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Di- μ_2 -isopropanolato-octamethylbis(μ -4-methyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-ido- κ^2 N¹:N²)di- μ_3 -oxido-tetratin(IV)

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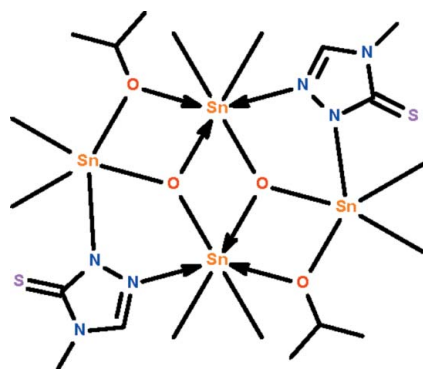
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Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{N}-\text{C}) = 0.004$ Å; disorder in main residue; R factor = 0.023; wR factor = 0.052; data-to-parameter ratio = 23.5.

The tetranuclear title compound, $[\text{Sn}_4(\text{CH}_3)_8(\text{C}_3\text{H}_7\text{O})_2\text{O}_2(\text{C}_3\text{H}_4\text{N}_3\text{S})_2]$, lies about a center of inversion; the molecule features a three-rung-staircase Sn_4O_4 core in which two Sn^{IV} atoms are bridged by the 4-methyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-ide group. The negatively charged N atom of the group binds to the terminal Sn^{IV} atom at a shorter distance [$\text{Sn}-\text{N} = 2.236$ (2) Å] compared with the neutral N atom that binds to the central Sn^{IV} atom [$\text{Sn}-\text{N} = 2.805$ (2) Å]. The terminal Sn^{IV} atom is five-coordinate in a *cis*- C_2SnNO_2 trigonal-bipyramidal geometry [$\text{C}-\text{Sn}-\text{C} = 136.4$ (1)°], whereas the central Sn^{IV} atom is six-coordinate in a C_2SnNO_3 skew-trapezoidal bipyramidal geometry [$\text{C}-\text{Sn}-\text{C} = 145.4$ (1)°]. The C atoms of the isopropoxy group are disordered over two positions in a 0.591 (7):0.409 (7) ratio.

Related literature

For the $[\text{Sn}_2\text{O}(\text{CH}_3)_4(\text{CH}_3\text{O})(\text{C}_3\text{H}_4\text{N}_3\text{S})_2]$ homolog, see: Najafi *et al.* (2011).



Experimental

Crystal data

$[\text{Sn}_4(\text{CH}_3)_8(\text{C}_3\text{H}_7\text{O})_2\text{O}_2(\text{C}_3\text{H}_4\text{N}_3\text{S})_2]$
 $M_r = 973.51$
 Monoclinic, $P2_1/c$
 $a = 9.6009$ (4) Å
 $b = 10.0839$ (4) Å
 $c = 18.3971$ (6) Å
 $\beta = 94.667$ (4)°
 $V = 1775.20$ (12) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 2.93$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.25 \times 0.20$ mm

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
 $T_{\text{min}} = 0.474$, $T_{\text{max}} = 0.592$
 17413 measured reflections
 4093 independent reflections
 3613 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.052$
 $S = 1.04$
 4093 reflections
 174 parameters
 21 restraints
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.49$ e Å⁻³

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT6864).

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supporting information

Acta Cryst. (2012). E68, m1546 [doi:10.1107/S160053681204771X]

Di- μ_2 -isopropanolato-octamethylbis(μ -4-methyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-ido- κ^2 N¹:N²)di- μ_3 -oxido-tetratin(IV)

Ezzatollah Najafi, Mostafa M. Amini and Seik Weng Ng

S1. Comment

The title compound (Scheme I, Fig. 1), a distannoxane, was the unexpected product from an attempt at synthesizing a dimethyltin 4-methyl-4*H*-1,2,4-triazol-3-thiolate that possesses a tin-sulfur linkage. In the reaction of diorganotin oxides with organic acids (particularly carboxylic acids), tetranuclear distannoxanes are sometimes formed; these compounds have four organic groups. In the present reaction, two of the four organic groups are replaced by ethoxide groups.

Tetranuclear Sn₄O₂(CH₃)₈(C₃H₇O)₂(C₃H₄N₃S)₂ lies about a center-of-inversion; the molecule features a three-rung-staircase Sn₄O₄ core in which two Sn atoms are bridged by the C₃H₄N₃S triazolate group. The negatively-charged N atom of the group binds to the terminal Sn atom at a shorter distance [Sn–N 2.236 (2) Å] compared with the neutral N atom that binds to the central Sn atom [Sn←N 2.805 (2) Å]. The terminal Sn atom is five-coordinate in a *cis*-C₃SnNO trigonal bipyramid whereas the central Sn atom is six-coordinate in a C₂SnNO₃ skew-trapezoidal bipyramidal geometry.

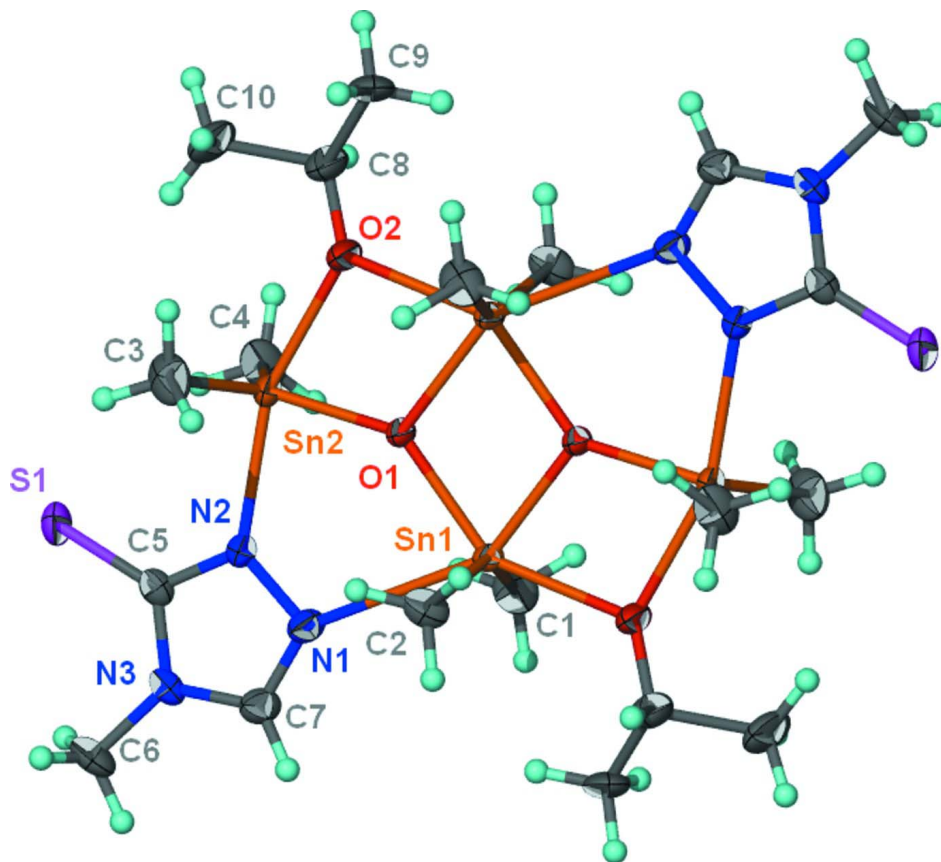
S2. Experimental

Dimethyltin diisothiocyanate (1 mmol), 4-methyl-4*H*-1,2,4-triazole-3-thiol (1 mmol) and 1,10-phenanthroline (1 mmol) were loaded into a convection tube; several drops of triethylamine were added. The tube was filled with dry 2-propanol and kept at 333 K. Colorless crystals were collected from the side arm after several days.

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 to 0.98 Å, $U_{\text{iso}}(\text{H})$ 1.2 to 1.5 $U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation.

The isopropoxy group is disordered over two positions in a 0.591 (7):0.409 ratio in respect of the carbon atoms. Pairs of 1,2-related distances were restrained to within 0.01 Å of each other, and the temperature factors of the primed atoms were set to those of the unprimed ones. The anisotropic temperatures were restrained to be nearly isotropic.

**Figure 1**

Thermal ellipsoid plot (Barbour, 2001) of $\text{Sn}_4\text{O}_2(\text{CH}_3)_8(\text{C}_3\text{H}_7\text{O})_2(\text{C}_3\text{H}_4\text{N}_3\text{S})_2$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius. The disorder is not shown.

Di- μ_2 -isopropanolato-octamethylbis(μ -4-methyl-5-sulfanylidene-4,5-dihydro-1*H*-1,2,4-triazol-1-ido- κ^2 N¹:N²)di- μ_3 -oxido- tetratin(IV)

Crystal data

$[\text{Sn}_4(\text{CH}_3)_8(\text{C}_3\text{H}_7\text{O})_2\text{O}_2(\text{C}_3\text{H}_4\text{N}_3\text{S})_2]$

$M_r = 973.51$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 9.6009(4)\ \text{\AA}$

$b = 10.0839(4)\ \text{\AA}$

$c = 18.3971(6)\ \text{\AA}$

$\beta = 94.667(4)^\circ$

$V = 1775.20(12)\ \text{\AA}^3$

$Z = 2$

$F(000) = 944$

$D_x = 1.821\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 6879 reflections

$\theta = 3.1\text{--}27.5^\circ$

$\mu = 2.93\ \text{mm}^{-1}$

$T = 100\ \text{K}$

Prism, colorless

$0.30 \times 0.25 \times 0.20\ \text{mm}$

Data collection

Agilent SuperNova (Dual, Cu at zero, Atlas) diffractometer

Radiation source: SuperNova (Mo) X-ray Source

Mirror monochromator

Detector resolution: $10.4041\ \text{pixels mm}^{-1}$

ω scan

Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)

$T_{\min} = 0.474$, $T_{\max} = 0.592$

17413 measured reflections

4093 independent reflections

3613 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.038$
 $\theta_{\text{max}} = 27.6^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -12 \rightarrow 12$
 $k = -13 \rightarrow 12$
 $l = -23 \rightarrow 23$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.052$
 $S = 1.04$
 4093 reflections
 174 parameters
 21 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
 $w = 1/[\sigma^2(F_o^2) + (0.0181P)^2 + 1.4453P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.003$
 $\Delta\rho_{\text{max}} = 0.55 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.49 \text{ e } \text{\AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
Sn1	0.652613 (19)	0.422511 (18)	0.513713 (9)	0.01404 (6)	
Sn2	0.52915 (2)	0.709776 (19)	0.634092 (9)	0.01671 (6)	
S1	0.77775 (9)	0.79225 (8)	0.78514 (4)	0.02858 (18)	
O1	0.5301 (2)	0.57582 (19)	0.55360 (9)	0.0169 (4)	
O2	0.3284 (2)	0.7351 (2)	0.57053 (11)	0.0276 (5)	
N1	0.8106 (3)	0.5270 (2)	0.63540 (12)	0.0203 (5)	
N2	0.7409 (2)	0.6280 (2)	0.66839 (11)	0.0177 (5)	
N3	0.9416 (2)	0.6003 (2)	0.73020 (12)	0.0190 (5)	
C1	0.6250 (4)	0.2782 (3)	0.59418 (17)	0.0299 (7)	
H1A	0.6127	0.3221	0.6408	0.045*	
H1B	0.7074	0.2206	0.5995	0.045*	
H1C	0.5421	0.2248	0.5797	0.045*	
C2	0.7985 (3)	0.5418 (3)	0.46418 (15)	0.0246 (7)	
H2A	0.8123	0.6249	0.4914	0.037*	
H2B	0.7633	0.5614	0.4138	0.037*	
H2C	0.8877	0.4946	0.4643	0.037*	
C3	0.6090 (4)	0.8948 (3)	0.60284 (19)	0.0347 (8)	
H3A	0.5315	0.9526	0.5850	0.052*	
H3B	0.6718	0.8814	0.5641	0.052*	
H3C	0.6607	0.9363	0.6450	0.052*	
C4	0.4407 (3)	0.6321 (4)	0.72647 (15)	0.0320 (8)	
H4A	0.3414	0.6558	0.7245	0.048*	
H4B	0.4893	0.6692	0.7708	0.048*	
H4C	0.4503	0.5354	0.7270	0.048*	
C5	0.8202 (3)	0.6727 (3)	0.72657 (14)	0.0191 (6)	
C6	1.0595 (3)	0.6163 (4)	0.78449 (16)	0.0287 (7)	
H6A	1.1257	0.5433	0.7801	0.043*	
H6B	1.0259	0.6153	0.8334	0.043*	
H6C	1.1062	0.7009	0.7766	0.043*	
C7	0.9295 (3)	0.5128 (3)	0.67331 (15)	0.0231 (6)	
H7	0.9990	0.4500	0.6629	0.028*	

C8	0.2044 (6)	0.7853 (7)	0.5959 (3)	0.0377 (16)	0.591 (7)
H8	0.1592	0.7218	0.6285	0.045*	0.591 (7)
C9	0.1067 (12)	0.8255 (19)	0.5272 (8)	0.038 (3)	0.591 (7)
H9A	0.0934	0.7491	0.4944	0.058*	0.591 (7)
H9B	0.1497	0.8983	0.5017	0.058*	0.591 (7)
H9C	0.0161	0.8542	0.5424	0.058*	0.591 (7)
C10	0.242 (2)	0.9267 (11)	0.6349 (6)	0.049 (3)	0.591 (7)
H10A	0.3190	0.9148	0.6726	0.074*	0.591 (7)
H10B	0.1597	0.9605	0.6572	0.074*	0.591 (7)
H10C	0.2697	0.9901	0.5984	0.074*	0.591 (7)
C8'	0.2376 (9)	0.8453 (9)	0.5658 (5)	0.0377 (16)	0.41
H8'	0.2723	0.9185	0.5353	0.045*	0.409 (7)
C9'	0.0850 (17)	0.802 (3)	0.5403 (13)	0.038 (3)	0.41
H9D	0.0874	0.7225	0.5100	0.058*	0.409 (7)
H9E	0.0381	0.8740	0.5119	0.058*	0.409 (7)
H9F	0.0337	0.7833	0.5830	0.058*	0.409 (7)
C10'	0.222 (3)	0.8905 (19)	0.6497 (8)	0.049 (3)	0.41
H10D	0.3053	0.8620	0.6804	0.074*	0.409 (7)
H10E	0.1390	0.8495	0.6673	0.074*	0.409 (7)
H10F	0.2140	0.9872	0.6520	0.074*	0.409 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.01409 (10)	0.01444 (11)	0.01334 (9)	0.00295 (7)	-0.00045 (7)	-0.00018 (7)
Sn2	0.01739 (10)	0.01539 (11)	0.01707 (10)	0.00134 (7)	-0.00036 (8)	-0.00515 (7)
S1	0.0253 (4)	0.0286 (5)	0.0312 (4)	-0.0025 (3)	-0.0012 (3)	-0.0154 (3)
O1	0.0166 (10)	0.0185 (11)	0.0149 (9)	0.0055 (8)	-0.0037 (8)	-0.0056 (7)
O2	0.0232 (11)	0.0292 (13)	0.0288 (11)	0.0121 (10)	-0.0074 (9)	-0.0140 (9)
N1	0.0213 (13)	0.0218 (14)	0.0179 (11)	0.0058 (10)	0.0015 (10)	-0.0026 (10)
N2	0.0180 (12)	0.0163 (13)	0.0185 (11)	0.0013 (10)	-0.0003 (10)	-0.0041 (9)
N3	0.0151 (12)	0.0247 (14)	0.0167 (11)	-0.0040 (10)	-0.0009 (9)	0.0004 (9)
C1	0.0340 (18)	0.0247 (18)	0.0297 (16)	-0.0028 (14)	-0.0043 (14)	0.0093 (13)
C2	0.0203 (15)	0.0321 (19)	0.0217 (14)	-0.0023 (13)	0.0037 (12)	0.0051 (13)
C3	0.041 (2)	0.0187 (18)	0.0428 (19)	-0.0071 (15)	-0.0072 (16)	0.0056 (14)
C4	0.0277 (17)	0.048 (2)	0.0213 (15)	-0.0071 (16)	0.0084 (13)	-0.0066 (14)
C5	0.0172 (14)	0.0211 (16)	0.0188 (13)	-0.0040 (12)	0.0005 (11)	0.0005 (11)
C6	0.0181 (15)	0.039 (2)	0.0281 (15)	-0.0024 (14)	-0.0070 (13)	0.0017 (14)
C7	0.0211 (15)	0.0291 (18)	0.0195 (13)	0.0050 (13)	0.0029 (12)	-0.0025 (12)
C8	0.029 (3)	0.041 (4)	0.042 (4)	0.015 (3)	-0.006 (2)	-0.018 (2)
C9	0.024 (4)	0.034 (6)	0.056 (5)	0.016 (3)	-0.004 (4)	-0.009 (4)
C10	0.045 (5)	0.039 (7)	0.063 (5)	0.021 (5)	-0.009 (4)	-0.030 (5)
C8'	0.029 (3)	0.041 (4)	0.042 (4)	0.015 (3)	-0.006 (2)	-0.018 (2)
C9'	0.024 (4)	0.034 (6)	0.056 (5)	0.016 (3)	-0.004 (4)	-0.009 (4)
C10'	0.045 (5)	0.039 (7)	0.063 (5)	0.021 (5)	-0.009 (4)	-0.030 (5)

Geometric parameters (Å, °)

Sn1—O1 ⁱ	2.0633 (18)	C3—H3A	0.9800
Sn1—C1	2.108 (3)	C3—H3B	0.9800
Sn1—C2	2.109 (3)	C3—H3C	0.9800
Sn1—O1	2.1101 (18)	C4—H4A	0.9800
Sn1—O2 ⁱ	2.2377 (19)	C4—H4B	0.9800
Sn1—N1	2.805 (2)	C4—H4C	0.9800
Sn2—O1	2.0050 (17)	C6—H6A	0.9800
Sn2—C4	2.111 (3)	C6—H6B	0.9800
Sn2—C3	2.115 (3)	C6—H6C	0.9800
Sn2—O2	2.187 (2)	C7—H7	0.9500
Sn2—N2	2.236 (2)	C8—C9	1.566 (9)
S1—C5	1.689 (3)	C8—C10	1.623 (9)
O1—Sn1 ⁱ	2.0633 (18)	C8—H8	1.0000
O2—C8	1.408 (5)	C9—H9A	0.9800
O2—C8'	1.411 (7)	C9—H9B	0.9800
O2—Sn1 ⁱ	2.2377 (19)	C9—H9C	0.9800
N1—C7	1.296 (4)	C10—H10A	0.9800
N1—N2	1.386 (3)	C10—H10B	0.9800
N2—C5	1.340 (3)	C10—H10C	0.9800
N3—C7	1.367 (4)	C8'—C9'	1.563 (11)
N3—C5	1.372 (4)	C8'—C10'	1.629 (10)
N3—C6	1.456 (3)	C8'—H8'	1.0000
C1—H1A	0.9800	C9'—H9D	0.9800
C1—H1B	0.9800	C9'—H9E	0.9800
C1—H1C	0.9800	C9'—H9F	0.9800
C2—H2A	0.9800	C10'—H10D	0.9800
C2—H2B	0.9800	C10'—H10E	0.9800
C2—H2C	0.9800	C10'—H10F	0.9800
O1 ⁱ —Sn1—C1	106.13 (11)	Sn2—C3—H3C	109.5
O1 ⁱ —Sn1—C2	107.34 (10)	H3A—C3—H3C	109.5
C1—Sn1—C2	145.41 (12)	H3B—C3—H3C	109.5
O1 ⁱ —Sn1—O1	74.45 (8)	Sn2—C4—H4A	109.5
C1—Sn1—O1	98.98 (11)	Sn2—C4—H4B	109.5
C2—Sn1—O1	98.10 (10)	H4A—C4—H4B	109.5
O1 ⁱ —Sn1—O2 ⁱ	72.74 (7)	Sn2—C4—H4C	109.5
C1—Sn1—O2 ⁱ	91.03 (11)	H4A—C4—H4C	109.5
C2—Sn1—O2 ⁱ	90.66 (11)	H4B—C4—H4C	109.5
O1—Sn1—O2 ⁱ	147.18 (7)	N2—C5—N3	106.6 (2)
O1 ⁱ —Sn1—N1	148.65 (7)	N2—C5—S1	126.7 (2)
C1—Sn1—N1	77.85 (10)	N3—C5—S1	126.6 (2)
C2—Sn1—N1	78.21 (9)	N3—C6—H6A	109.5
O1—Sn1—N1	74.22 (7)	N3—C6—H6B	109.5
O2 ⁱ —Sn1—N1	138.60 (7)	H6A—C6—H6B	109.5
O1—Sn2—C4	111.77 (11)	N3—C6—H6C	109.5
O1—Sn2—C3	111.73 (11)	H6A—C6—H6C	109.5

C4—Sn2—C3	136.43 (14)	H6B—C6—H6C	109.5
O1—Sn2—O2	74.96 (7)	N1—C7—N3	110.9 (3)
C4—Sn2—O2	94.53 (11)	N1—C7—H7	124.5
C3—Sn2—O2	94.29 (11)	N3—C7—H7	124.5
O1—Sn2—N2	84.34 (8)	O2—C8—C9	106.9 (8)
C4—Sn2—N2	92.98 (11)	O2—C8—C10	107.4 (8)
C3—Sn2—N2	93.49 (12)	C9—C8—C10	103.1 (10)
O2—Sn2—N2	159.29 (8)	O2—C8—H8	112.9
Sn2—O1—Sn1 ⁱ	112.53 (9)	C9—C8—H8	112.9
Sn2—O1—Sn1	141.87 (9)	C10—C8—H8	112.9
Sn1 ⁱ —O1—Sn1	105.55 (8)	C8—C9—H9A	109.5
C8—O2—Sn2	126.6 (3)	C8—C9—H9B	109.5
C8'—O2—Sn2	129.7 (4)	H9A—C9—H9B	109.5
C8—O2—Sn1 ⁱ	127.2 (3)	C8—C9—H9C	109.5
C8'—O2—Sn1 ⁱ	126.9 (4)	H9A—C9—H9C	109.5
Sn2—O2—Sn1 ⁱ	99.75 (8)	H9B—C9—H9C	109.5
C7—N1—N2	106.3 (2)	C8—C10—H10A	109.5
C7—N1—Sn1	141.58 (19)	C8—C10—H10B	109.5
N2—N1—Sn1	112.10 (15)	H10A—C10—H10B	109.5
C5—N2—N1	109.5 (2)	C8—C10—H10C	109.5
C5—N2—Sn2	123.10 (19)	H10A—C10—H10C	109.5
N1—N2—Sn2	127.45 (16)	H10B—C10—H10C	109.5
C7—N3—C5	106.7 (2)	O2—C8'—C9'	111.1 (13)
C7—N3—C6	127.5 (3)	O2—C8'—C10'	105.3 (11)
C5—N3—C6	125.8 (2)	C9'—C8'—C10'	102.0 (16)
Sn1—C1—H1A	109.5	O2—C8'—H8'	112.6
Sn1—C1—H1B	109.5	C9'—C8'—H8'	112.6
H1A—C1—H1B	109.5	C10'—C8'—H8'	112.6
Sn1—C1—H1C	109.5	C8'—C9'—H9D	109.5
H1A—C1—H1C	109.5	C8'—C9'—H9E	109.5
H1B—C1—H1C	109.5	H9D—C9'—H9E	109.5
Sn1—C2—H2A	109.5	C8'—C9'—H9F	109.5
Sn1—C2—H2B	109.5	H9D—C9'—H9F	109.5
H2A—C2—H2B	109.5	H9E—C9'—H9F	109.5
Sn1—C2—H2C	109.5	C8'—C10'—H10D	109.5
H2A—C2—H2C	109.5	C8'—C10'—H10E	109.5
H2B—C2—H2C	109.5	H10D—C10'—H10E	109.5
Sn2—C3—H3A	109.5	C8'—C10'—H10F	109.5
Sn2—C3—H3B	109.5	H10D—C10'—H10F	109.5
H3A—C3—H3B	109.5	H10E—C10'—H10F	109.5
C4—Sn2—O1—Sn1 ⁱ	87.73 (13)	O1—Sn1—N1—N2	1.24 (17)
C3—Sn2—O1—Sn1 ⁱ	-89.81 (13)	O2 ⁱ —Sn1—N1—N2	-179.37 (16)
O2—Sn2—O1—Sn1 ⁱ	-1.17 (9)	C7—N1—N2—C5	-0.3 (3)
N2—Sn2—O1—Sn1 ⁱ	178.69 (11)	Sn1—N1—N2—C5	179.15 (17)
C4—Sn2—O1—Sn1	-88.87 (19)	C7—N1—N2—Sn2	179.8 (2)
C3—Sn2—O1—Sn1	93.60 (19)	Sn1—N1—N2—Sn2	-0.7 (3)
O2—Sn2—O1—Sn1	-177.76 (18)	O1—Sn2—N2—C5	179.9 (2)

N2—Sn2—O1—Sn1	2.09 (16)	C4—Sn2—N2—C5	-68.5 (2)
O1 ⁱ —Sn1—O1—Sn2	176.7 (2)	C3—Sn2—N2—C5	68.4 (2)
C1—Sn1—O1—Sn2	72.38 (18)	O2—Sn2—N2—C5	-179.7 (2)
C2—Sn1—O1—Sn2	-77.43 (18)	O1—Sn2—N2—N1	-0.2 (2)
O2 ⁱ —Sn1—O1—Sn2	178.55 (13)	C4—Sn2—N2—N1	111.4 (2)
N1—Sn1—O1—Sn2	-2.19 (15)	C3—Sn2—N2—N1	-111.8 (2)
O1 ⁱ —Sn1—O1—Sn1 ⁱ	0.0	O2—Sn2—N2—N1	0.2 (4)
C1—Sn1—O1—Sn1 ⁱ	-104.36 (11)	N1—N2—C5—N3	0.5 (3)
C2—Sn1—O1—Sn1 ⁱ	105.84 (11)	Sn2—N2—C5—N3	-179.64 (17)
O2 ⁱ —Sn1—O1—Sn1 ⁱ	1.82 (19)	N1—N2—C5—S1	-178.2 (2)
N1—Sn1—O1—Sn1 ⁱ	-178.92 (10)	Sn2—N2—C5—S1	1.6 (4)
O1—Sn2—O2—C8	154.1 (4)	C7—N3—C5—N2	-0.5 (3)
C4—Sn2—O2—C8	42.7 (4)	C6—N3—C5—N2	179.2 (3)
C3—Sn2—O2—C8	-94.6 (4)	C7—N3—C5—S1	178.3 (2)
N2—Sn2—O2—C8	153.7 (4)	C6—N3—C5—S1	-2.1 (4)
O1—Sn2—O2—C8'	-158.3 (6)	N2—N1—C7—N3	0.0 (3)
C4—Sn2—O2—C8'	90.3 (6)	Sn1—N1—C7—N3	-179.2 (2)
C3—Sn2—O2—C8'	-47.0 (6)	C5—N3—C7—N1	0.3 (3)
N2—Sn2—O2—C8'	-158.7 (6)	C6—N3—C7—N1	-179.4 (3)
O1—Sn2—O2—Sn1 ⁱ	1.01 (8)	C8'—O2—C8—C9	52.9 (10)
C4—Sn2—O2—Sn1 ⁱ	-110.34 (12)	Sn2—O2—C8—C9	162.6 (6)
C3—Sn2—O2—Sn1 ⁱ	112.37 (12)	Sn1 ⁱ —O2—C8—C9	-51.5 (9)
N2—Sn2—O2—Sn1 ⁱ	0.6 (3)	C8'—O2—C8—C10	-57.2 (10)
O1 ⁱ —Sn1—N1—C7	178.4 (3)	Sn2—O2—C8—C10	52.5 (8)
C1—Sn1—N1—C7	77.3 (3)	Sn1 ⁱ —O2—C8—C10	-161.6 (5)
C2—Sn1—N1—C7	-77.5 (3)	C8—O2—C8'—C9'	-56.5 (13)
O1—Sn1—N1—C7	-179.6 (3)	Sn2—O2—C8'—C9'	-157.3 (11)
O2 ⁱ —Sn1—N1—C7	-0.2 (4)	Sn1 ⁱ —O2—C8'—C9'	48.5 (14)
O1 ⁱ —Sn1—N1—N2	-0.8 (3)	C8—O2—C8'—C10'	53.2 (12)
C1—Sn1—N1—N2	-101.9 (2)	Sn2—O2—C8'—C10'	-47.6 (13)
C2—Sn1—N1—N2	103.28 (19)	Sn1 ⁱ —O2—C8'—C10'	158.2 (10)

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