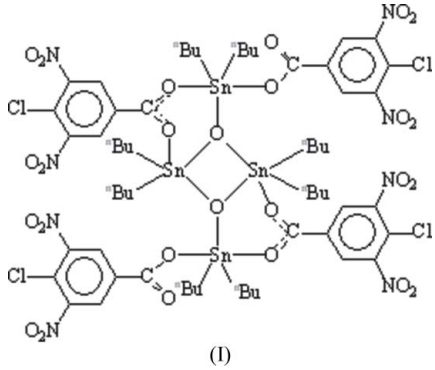
The title compound, $[Sn_4O_2(C_7H_2ClN_2O_6)_4(C_4H_9)_8]$, is a centrosymmetric dimer of an oxoditin(IV) complex. Two dibutylbis[4-chloro-3,5-dinitrobenzoate]tin(IV) units containing monodentate and bridging bidentate carboxylate ligands are connected to the central Sn_2O_2 core. Each Sn atom adopts a distorted trigonal–bipyramidal geometry, with Sn—C distances lying in the narrow range 2.119 (3)–2.135 (3) Å, while Sn—O distances range between 2.037 (2) and 2.286 (2) Å.

Comment

There have been several reports dealing with the impact of organotin chemistry in the biosphere (Gielen, 1994; Ng *et al.*, 1991). Exploration of the structure–activity relationships of such systems has led to numerous reports in recent years (Gielen, 1994; Selvaratnam *et al.*, 1994; McManus *et al.*, 1994). The structural chemistry of organotin carboxylic acid esters has been extensively explored because of the rich diversity of structural motifs (Tiekink, 1994). Among organotin carboxylates, dimeric distannoxanes comprise the most interesting class with respect to their structural chemistry. Reports on crystallographic studies show that these compounds may adopt a variety of structural modes depending on the nature of organic substituents at the Sn atom or carboxylate ligand (Danish *et al.*, 1996). There have been numerous crystallographic reports on these compounds describing their dimeric nature and there are at least five distinct structural types known for them (Tiekink, 1991). In continuation of our studies of organotin(IV) carboxylates (Sadiq-ur-Rehman *et al.*, 2006), we have synthesized the title compound (I), the crystal structure of which is reported here.



(I)

The structure of (I) is composed of a centrosymmetric dimer of oxoditin units (Fig. 1). The endocyclic Sn—O distance in the central core [Sn1—O7 of 2.286 (2) Å] and the endocyclic distance [Sn1—O1 = 2.188 (2) Å] are quite similar

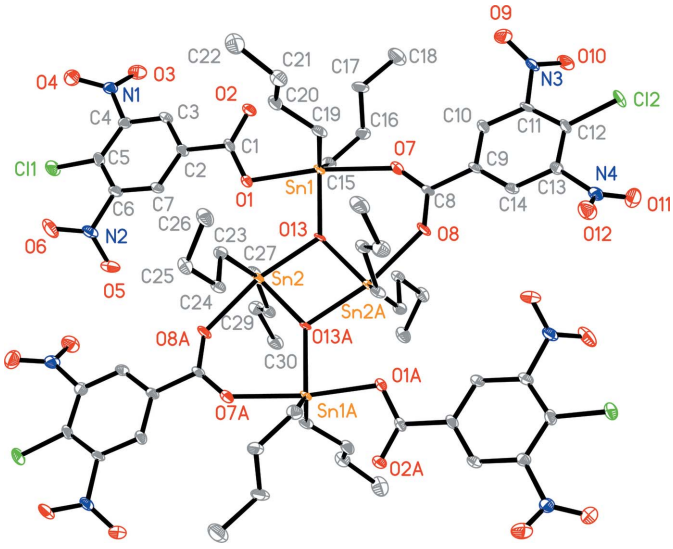


Figure 1
Structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The atoms labelled with A are at the symmetry position ($-x$, $-y$, $-z$). H atoms have been omitted. For clarity, only one component of the disordered butyl group (C15–C18) is shown.

to those observed in the tetrabutylbis(*N*-phthaloylglycinato)-distannoxane dimer (Parvez *et al.*, 2000) and the tetrabutyl-bis(*N*-phthaloylphenylalaninato)distannoxane dimer (Hans *et al.*, 2002). Both independent Sn atoms in (I) are in a five-coordinate O_3C_2Sn distorted trigonal–bipyramidal geometry. The carboxylate ligand shows different modes of coordination with Sn. Firstly, it acts as monodentate, coordinated to Sn1 *via* O1; the Sn1···O2 distance is 2.883 (2) Å, *i.e.* too long to be considered bonding [likewise, the Sn2···O1 distance of 2.913 (2) Å]. In the other coordination mode, the ligand bridges two Sn atoms in a bidentate fashion, thus resulting in a six-membered Sn1—O7—C8—O8—Sn2^{i}—O13 ring [symmetry code: (i) $-x$, $-y$, $-z$]. The Sn—C distances lie in the very narrow range 2.119 (3)–2.135 (3) Å, while the Sn—O distances range between 2.037 (2) and 2.286 (2) Å (Table 1).

Experimental

A mixture of 3,5-dinitro-4-chlorobenzoic acid (2 g, 1 mmol) and di-*n*-butyltin oxide (2.02 g, 1 mmol) was refluxed in dry toluene (150 ml) for 5–6 h using a Dean and Stark trap. The reaction mixture was cooled to room temperature and solvent was evaporated under reduced pressure. The solid product was recrystallized from chloroform, resulting in rod-shaped crystals of (I) (yield 85%, m.p. 513–514 K).

Crystal data

$[Sn_4O_2(C_7H_2ClN_2O_6)_4(C_4H_9)_8]$
M_r = 1945.88
Triclinic, $P\overline{1}$
a = 12.1784 (11) Å
b = 12.5143 (12) Å
c = 13.5682 (12) Å
α = 104.597 (1)°
β = 110.770 (1)°
γ = 95.960 (1)°
V = 1827.9 (3) Å^3
Z = 1
D_x = 1.768 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.58 mm^{-1}
T = 100 (2) K
Rod, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.571, T_{max} = 0.743
14580 measured reflections
7352 independent reflections
6497 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 26.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.086
S = 1.02
7352 reflections
482 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.61 e Å^{-3}
$\Delta\rho_{min}$ = −1.47 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Sn1—O13	2.0391 (19)	Sn2—C23	2.119 (3)
Sn1—C19	2.124 (3)	Sn2—C27	2.125 (3)
Sn1—C15	2.135 (3)	Sn2—O13	2.1708 (19)
Sn1—O1	2.188 (2)	Sn2—O8^{i}	2.276 (2)
Sn1—O7	2.286 (2)	Sn2···Sn2^{i}	3.2908 (5)
Sn2—O13^{i}	2.0372 (19)		
O13—Sn1—C19	106.03 (10)	O13^{i}—Sn2—C23	108.48 (10)
O13—Sn1—C15	108.78 (10)	O13^{i}—Sn2—C27	114.33 (10)
C19—Sn1—C15	144.19 (12)	C23—Sn2—C27	136.69 (12)
O13—Sn1—O1	83.08 (8)	O13^{i}—Sn2—O13	77.16 (8)
C19—Sn1—O1	99.15 (10)	C23—Sn2—O13	97.19 (10)
C15—Sn1—O1	93.09 (10)	C27—Sn2—O13	98.24 (10)
O13—Sn1—O7	89.89 (8)	O13^{i}—Sn2—O8^{i}	91.86 (8)
C19—Sn1—O7	86.80 (10)	C23—Sn2—O8^{i}	89.20 (10)
C15—Sn1—O7	85.19 (11)	C27—Sn2—O8^{i}	83.31 (10)
O1—Sn1—O7	171.81 (8)	O13—Sn2—O8^{i}	168.58 (8)

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

H atoms were included in calculated positions using the riding model, with C—H = 0.95–0.99 Å and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5U_{eq}(C) for methyl groups. In one of the butyl groups (C15–C18), atoms C16 and C17 are disordered over two sites (C16/C17 and C16*A*/C17*A*); the occupancies refined to 0.496 (15) and 0.504 (15), respectively, and were fixed at 0.5 for the final cycles of refinement. The highest residual density peak is located 0.95 Å from atom Sn2 and the deepest hole is located 0.98 Å from atom Sn1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

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supporting information

Acta Cryst. (2006). E**62**, m1734–m1736 [https://doi.org/10.1107/S1600536806024627]

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$\beta = 110.770$ (1)°
$\gamma = 95.960$ (1)°
$V = 1827.9$ (3) Å^3
$Z = 1$
$F(000) = 972$
$D_x = 1.768$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7196 reflections
$\theta = 2.5$–$26.5°$
$\mu = 1.58$ mm^{-1}
$T = 100$ K
Rod, colourless
0.40 × 0.20 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2001)
$T_{min} = 0.571$, $T_{max} = 0.743$
14580 measured reflections
7352 independent reflections
6497 reflections with $I > 2\sigma(I)$
$R_{int} = 0.030$
$\theta_{max} = 26.5°$, $\theta_{min} = 1.7°$
$h = -15 \rightarrow 15$
$k = -15 \rightarrow 15$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.032$
$wR(F^2) = 0.086$
$S = 1.02$
7352 reflections
482 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
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 0.862P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.61$ e Å^{-3}
$\Delta\rho_{min} = -1.47$ e Å^{-3}

Special details

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

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.186221 (17)	0.253668 (16)	0.122415 (16)	0.01147 (7)	
Sn2	−0.027218 (17)	0.018653 (16)	0.112909 (16)	0.01035 (7)	
Cl1	−0.01669 (8)	0.36631 (7)	0.69264 (7)	0.02520 (19)	
Cl2	0.45592 (7)	0.35195 (7)	−0.38525 (7)	0.02411 (18)	
O1	0.13859 (19)	0.23175 (17)	0.25822 (17)	0.0145 (4)	
O2	0.24963 (19)	0.40626 (18)	0.34197 (18)	0.0186 (5)	
O3	0.1447 (2)	0.63958 (19)	0.6391 (2)	0.0255 (5)	
O4	0.1710 (2)	0.5649 (2)	0.7714 (2)	0.0308 (6)	
O5	−0.1153 (3)	0.0890 (2)	0.4346 (2)	0.0396 (7)	
O6	−0.0075 (2)	0.1239 (2)	0.6087 (2)	0.0308 (6)	
O7	0.2093 (2)	0.26123 (18)	−0.03587 (18)	0.0194 (5)	
O8	0.15698 (19)	0.08706 (18)	−0.15554 (18)	0.0176 (5)	
O9	0.4734 (2)	0.5540 (2)	−0.0914 (2)	0.0286 (6)	
O10	0.3987 (2)	0.5486 (2)	−0.2633 (2)	0.0274 (6)	
O11	0.3030 (2)	0.1292 (2)	−0.5220 (2)	0.0298 (6)	
O12	0.3576 (2)	0.0202 (2)	−0.4196 (2)	0.0276 (6)	
O13	0.07587 (17)	0.09778 (16)	0.03868 (16)	0.0119 (4)	
N1	0.1459 (2)	0.5598 (2)	0.6743 (2)	0.0184 (6)	
N2	−0.0361 (2)	0.1466 (2)	0.5220 (2)	0.0187 (6)	
N3	0.4189 (2)	0.5049 (2)	−0.1891 (2)	0.0175 (6)	
N4	0.3303 (2)	0.1077 (2)	−0.4353 (2)	0.0191 (6)	
C1	0.1812 (3)	0.3254 (3)	0.3390 (2)	0.0137 (6)	
C2	0.1381 (3)	0.3335 (3)	0.4312 (3)	0.0146 (6)	
C3	0.1615 (3)	0.4372 (3)	0.5100 (3)	0.0153 (6)	
H3	0.2068	0.5021	0.5072	0.018*	
C4	0.1184 (3)	0.4461 (3)	0.5932 (3)	0.0151 (6)	
C5	0.0508 (3)	0.3531 (3)	0.6002 (3)	0.0166 (6)	
C6	0.0321 (3)	0.2503 (3)	0.5212 (3)	0.0162 (6)	
C7	0.0727 (3)	0.2397 (3)	0.4367 (3)	0.0146 (6)	
H7	0.0557	0.1682	0.3828	0.018*	
C8	0.2047 (2)	0.1898 (2)	−0.1208 (2)	0.0120 (6)	
C9	0.2660 (3)	0.2319 (3)	−0.1876 (2)	0.0131 (6)	
C10	0.3160 (3)	0.3458 (3)	−0.1589 (3)	0.0145 (6)	
H10A	0.3133	0.3986	−0.0961	0.017*	
C11	0.3698 (3)	0.3818 (3)	−0.2229 (2)	0.0148 (6)	

C12	0.3781 (3)	0.3081 (3)	−0.3143 (3)	0.0163 (6)	
C13	0.3281 (3)	0.1939 (3)	−0.3396 (3)	0.0161 (6)	
C14	0.2737 (3)	0.1564 (3)	−0.2773 (2)	0.0152 (6)	
H14	0.2413	0.0781	−0.2964	0.018*	
C15	0.0822 (3)	0.3791 (3)	0.0976 (3)	0.0177 (7)	
H15A	0.0004	0.3403	0.0420	0.021*	0.50
H15B	0.0747	0.4150	0.1681	0.021*	0.50
C16	0.1275 (6)	0.4707 (6)	0.0605 (7)	0.0198 (14)	0.50
H16A	0.0779	0.5284	0.0628	0.024*	0.50
H16B	0.1177	0.4383	−0.0174	0.024*	0.50
C17	0.2593 (7)	0.5278 (6)	0.1315 (7)	0.0220 (16)	0.50
H17A	0.3096	0.4708	0.1286	0.026*	0.50
H17B	0.2698	0.5603	0.2096	0.026*	0.50
C18	0.3029 (4)	0.6251 (3)	0.0896 (3)	0.0321 (9)	
H18A	0.3879	0.6594	0.1360	0.048*	0.50
H18B	0.2549	0.6828	0.0945	0.048*	0.50
H18C	0.2929	0.5931	0.0124	0.048*	0.50
H15C	0.0261	0.3560	0.0187	0.021*	0.50
H15D	0.0335	0.3827	0.1428	0.021*	0.50
C16A	0.1605 (6)	0.5005 (6)	0.1290 (7)	0.0201 (14)	0.50
H16C	0.1058	0.5536	0.1177	0.024*	0.50
H16D	0.2129	0.5247	0.2091	0.024*	0.50
C17A	0.2387 (7)	0.5117 (6)	0.0658 (8)	0.0246 (16)	0.50
H17C	0.2980	0.4634	0.0820	0.030*	0.50
H17D	0.1875	0.4820	−0.0145	0.030*	0.50
H18D	0.3870	0.6345	0.1390	0.048*	0.50
H18E	0.2659	0.6797	0.1256	0.048*	0.50
H18F	0.2993	0.6379	0.0203	0.048*	0.50
C19	0.3640 (3)	0.2258 (3)	0.1793 (3)	0.0166 (6)	
H19A	0.3602	0.1455	0.1429	0.020*	
H19B	0.4113	0.2717	0.1524	0.020*	
C20	0.4341 (3)	0.2511 (3)	0.3031 (3)	0.0186 (7)	
H20A	0.3863	0.2099	0.3330	0.022*	
H20B	0.4472	0.3330	0.3406	0.022*	
C21	0.5552 (3)	0.2169 (3)	0.3284 (3)	0.0218 (7)	
H21A	0.5994	0.2522	0.2919	0.026*	
H21B	0.5416	0.1339	0.2968	0.026*	
C22	0.6319 (3)	0.2518 (4)	0.4523 (3)	0.0303 (8)	
H22A	0.6421	0.3334	0.4848	0.045*	
H22B	0.7108	0.2332	0.4640	0.045*	
H22C	0.5921	0.2114	0.4878	0.045*	
C23	0.1182 (3)	−0.0223 (3)	0.2289 (3)	0.0157 (6)	
H23A	0.1939	0.0247	0.2382	0.019*	
H23B	0.1110	−0.0014	0.3014	0.019*	
C24	0.1273 (3)	−0.1455 (3)	0.1987 (3)	0.0165 (6)	
H24A	0.1402	−0.1661	0.1289	0.020*	
H24B	0.0507	−0.1937	0.1859	0.020*	
C25	0.2304 (3)	−0.1686 (3)	0.2899 (3)	0.0188 (7)	

H25A	0.2181	−0.1458	0.3599	0.023*
H25B	0.2274	−0.2509	0.2699	0.023*
C26	0.3545 (3)	−0.1071 (3)	0.3097 (3)	0.0229 (7)
H26A	0.3680	−0.1296	0.2410	0.034*
H26B	0.4157	−0.1269	0.3679	0.034*
H26C	0.3597	−0.0253	0.3328	0.034*
C27	−0.1432 (3)	0.1336 (3)	0.1186 (3)	0.0154 (6)
H27A	−0.1485	0.1516	0.1919	0.018*
H27B	−0.1067	0.2048	0.1123	0.018*
C28	−0.2705 (3)	0.0910 (3)	0.0283 (3)	0.0155 (6)
H28A	−0.2678	0.0888	−0.0442	0.019*
H28B	−0.3018	0.0130	0.0241	0.019*
C29	−0.3550 (3)	0.1654 (3)	0.0506 (3)	0.0205 (7)
H29A	−0.3175	0.2451	0.0658	0.025*
H29B	−0.3661	0.1590	0.1179	0.025*
C30	−0.4784 (3)	0.1352 (3)	−0.0454 (3)	0.0233 (7)
H30A	−0.4686	0.1441	−0.1117	0.035*
H30B	−0.5289	0.1855	−0.0254	0.035*
H30C	−0.5167	0.0567	−0.0605	0.035*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01090 (11)	0.01017 (12)	0.01361 (12)	−0.00227 (8)	0.00649 (8)	0.00355 (8)
Sn2	0.00895 (11)	0.01034 (11)	0.01277 (12)	−0.00108 (8)	0.00595 (8)	0.00414 (8)
Cl1	0.0278 (4)	0.0263 (4)	0.0256 (4)	−0.0011 (3)	0.0203 (4)	0.0033 (4)
Cl2	0.0225 (4)	0.0313 (5)	0.0255 (4)	−0.0012 (3)	0.0167 (3)	0.0129 (4)
O1	0.0155 (11)	0.0149 (11)	0.0153 (11)	0.0001 (9)	0.0091 (9)	0.0051 (9)
O2	0.0185 (11)	0.0171 (12)	0.0203 (12)	−0.0032 (9)	0.0113 (9)	0.0033 (9)
O3	0.0248 (13)	0.0165 (12)	0.0315 (14)	0.0029 (10)	0.0101 (11)	0.0032 (11)
O4	0.0393 (15)	0.0257 (14)	0.0228 (14)	−0.0040 (12)	0.0155 (12)	−0.0004 (11)
O5	0.0429 (17)	0.0287 (15)	0.0322 (15)	−0.0214 (13)	0.0130 (13)	−0.0010 (12)
O6	0.0269 (14)	0.0370 (15)	0.0385 (15)	0.0030 (12)	0.0159 (12)	0.0255 (13)
O7	0.0226 (12)	0.0162 (11)	0.0205 (12)	−0.0034 (9)	0.0122 (10)	0.0054 (10)
O8	0.0184 (11)	0.0146 (11)	0.0236 (12)	−0.0025 (9)	0.0137 (10)	0.0069 (9)
O9	0.0353 (14)	0.0179 (12)	0.0244 (13)	−0.0069 (11)	0.0085 (11)	0.0027 (10)
O10	0.0307 (14)	0.0219 (13)	0.0293 (13)	−0.0057 (11)	0.0099 (11)	0.0148 (11)
O11	0.0300 (14)	0.0369 (15)	0.0203 (13)	0.0040 (12)	0.0108 (11)	0.0054 (11)
O12	0.0297 (14)	0.0231 (13)	0.0349 (14)	0.0055 (11)	0.0194 (12)	0.0075 (11)
O13	0.0117 (10)	0.0093 (10)	0.0139 (10)	−0.0050 (8)	0.0074 (8)	0.0015 (8)
N1	0.0131 (13)	0.0207 (15)	0.0193 (14)	−0.0009 (11)	0.0079 (11)	0.0022 (12)
N2	0.0164 (14)	0.0154 (14)	0.0265 (15)	−0.0002 (11)	0.0130 (12)	0.0050 (12)
N3	0.0143 (13)	0.0187 (14)	0.0212 (15)	−0.0020 (11)	0.0090 (11)	0.0086 (12)
N4	0.0115 (13)	0.0222 (15)	0.0226 (15)	−0.0010 (11)	0.0097 (11)	0.0030 (12)
C1	0.0114 (14)	0.0181 (16)	0.0156 (15)	0.0028 (12)	0.0073 (12)	0.0093 (13)
C2	0.0101 (14)	0.0189 (16)	0.0174 (15)	0.0013 (12)	0.0076 (12)	0.0075 (13)
C3	0.0113 (14)	0.0150 (15)	0.0197 (16)	−0.0005 (12)	0.0070 (12)	0.0059 (13)
C4	0.0110 (14)	0.0164 (16)	0.0163 (15)	0.0009 (12)	0.0051 (12)	0.0035 (13)

C5	0.0149 (15)	0.0221 (17)	0.0161 (15)	0.0028 (13)	0.0092 (12)	0.0075 (13)
C6	0.0125 (15)	0.0156 (16)	0.0199 (16)	−0.0008 (12)	0.0058 (12)	0.0068 (13)
C7	0.0099 (14)	0.0156 (16)	0.0173 (15)	−0.0010 (12)	0.0057 (12)	0.0044 (13)
C8	0.0052 (13)	0.0142 (15)	0.0170 (15)	−0.0004 (11)	0.0043 (11)	0.0068 (12)
C9	0.0070 (13)	0.0149 (15)	0.0171 (15)	−0.0004 (11)	0.0031 (11)	0.0081 (12)
C10	0.0114 (14)	0.0189 (16)	0.0158 (15)	0.0021 (12)	0.0065 (12)	0.0085 (13)
C11	0.0106 (14)	0.0133 (15)	0.0183 (16)	−0.0039 (12)	0.0033 (12)	0.0074 (13)
C12	0.0115 (14)	0.0240 (17)	0.0158 (15)	−0.0002 (13)	0.0062 (12)	0.0107 (13)
C13	0.0097 (14)	0.0217 (17)	0.0159 (15)	0.0001 (12)	0.0059 (12)	0.0043 (13)
C14	0.0084 (14)	0.0175 (16)	0.0171 (15)	−0.0021 (12)	0.0039 (12)	0.0048 (13)
C15	0.0183 (16)	0.0145 (16)	0.0198 (16)	0.0039 (13)	0.0057 (13)	0.0072 (13)
C16	0.022 (4)	0.014 (3)	0.019 (4)	−0.002 (3)	0.005 (3)	0.004 (3)
C17	0.020 (4)	0.014 (4)	0.027 (4)	−0.005 (3)	0.008 (4)	0.003 (4)
C18	0.035 (2)	0.026 (2)	0.041 (2)	0.0011 (17)	0.0214 (18)	0.0126 (18)
C16A	0.022 (4)	0.013 (3)	0.025 (4)	0.001 (3)	0.010 (3)	0.005 (3)
C17A	0.022 (4)	0.014 (4)	0.038 (5)	0.000 (3)	0.014 (4)	0.006 (4)
C19	0.0125 (15)	0.0155 (16)	0.0228 (17)	−0.0008 (12)	0.0100 (13)	0.0048 (13)
C20	0.0139 (15)	0.0232 (17)	0.0217 (17)	0.0015 (13)	0.0088 (13)	0.0103 (14)
C21	0.0195 (17)	0.0227 (18)	0.0256 (18)	0.0044 (14)	0.0097 (14)	0.0106 (15)
C22	0.0163 (17)	0.046 (2)	0.033 (2)	0.0088 (16)	0.0083 (15)	0.0207 (18)
C23	0.0147 (15)	0.0143 (15)	0.0171 (15)	0.0014 (12)	0.0048 (12)	0.0062 (13)
C24	0.0138 (15)	0.0161 (16)	0.0203 (16)	−0.0004 (12)	0.0077 (13)	0.0065 (13)
C25	0.0176 (16)	0.0212 (17)	0.0224 (17)	0.0055 (13)	0.0097 (13)	0.0117 (14)
C26	0.0175 (17)	0.0287 (19)	0.0281 (18)	0.0051 (14)	0.0118 (14)	0.0138 (15)
C27	0.0100 (14)	0.0158 (15)	0.0210 (16)	0.0001 (12)	0.0075 (12)	0.0060 (13)
C28	0.0115 (14)	0.0172 (16)	0.0192 (16)	0.0017 (12)	0.0072 (12)	0.0071 (13)
C29	0.0138 (15)	0.0229 (18)	0.0251 (18)	0.0046 (13)	0.0072 (13)	0.0083 (15)
C30	0.0107 (15)	0.031 (2)	0.0315 (19)	0.0037 (14)	0.0080 (14)	0.0149 (16)

Geometric parameters (Å, º)

Sn1—O13	2.0391 (19)	C16—C17	1.528 (10)
Sn1—C19	2.124 (3)	C16—H16A	0.9900
Sn1—C15	2.135 (3)	C16—H16B	0.9900
Sn1—O1	2.188 (2)	C17—C18	1.585 (8)
Sn1—O7	2.286 (2)	C17—H17A	0.9900
Sn2—O13^{i}	2.0372 (19)	C17—H17B	0.9900
Sn2—C23	2.119 (3)	C18—H18A	0.9800
Sn2—C27	2.125 (3)	C18—H18B	0.9800
Sn2—O13	2.1708 (19)	C18—H18C	0.9800
Sn2—O8^{i}	2.276 (2)	C18—H18D	0.9800
Sn2—Sn2^{i}	3.2908 (5)	C18—H18E	0.9800
Cl1—C5	1.712 (3)	C18—H18F	0.9800
Cl2—C12	1.712 (3)	C16A—C17A	1.508 (11)
O1—C1	1.291 (4)	C16A—H16C	0.9900
O2—C1	1.225 (4)	C16A—H16D	0.9900
O3—N1	1.210 (3)	C17A—H17C	0.9900
O4—N1	1.225 (4)	C17A—H17D	0.9900

O5—N2	1.213 (4)	C19—C20	1.520 (4)
O6—N2	1.219 (4)	C19—H19A	0.9900
O7—C8	1.247 (4)	C19—H19B	0.9900
O8—C8	1.249 (4)	C20—C21	1.523 (4)
O8—Sn2^{i}	2.276 (2)	C20—H20A	0.9900
O9—N3	1.206 (3)	C20—H20B	0.9900
O10—N3	1.226 (3)	C21—C22	1.524 (5)
O11—N4	1.212 (4)	C21—H21A	0.9900
O12—N4	1.223 (4)	C21—H21B	0.9900
O13—Sn2^{i}	2.0373 (19)	C22—H22A	0.9800
N1—C4	1.483 (4)	C22—H22B	0.9800
N2—C6	1.470 (4)	C22—H22C	0.9800
N3—C11	1.483 (4)	C23—C24	1.520 (4)
N4—C13	1.474 (4)	C23—H23A	0.9900
C1—C2	1.504 (4)	C23—H23B	0.9900
C2—C7	1.383 (4)	C24—C25	1.531 (4)
C2—C3	1.384 (4)	C24—H24A	0.9900
C3—C4	1.390 (4)	C24—H24B	0.9900
C3—H3	0.9500	C25—C26	1.522 (4)
C4—C5	1.397 (4)	C25—H25A	0.9900
C5—C6	1.389 (4)	C25—H25B	0.9900
C6—C7	1.384 (4)	C26—H26A	0.9800
C7—H7	0.9500	C26—H26B	0.9800
C8—C9	1.515 (4)	C26—H26C	0.9800
C9—C14	1.379 (4)	C27—C28	1.530 (4)
C9—C10	1.388 (4)	C27—H27A	0.9900
C10—C11	1.388 (4)	C27—H27B	0.9900
C10—H10A	0.9500	C28—C29	1.515 (4)
C11—C12	1.390 (4)	C28—H28A	0.9900
C12—C13	1.398 (4)	C28—H28B	0.9900
C13—C14	1.381 (4)	C29—C30	1.531 (4)
C14—H14	0.9500	C29—H29A	0.9900
C15—C16	1.492 (7)	C29—H29B	0.9900
C15—H15A	0.9900	C30—H30A	0.9800
C15—H15B	0.9900	C30—H30B	0.9800
C15—H15C	0.9900	C30—H30C	0.9800
C15—H15D	0.9900		

O13—Sn1—C19	106.03 (10)	C15—C16—H16B	108.9
O13—Sn1—C15	108.78 (10)	C17—C16—H16B	108.9
C19—Sn1—C15	144.19 (12)	H16A—C16—H16B	107.7
O13—Sn1—O1	83.08 (8)	C16—C17—C18	111.4 (6)
C19—Sn1—O1	99.15 (10)	C16—C17—H17A	109.3
C15—Sn1—O1	93.09 (10)	C18—C17—H17A	109.3
O13—Sn1—O7	89.89 (8)	C16—C17—H17B	109.3
C19—Sn1—O7	86.80 (10)	C18—C17—H17B	109.3
C15—Sn1—O7	85.19 (11)	H17A—C17—H17B	108.0
O1—Sn1—O7	171.81 (8)	C17—C18—H18A	109.5

O13^{i}—Sn2—C23	108.48 (10)	C17—C18—H18B	109.5
O13^{i}—Sn2—C27	114.33 (10)	H18A—C18—H18B	109.5
C23—Sn2—C27	136.69 (12)	C17—C18—H18C	109.5
O13^{i}—Sn2—O13	77.16 (8)	H18A—C18—H18C	109.5
C23—Sn2—O13	97.19 (10)	H18B—C18—H18C	109.5
C27—Sn2—O13	98.24 (10)	C17A—C18—H18D	109.5
O13^{i}—Sn2—O8^{i}	91.86 (8)	C17A—C18—H18E	109.5
C23—Sn2—O8^{i}	89.20 (10)	H18D—C18—H18E	109.5
C27—Sn2—O8^{i}	83.31 (10)	C17A—C18—H18F	109.5
O13—Sn2—O8^{i}	168.58 (8)	H18D—C18—H18F	109.5
O13^{i}—Sn2—Sn2^{i}	40.03 (5)	H18E—C18—H18F	109.5
C23—Sn2—Sn2^{i}	106.19 (9)	C17A—C16A—H16C	108.2
C27—Sn2—Sn2^{i}	110.47 (9)	C17A—C16A—H16D	108.2
O13—Sn2—Sn2^{i}	37.13 (5)	H16C—C16A—H16D	107.4
O8^{i}—Sn2—Sn2^{i}	131.81 (6)	C16A—C17A—H17C	108.4
C1—O1—Sn1	108.57 (18)	C16A—C17A—H17D	108.4
C8—O7—Sn1	135.05 (19)	H17C—C17A—H17D	107.5
C8—O8—Sn2^{i}	133.1 (2)	C20—C19—Sn1	118.8 (2)
Sn2^{i}—O13—Sn1	136.33 (10)	C20—C19—H19A	107.6
Sn2^{i}—O13—Sn2	102.84 (8)	Sn1—C19—H19A	107.6
Sn1—O13—Sn2	120.82 (9)	C20—C19—H19B	107.6
O3—N1—O4	125.8 (3)	Sn1—C19—H19B	107.6
O3—N1—C4	117.0 (3)	H19A—C19—H19B	107.0
O4—N1—C4	117.2 (3)	C19—C20—C21	111.8 (3)
O5—N2—O6	125.2 (3)	C19—C20—H20A	109.2
O5—N2—C6	116.6 (3)	C21—C20—H20A	109.2
O6—N2—C6	118.2 (3)	C19—C20—H20B	109.2
O9—N3—O10	125.5 (3)	C21—C20—H20B	109.2
O9—N3—C11	117.7 (3)	H20A—C20—H20B	107.9
O10—N3—C11	116.8 (3)	C20—C21—C22	112.6 (3)
O11—N4—O12	126.3 (3)	C20—C21—H21A	109.1
O11—N4—C13	117.1 (3)	C22—C21—H21A	109.1
O12—N4—C13	116.5 (3)	C20—C21—H21B	109.1
O2—C1—O1	124.0 (3)	C22—C21—H21B	109.1
O2—C1—C2	120.0 (3)	H21A—C21—H21B	107.8
O1—C1—C2	116.0 (3)	C21—C22—H22A	109.5
C7—C2—C3	119.5 (3)	C21—C22—H22B	109.5
C7—C2—C1	121.1 (3)	H22A—C22—H22B	109.5
C3—C2—C1	119.4 (3)	C21—C22—H22C	109.5
C2—C3—C4	119.7 (3)	H22A—C22—H22C	109.5
C2—C3—H3	120.1	H22B—C22—H22C	109.5
C4—C3—H3	120.1	C24—C23—Sn2	115.5 (2)
C3—C4—C5	122.1 (3)	C24—C23—H23A	108.4
C3—C4—N1	116.9 (3)	Sn2—C23—H23A	108.4
C5—C4—N1	121.0 (3)	C24—C23—H23B	108.4
C6—C5—C4	116.2 (3)	Sn2—C23—H23B	108.4
C6—C5—Cl1	121.3 (2)	H23A—C23—H23B	107.5
C4—C5—Cl1	122.2 (2)	C23—C24—C25	111.9 (3)

C7—C6—C5	122.7 (3)	C23—C24—H24A	109.2
C7—C6—N2	116.5 (3)	C25—C24—H24A	109.2
C5—C6—N2	120.8 (3)	C23—C24—H24B	109.2
C2—C7—C6	119.7 (3)	C25—C24—H24B	109.2
C2—C7—H7	120.1	H24A—C24—H24B	107.9
C6—C7—H7	120.1	C26—C25—C24	114.0 (3)
O7—C8—O8	127.0 (3)	C26—C25—H25A	108.7
O7—C8—C9	116.4 (3)	C24—C25—H25A	108.7
O8—C8—C9	116.5 (3)	C26—C25—H25B	108.7
C14—C9—C10	119.3 (3)	C24—C25—H25B	108.7
C14—C9—C8	119.9 (3)	H25A—C25—H25B	107.6
C10—C9—C8	120.7 (3)	C25—C26—H26A	109.5
C11—C10—C9	119.2 (3)	C25—C26—H26B	109.5
C11—C10—H10A	120.4	H26A—C26—H26B	109.5
C9—C10—H10A	120.4	C25—C26—H26C	109.5
C10—C11—C12	122.8 (3)	H26A—C26—H26C	109.5
C10—C11—N3	116.4 (3)	H26B—C26—H26C	109.5
C12—C11—N3	120.7 (3)	C28—C27—Sn2	114.8 (2)
C11—C12—C13	116.2 (3)	C28—C27—H27A	108.6
C11—C12—Cl2	122.2 (2)	Sn2—C27—H27A	108.6
C13—C12—Cl2	121.4 (2)	C28—C27—H27B	108.6
C14—C13—C12	121.9 (3)	Sn2—C27—H27B	108.6
C14—C13—N4	116.8 (3)	H27A—C27—H27B	107.5
C12—C13—N4	121.3 (3)	C29—C28—C27	112.0 (3)
C9—C14—C13	120.5 (3)	C29—C28—H28A	109.2
C9—C14—H14	119.8	C27—C28—H28A	109.2
C13—C14—H14	119.8	C29—C28—H28B	109.2
C16—C15—Sn1	117.4 (3)	C27—C28—H28B	109.2
C16—C15—H15A	107.9	H28A—C28—H28B	107.9
Sn1—C15—H15A	107.9	C28—C29—C30	113.5 (3)
C16—C15—H15B	107.9	C28—C29—H29A	108.9
Sn1—C15—H15B	107.9	C30—C29—H29A	108.9
H15A—C15—H15B	107.2	C28—C29—H29B	108.9
C16A—C15—H15C	108.9	C30—C29—H29B	108.9
Sn1—C15—H15C	108.9	H29A—C29—H29B	107.7
C16A—C15—H15D	108.9	C29—C30—H30A	109.5
Sn1—C15—H15D	108.9	C29—C30—H30B	109.5
H15C—C15—H15D	107.7	H30A—C30—H30B	109.5
C15—C16—C17	113.3 (6)	C29—C30—H30C	109.5
C15—C16—H16A	108.9	H30A—C30—H30C	109.5
C17—C16—H16A	108.9	H30B—C30—H30C	109.5

O13—Sn1—O1—C1	−172.38 (19)	$Sn2^{i}$—O8—C8—O7	13.9 (5)
C19—Sn1—O1—C1	82.4 (2)	$Sn2^{i}$—O8—C8—C9	−167.43 (18)
C15—Sn1—O1—C1	−63.8 (2)	O7—C8—C9—C14	174.6 (3)
O7—Sn1—O1—C1	−141.4 (5)	O8—C8—C9—C14	−4.1 (4)
O13—Sn1—O7—C8	−27.5 (3)	O7—C8—C9—C10	−4.7 (4)
C19—Sn1—O7—C8	78.6 (3)	O8—C8—C9—C10	176.5 (3)

C15—Sn1—O7—C8	−136.3 (3)	C14—C9—C10—C11	1.6 (4)
O1—Sn1—O7—C8	−58.2 (7)	C8—C9—C10—C11	−179.0 (3)
C19—Sn1—O13—Sn2^{i}	−76.86 (17)	C9—C10—C11—C12	−1.1 (5)
C15—Sn1—O13—Sn2^{i}	94.65 (17)	C9—C10—C11—N3	178.7 (3)
O1—Sn1—O13—Sn2^{i}	−174.43 (16)	O9—N3—C11—C10	42.5 (4)
O7—Sn1—O13—Sn2^{i}	9.78 (15)	O10—N3—C11—C10	−136.3 (3)
C19—Sn1—O13—Sn2	103.91 (13)	O9—N3—C11—C12	−137.7 (3)
C15—Sn1—O13—Sn2	−84.58 (14)	O10—N3—C11—C12	43.5 (4)
O1—Sn1—O13—Sn2	6.34 (10)	C10—C11—C12—C13	0.3 (5)
O7—Sn1—O13—Sn2	−169.46 (11)	N3—C11—C12—C13	−179.5 (3)
O13^{i}—Sn2—O13—Sn2^{i}	0.0	C10—C11—C12—Cl2	−174.3 (2)
C23—Sn2—O13—Sn2^{i}	107.39 (11)	N3—C11—C12—Cl2	5.9 (4)
C27—Sn2—O13—Sn2^{i}	−113.20 (11)	C11—C12—C13—C14	0.0 (5)
O8^{i}—Sn2—O13—Sn2^{i}	−16.2 (4)	Cl2—C12—C13—C14	174.6 (2)
O13^{i}—Sn2—O13—Sn1	179.46 (17)	C11—C12—C13—N4	179.5 (3)
C23—Sn2—O13—Sn1	−73.15 (13)	Cl2—C12—C13—N4	−5.9 (4)
C27—Sn2—O13—Sn1	66.25 (13)	O11—N4—C13—C14	134.2 (3)
O8^{i}—Sn2—O13—Sn1	163.3 (3)	O12—N4—C13—C14	−44.5 (4)
Sn2^{i}—Sn2—O13—Sn1	179.46 (17)	O11—N4—C13—C12	−45.3 (4)
Sn1—O1—C1—O2	−8.7 (4)	O12—N4—C13—C12	136.0 (3)
Sn1—O1—C1—C2	169.0 (2)	C10—C9—C14—C13	−1.4 (4)
O2—C1—C2—C7	−172.2 (3)	C8—C9—C14—C13	179.2 (3)
O1—C1—C2—C7	10.0 (4)	C12—C13—C14—C9	0.6 (5)
O2—C1—C2—C3	9.6 (4)	N4—C13—C14—C9	−178.9 (3)
O1—C1—C2—C3	−168.2 (3)	O13—Sn1—C15—C16	−129.3 (4)
C7—C2—C3—C4	−0.5 (5)	C19—Sn1—C15—C16	36.7 (5)
C1—C2—C3—C4	177.8 (3)	O1—Sn1—C15—C16	147.0 (4)
C2—C3—C4—C5	−0.3 (5)	O7—Sn1—C15—C16	−41.0 (4)
C2—C3—C4—N1	−179.6 (3)	Sn1—C15—C16—C17	−50.5 (7)
O3—N1—C4—C3	37.1 (4)	C15—C16—C17—C18	−179.5 (5)
O4—N1—C4—C3	−141.0 (3)	O13—Sn1—C19—C20	−112.1 (2)
O3—N1—C4—C5	−142.2 (3)	C15—Sn1—C19—C20	81.7 (3)
O4—N1—C4—C5	39.7 (4)	O1—Sn1—C19—C20	−26.8 (2)
C3—C4—C5—C6	1.8 (5)	O7—Sn1—C19—C20	158.9 (2)
N1—C4—C5—C6	−178.9 (3)	Sn1—C19—C20—C21	175.1 (2)
C3—C4—C5—Cl1	−172.5 (2)	C19—C20—C21—C22	174.5 (3)
N1—C4—C5—Cl1	6.8 (4)	O13^{i}—Sn2—C23—C24	−24.4 (2)
C4—C5—C6—C7	−2.8 (5)	C27—Sn2—C23—C24	146.7 (2)
Cl1—C5—C6—C7	171.6 (2)	O13—Sn2—C23—C24	−103.2 (2)
C4—C5—C6—N2	179.0 (3)	O8^{i}—Sn2—C23—C24	67.3 (2)
Cl1—C5—C6—N2	−6.6 (4)	Sn2^{i}—Sn2—C23—C24	−66.3 (2)
O5—N2—C6—C7	−47.5 (4)	Sn2—C23—C24—C25	−176.8 (2)
O6—N2—C6—C7	131.0 (3)	C23—C24—C25—C26	−64.2 (4)
O5—N2—C6—C5	130.8 (3)	O13^{i}—Sn2—C27—C28	23.0 (2)
O6—N2—C6—C5	−50.7 (4)	C23—Sn2—C27—C28	−147.6 (2)
C3—C2—C7—C6	−0.4 (5)	O13—Sn2—C27—C28	102.6 (2)
C1—C2—C7—C6	−178.6 (3)	O8^{i}—Sn2—C27—C28	−66.0 (2)
C5—C6—C7—C2	2.1 (5)	Sn2^{i}—Sn2—C27—C28	66.3 (2)

N2—C6—C7—C2	−179.6 (3)	Sn2—C27—C28—C29	168.3 (2)
Sn1—O7—C8—O8	18.7 (5)	C27—C28—C29—C30	172.0 (3)
Sn1—O7—C8—C9	−159.9 (2)		

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