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# Bis($\mu_2$-4-amino-3-nitrobenzoato)bis(4-amino-3-nitrobenzoato)octabutyldi-$\mu_3$-oxido-tetratin(IV)

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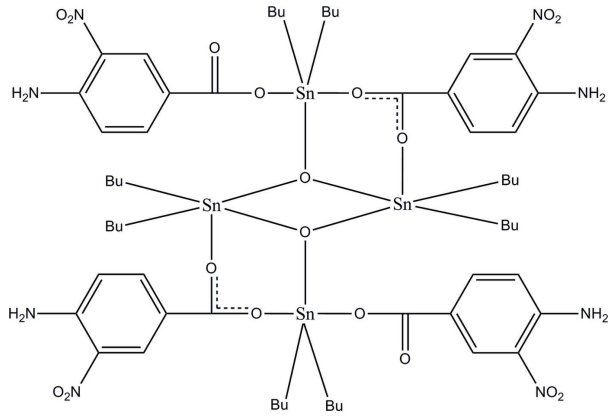
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.006 Å; $R$ factor = 0.037; $wR$ factor = 0.116; data-to-parameter ratio = 27.7.

The tetranuclear molecules of the title compound, $[Sn_4(C_4H_9)_8(C_7H_5N_2O_4)_4O_2]$, reside on a crystallographic inversion center. Both the two independent Sn atoms are five-coordinate, with distorted trigonal–bipyramidal geometries. One Sn atom is coordinated by two O atoms of the carboxylate anions, one bridging O atom and two butyl groups and the other Sn atom is coordinated by an O atom of the carboxylate anion, two bridging O atoms and two butyl groups. All the butyl groups are equatorial with respect to the $SnO_3$ trigonal plane. The molecular structure is stabilized by intramolecular N—H···O hydrogen bonds. In the crystal, pairs of intermolecular bifurcated acceptor N—H···O and C—H···O hydrogen bonds link the molecules into chains along [10$\bar{1}$]. Weak intermolecular C—H···$\pi$ and $\pi$–$\pi$ interactions [centroid–centroid distance = 3.713 (2) Å] are also observed.

## Related literature

For general background to and applications of the title complex, see: Khoo & Hazell (1999); Parvez *et al.* (2004); Li *et al.* (2006); Win *et al.* (2008*a*,*b*). For closely related structures, see: Khoo & Hazell (1999); Parvez *et al.* (2004); Li *et al.* (2006); Win *et al.* (2008*b*). For graph-set motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



## Experimental

### Crystal data

$[Sn_4(C_4H_9)_8(C_7H_5N_2O_4)_4O_2]$
$M_r$ = 1688.18
Triclinic, $P\bar{1}$
$a$ = 11.9585 (9) Å
$b$ = 13.0679 (10) Å
$c$ = 13.1897 (10) Å
$\alpha$ = 76.256 (2)°
$\beta$ = 67.445 (2)°
$\gamma$ = 66.108 (2)°
$V$ = 1732.1 (2) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 1.50 mm$^{-1}$
$T$ = 100 K
0.20 × 0.15 × 0.06 mm

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.758, $T_{max}$ = 0.912
32184 measured reflections
11359 independent reflections
8603 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.116
$S$ = 1.04
11359 reflections
410 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.18 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

*Cg*1 is the centroid of the C16–C21 phenyl ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*1···O6 | 0.91 | 2.59 | 3.422 (4) | 153 |
| N1—H2*N*1···O1 | 1.03 | 1.83 | 2.644 (5) | 133 |
| N3—H1*N*3···O4$^{i}$ | 0.88 | 2.04 | 2.910 (4) | 167 |
| N3—H2*N*3···O5 | 0.88 | 2.06 | 2.669 (4) | 125 |
| C17—H17*A*···O4$^{i}$ | 0.93 | 2.51 | 3.246 (5) | 137 |
| C30—H30*A*···*Cg*1$^{ii}$ | 0.96 | 2.80 | 3.584 (5) | 139 |

Symmetry codes: (i) $x+1, y, z-1$; (ii) $-x+1, -y+1, -z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2350).

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Win, Y. F., Teoh, S. G., Lim, E. K., Ng, S. L. & Fun, H. K. (2008*a*). *J. Chem. Crystallogr.* **38**, 345–350.

# supporting information

*Acta Cryst.* (2010). E**66**, m1406–m1407 [https://doi.org/10.1107/S1600536810040146]

## Bis($\mu_2$-4-amino-3-nitrobenzoato)bis(4-amino-3-nitrobenzoato)octabutyldi-$\mu_3$-oxido-tetratin(IV)

**Yip-Foo Win, Chen-Shang Choong, Siang-Guan Teoh, Jia Hao Goh and Hoong-Kun Fun**

### S1. Comment

In general, there are many well-documented structures on complexes isolated from 1:1 molar ratio reaction between diorganotin(IV) with the respective organic acids (Khoo & Hazell, 1999; Parvez *et al.*, 2004; Li *et al.*, 2006; Win *et al.*, 2008*a*,*b*). This dimeric structure is known as organodistannoxane dimer with the core geometry consisting of a centrosymmetric planar $Sn_2O_2$ group (Win *et al.*, 2008*a*,*b*). The centrosymmetric planar $Sn_2O_2$ group is bonded to the exo- and endocyclic tin(IV) atom moiety *via* the bridging oxygen atoms so that the oxygen atoms are tri-coordinated (Khoo & Hazell, 1999; Parvez *et al.*, 2004; Li *et al.*, 2006). In this study, the crystal structure of the title complex is similar to bis(2,3-dibromopropionato)tetrabutyldistannoxane(IV) dimer and consists of a centrosymmetric planar $Sn_2O_2$ group (Win *et al.*, 2008*b*). The only exception is 4-amino-3-nitrobenzoic acid is utilized in the reaction to obtain the title complex.

The asymmetric unit of the title complex (Fig. 1) lies on a crystallographic inversion center and comprises of one-half molecule, with the other half of the molecule is generated by symmetry code -x, -y+1, -z. The Sn1 atom is five-coordinated by two butyl groups in equatorial position, an O atom of the monodentate carboxylate anion, an O atom of the bridging carboxylate atom and one bridging O atom in a distorted trigonal bipiramidal geometry. The Sn2 atom also has a distorted trigonal bipiramidal geometry, being coordinated by two butyl groups in equatorial position, one bridging carboxylate O atom and two bridging O atoms. Intramolecular N1—H2N1···O1 and N3—H2N3···O5 hydrogen bonds (Table 1) form two different six-membered rings, generating *S*(6) ring motifs (Bernstein *et al.*, 1995) which help to stabilize the molecular structure. All geometric parameters are consistent to those observed in closely related structures (Khoo & Hazell, 1999; Parvez *et al.*, 2004; Li *et al.*, 2006; Win *et al.*, 2008*b*).

In the crystal structure, pairs of intermolecular bifurcated acceptor N3—H1N3···O4 and C17—H17A···O4 hydrogen bonds (Table 1) link adjacent molecules into one-dimensional chains incorporating $R^2_1(6)$ hydrogen bond ring motifs along the [10$\bar{1}$] direction (Bernstein *et al.*, 1995, Fig. 2). Further stabilization of the crystal structure is provided by weak intermolecular C30—H30A···*Cg*1 interactions (Table 1) as well as *Cg*1···*Cg*2 aromatic stacking interactions where *Cg*1 and *Cg* 2 are the centroids of the C16-C21 and C1-C6 benzene rings.

### S2. Experimental

The title complex was obtained by heating under reflux in a 1:1 molar mixture of dibutyltin(IV) oxide (0.50 g, 2 mmol) and 4-amino-3-nitrobenzoic acid (0.36 g, 2 mmol) in methanol (50 ml) for 4 h. Clear yellowish solution was isolated by filtration and kept in a bottle. After 12 days, yellow single crystals (0.71 g, 75.8 % yeild) were collected. *M.p.* 525.8–527.4 K. Analysis found for $C_{60}H_{92}N_8O_{18}Sn_4$: C, 42.84; H, 5.43; N, 6.49; Sn, 28.28 %. Calculated found for $C_{60}H_{92}N_8O_{18}Sn_4$: C, 42.68; H, 5.49; N, 6.64; Sn, 28.13 %.

## S3. Refinement

The amino group H atoms were located from the difference Fourier map and constrained to ride with the parent atom with $U_{iso}$ = 1.2 $U_{eq}$(N). All other H atoms were placed in their calculated positions, with C—H = 0.93 – 0.97 Å, and refined using a riding model with $U_{iso}$ = 1.2 or 1.5 $U_{eq}$(C). The rotating group model was used for the methyl groups. The highest residual electron density peak and the deepest hole were located at 0.72 Å from atom Sn1.

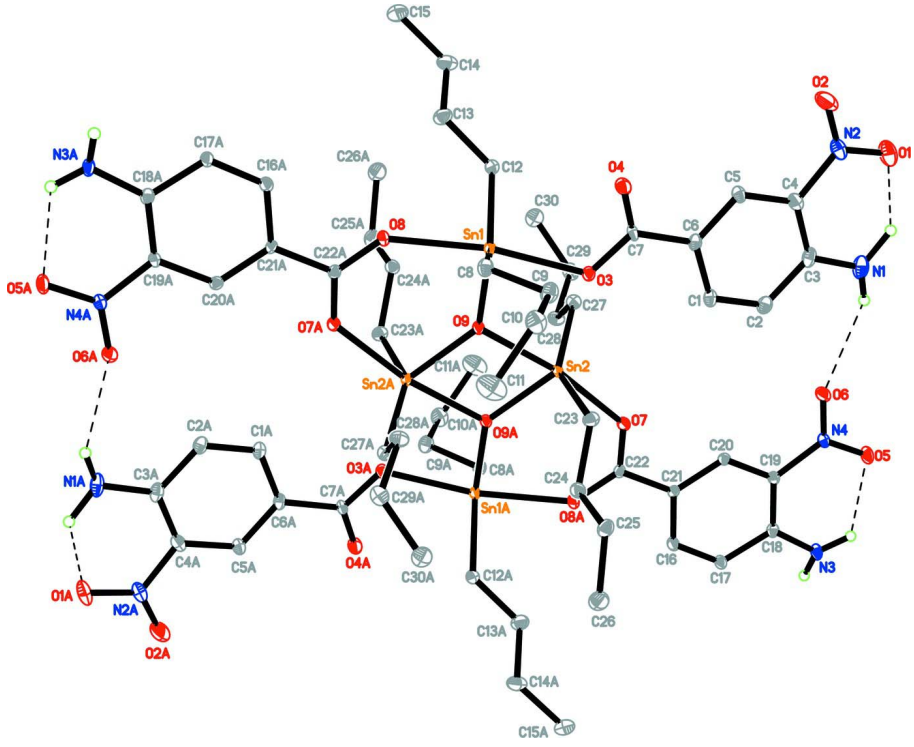


**Figure 1**

The molecular structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The suffix A corresponds to symmetry code [-x, -y+1, -z]. Intramolecular hydrogen bonds are shown as dashed lines and all C-bound H atoms were omitted for clarity.

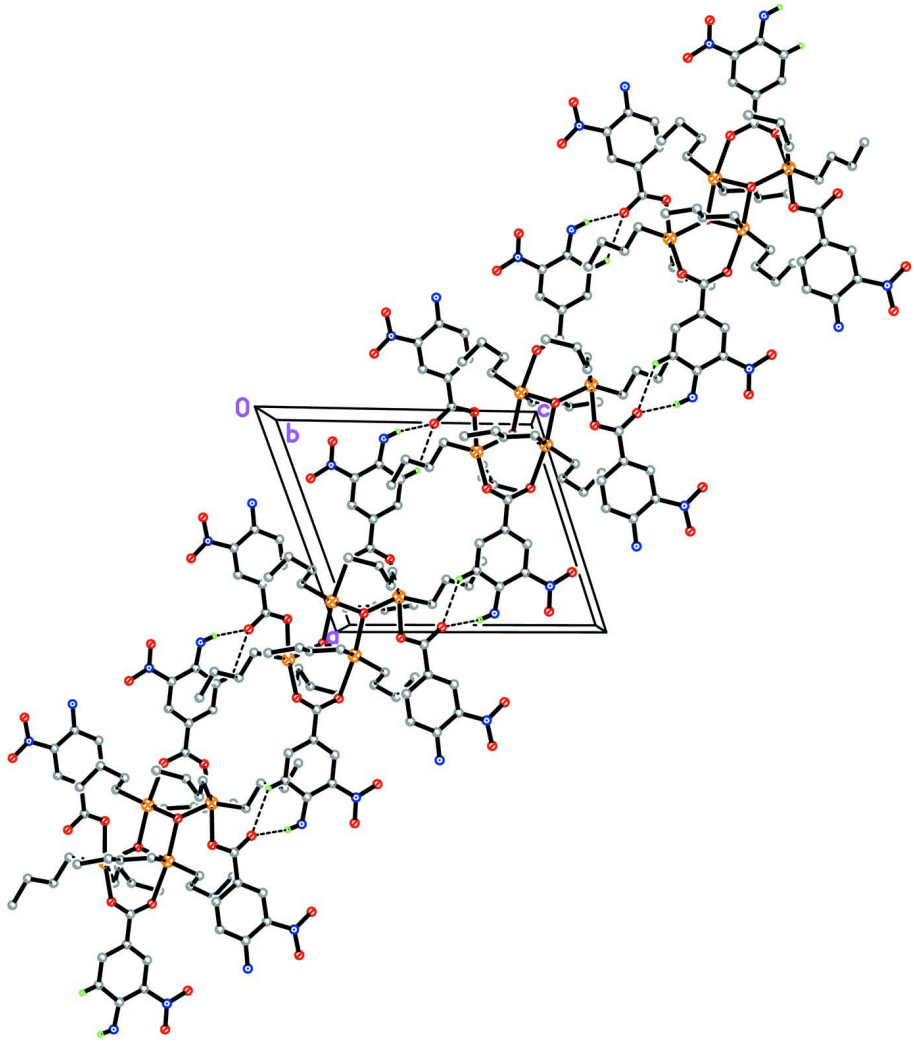


**Figure 2**

The crystal structure of the title complex, viewed along the *b* axis, showing a one-dimensional chain along the [10$\bar{1}$] direction. H atoms not involved in intermolecular hydrogen bonds (dashed lines) have been omitted for clarity.

**Bis($\mu_2$-4-amino-3-nitrobenzoato)bis(4-amino-3-nitrobenzoato)octabutyldi- $\mu_3$-oxido-tetratin(IV)**

*Crystal data*

$[Sn_4(C_4H_9)_8(C_7H_5N_2O_4)_4O_2]$
$M_r$ = 1688.18
Triclinic, $P\bar{1}$
Hall symbol: -P 1
$a$ = 11.9585 (9) Å
$b$ = 13.0679 (10) Å
$c$ = 13.1897 (10) Å
$\alpha$ = 76.256 (2)°
$\beta$ = 67.445 (2)°
$\gamma$ = 66.108 (2)°
$V$ = 1732.1 (2) Å$^3$
$Z$ = 1
$F$(000) = 852
$D_x$ = 1.618 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5645 reflections
$\theta$ = 3.4–33.2°
$\mu$ = 1.50 mm$^{-1}$
$T$ = 100 K
Block, yellow
0.20 × 0.15 × 0.06 mm

*Data collection*

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.758, $T_{max}$ = 0.912
32184 measured reflections
11359 independent reflections
8603 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.055
$\theta_{max}$ = 31.5°, $\theta_{min}$ = 1.7°
$h$ = −17→17
$k$ = −19→18
$l$ = −19→19

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.116
$S$ = 1.04
11359 reflections
410 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
$w = 1/[\sigma^2(F_o^2) + (0.0611P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.26 e Å$^{-3}$
$\Delta\rho_{min}$ = −1.18 e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1)K.

**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**. 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 $F^2 > 2$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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Sn1 | −0.15407 (2) | 0.426491 (18) | 0.258267 (17) | 0.01235 (6) |
| Sn2 | 0.126384 (19) | 0.388757 (17) | 0.012249 (17) | 0.01183 (6) |
| O1 | 0.5285 (3) | −0.1013 (3) | 0.4294 (3) | 0.0452 (9) |
| O2 | 0.3268 (4) | −0.0394 (3) | 0.5298 (3) | 0.0469 (9) |
| O3 | 0.0372 (2) | 0.29294 (19) | 0.21639 (19) | 0.0150 (5) |
| O4 | −0.0160 (2) | 0.2104 (2) | 0.3863 (2) | 0.0230 (5) |
| O5 | 0.9029 (2) | −0.0002 (2) | −0.1901 (2) | 0.0233 (5) |
| O6 | 0.7210 (3) | 0.0470 (2) | −0.0558 (2) | 0.0254 (6) |
| O7 | 0.3299 (2) | 0.3217 (2) | −0.10236 (19) | 0.0183 (5) |
| O8 | −0.3316 (2) | 0.5805 (2) | 0.2675 (2) | 0.0187 (5) |
| O9 | −0.0734 (2) | 0.47928 (19) | 0.09963 (18) | 0.0133 (4) |
| N1 | 0.5993 (3) | −0.0496 (3) | 0.2134 (3) | 0.0313 (8) |
| H1N1 | 0.6573 | −0.0435 | 0.1450 | 0.038* |
| H2N1 | 0.6222 | −0.0939 | 0.2830 | 0.038* |

| | | | | |
|---|---|---|---|---|
| N2 | 0.4123 (4) | −0.0430 (3) | 0.4400 (3) | 0.0315 (8) |
| N3 | 0.9151 (3) | 0.0899 (3) | −0.3964 (2) | 0.0192 (6) |
| H1N3 | 0.9467 | 0.1258 | −0.4600 | 0.023* |
| H2N3 | 0.9574 | 0.0317 | −0.3594 | 0.023* |
| N4 | 0.7854 (3) | 0.0571 (2) | −0.1543 (2) | 0.0173 (6) |
| C1 | 0.2968 (3) | 0.1390 (3) | 0.1681 (3) | 0.0186 (7) |
| H1A | 0.2693 | 0.1787 | 0.1084 | 0.022* |
| C2 | 0.4240 (3) | 0.0748 (3) | 0.1495 (3) | 0.0212 (7) |
| H2A | 0.4809 | 0.0718 | 0.0776 | 0.025* |
| C3 | 0.4715 (3) | 0.0126 (3) | 0.2369 (3) | 0.0213 (7) |
| C4 | 0.3797 (4) | 0.0193 (3) | 0.3434 (3) | 0.0211 (7) |
| C5 | 0.2486 (3) | 0.0864 (3) | 0.3609 (3) | 0.0182 (6) |
| H5A | 0.1902 | 0.0895 | 0.4322 | 0.022* |
| C6 | 0.2058 (3) | 0.1470 (3) | 0.2745 (3) | 0.0163 (6) |
| C7 | 0.0658 (3) | 0.2188 (3) | 0.2964 (3) | 0.0161 (6) |
| C8 | −0.2737 (3) | 0.3386 (3) | 0.2691 (3) | 0.0190 (7) |
| H8A | −0.3379 | 0.3446 | 0.3420 | 0.023* |
| H8B | −0.3195 | 0.3771 | 0.2164 | 0.023* |
| C9 | −0.2096 (4) | 0.2138 (3) | 0.2494 (3) | 0.0238 (7) |
| H9A | −0.1820 | 0.1707 | 0.3118 | 0.029* |
| H9B | −0.1334 | 0.2038 | 0.1843 | 0.029* |
| C10 | −0.3018 (4) | 0.1683 (3) | 0.2336 (4) | 0.0283 (8) |
| H10A | −0.2612 | 0.0875 | 0.2313 | 0.034* |
| H10B | −0.3802 | 0.1828 | 0.2968 | 0.034* |
| C11 | −0.3378 (6) | 0.2205 (5) | 0.1287 (4) | 0.0438 (12) |
| H11A | −0.3958 | 0.1894 | 0.1240 | 0.066* |
| H11B | −0.2611 | 0.2043 | 0.0655 | 0.066* |
| H11C | −0.3793 | 0.3004 | 0.1307 | 0.066* |
| C12 | −0.1180 (3) | 0.4888 (3) | 0.3732 (3) | 0.0191 (7) |
| H12A | −0.0676 | 0.4252 | 0.4117 | 0.023* |
| H12B | −0.0650 | 0.5344 | 0.3321 | 0.023* |
| C13 | −0.2355 (4) | 0.5582 (4) | 0.4589 (3) | 0.0248 (8) |
| H13A | −0.2862 | 0.6223 | 0.4211 | 0.030* |
| H13B | −0.2886 | 0.5128 | 0.5010 | 0.030* |
| C14 | −0.2041 (4) | 0.6002 (4) | 0.5377 (3) | 0.0280 (8) |
| H14A | −0.1521 | 0.6466 | 0.4963 | 0.034* |
| H14B | −0.1533 | 0.5365 | 0.5758 | 0.034* |
| C15 | −0.3241 (5) | 0.6682 (4) | 0.6222 (4) | 0.0352 (10) |
| H15A | −0.2992 | 0.6927 | 0.6707 | 0.053* |
| H15B | −0.3754 | 0.6224 | 0.6644 | 0.053* |
| H15C | −0.3737 | 0.7325 | 0.5851 | 0.053* |
| C16 | 0.5905 (3) | 0.2917 (3) | −0.3655 (3) | 0.0166 (6) |
| H16A | 0.5465 | 0.3451 | −0.4107 | 0.020* |
| C17 | 0.7173 (3) | 0.2297 (3) | −0.4104 (3) | 0.0178 (6) |
| H17A | 0.7574 | 0.2407 | −0.4859 | 0.021* |
| C18 | 0.7904 (3) | 0.1483 (3) | −0.3449 (3) | 0.0152 (6) |
| C19 | 0.7236 (3) | 0.1349 (3) | −0.2307 (3) | 0.0135 (6) |
| C20 | 0.5918 (3) | 0.1990 (3) | −0.1861 (3) | 0.0133 (6) |

| | | | | |
|---|---|---|---|---|
| H20A | 0.5499 | 0.1885 | −0.1109 | 0.016* |
| C21 | 0.5243 (3) | 0.2764 (3) | −0.2514 (3) | 0.0136 (6) |
| C22 | 0.3840 (3) | 0.3441 (3) | −0.2034 (3) | 0.0138 (6) |
| C23 | 0.0916 (4) | 0.2564 (3) | −0.0232 (3) | 0.0194 (7) |
| H23A | 0.1537 | 0.1853 | −0.0055 | 0.023* |
| H23B | 0.0061 | 0.2570 | 0.0241 | 0.023* |
| C24 | 0.1005 (3) | 0.2635 (3) | −0.1432 (3) | 0.0183 (6) |
| H24A | 0.0363 | 0.3332 | −0.1604 | 0.022* |
| H24B | 0.1850 | 0.2651 | −0.1908 | 0.022* |
| C25 | 0.0794 (4) | 0.1652 (3) | −0.1674 (3) | 0.0215 (7) |
| H25A | 0.1367 | 0.0952 | −0.1421 | 0.026* |
| H25B | −0.0088 | 0.1689 | −0.1266 | 0.026* |
| C26 | 0.1044 (4) | 0.1659 (4) | −0.2894 (4) | 0.0301 (9) |
| H26A | 0.1004 | 0.0983 | −0.3020 | 0.045* |
| H26B | 0.1885 | 0.1701 | −0.3309 | 0.045* |
| H26C | 0.0400 | 0.2299 | −0.3125 | 0.045* |
| C27 | 0.2107 (3) | 0.4357 (3) | 0.1018 (3) | 0.0174 (6) |
| H27A | 0.1436 | 0.4668 | 0.1682 | 0.021* |
| H27B | 0.2737 | 0.3685 | 0.1245 | 0.021* |
| C28 | 0.2768 (4) | 0.5210 (3) | 0.0386 (3) | 0.0202 (7) |
| H28A | 0.3422 | 0.4917 | −0.0292 | 0.024* |
| H28B | 0.2134 | 0.5900 | 0.0189 | 0.024* |
| C29 | 0.3397 (3) | 0.5474 (3) | 0.1050 (3) | 0.0221 (7) |
| H29A | 0.3960 | 0.4773 | 0.1313 | 0.027* |
| H29B | 0.3931 | 0.5906 | 0.0567 | 0.027* |
| C30 | 0.2445 (4) | 0.6125 (4) | 0.2031 (3) | 0.0269 (8) |
| H30A | 0.2908 | 0.6194 | 0.2452 | 0.040* |
| H30B | 0.1869 | 0.5733 | 0.2487 | 0.040* |
| H30C | 0.1957 | 0.6860 | 0.1774 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Sn1 | 0.01042 (10) | 0.01296 (11) | 0.01006 (10) | −0.00221 (7) | −0.00232 (7) | 0.00013 (8) |
| Sn2 | 0.01123 (10) | 0.01097 (10) | 0.01065 (10) | −0.00180 (7) | −0.00337 (7) | −0.00046 (7) |
| O1 | 0.0303 (17) | 0.047 (2) | 0.053 (2) | 0.0028 (14) | −0.0281 (16) | −0.0003 (17) |
| O2 | 0.042 (2) | 0.059 (2) | 0.0247 (16) | −0.0027 (16) | −0.0162 (15) | 0.0049 (15) |
| O3 | 0.0112 (10) | 0.0149 (11) | 0.0138 (10) | −0.0025 (8) | −0.0021 (8) | 0.0003 (9) |
| O4 | 0.0167 (12) | 0.0256 (14) | 0.0165 (12) | −0.0040 (9) | −0.0023 (10) | 0.0045 (10) |
| O5 | 0.0134 (11) | 0.0237 (13) | 0.0247 (13) | 0.0002 (9) | −0.0071 (10) | 0.0013 (10) |
| O6 | 0.0214 (13) | 0.0294 (15) | 0.0150 (12) | −0.0009 (10) | −0.0053 (10) | 0.0010 (10) |
| O7 | 0.0117 (11) | 0.0233 (13) | 0.0119 (10) | −0.0004 (9) | −0.0021 (9) | −0.0007 (9) |
| O8 | 0.0135 (11) | 0.0199 (12) | 0.0174 (11) | 0.0010 (9) | −0.0068 (9) | −0.0017 (9) |
| O9 | 0.0116 (10) | 0.0127 (10) | 0.0117 (10) | −0.0025 (8) | −0.0029 (8) | 0.0009 (8) |
| N1 | 0.0133 (14) | 0.0299 (18) | 0.043 (2) | −0.0003 (12) | −0.0082 (14) | −0.0053 (16) |
| N2 | 0.0276 (18) | 0.0309 (19) | 0.0340 (19) | −0.0016 (13) | −0.0198 (15) | 0.0013 (15) |
| N3 | 0.0104 (12) | 0.0188 (14) | 0.0184 (14) | −0.0006 (10) | −0.0018 (10) | 0.0026 (11) |
| N4 | 0.0149 (13) | 0.0170 (14) | 0.0190 (14) | −0.0021 (10) | −0.0088 (11) | −0.0010 (11) |

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|---|---|---|---|---|---|---|
| C1 | 0.0141 (15) | 0.0159 (15) | 0.0233 (17) | −0.0039 (11) | −0.0057 (13) | −0.0005 (13) |
| C2 | 0.0146 (15) | 0.0217 (17) | 0.0237 (17) | −0.0053 (12) | −0.0027 (13) | −0.0040 (14) |
| C3 | 0.0149 (15) | 0.0163 (16) | 0.0331 (19) | −0.0041 (12) | −0.0078 (14) | −0.0057 (14) |
| C4 | 0.0245 (18) | 0.0179 (16) | 0.0251 (17) | −0.0081 (13) | −0.0140 (14) | 0.0015 (14) |
| C5 | 0.0148 (15) | 0.0182 (16) | 0.0206 (16) | −0.0051 (11) | −0.0073 (13) | 0.0014 (13) |
| C6 | 0.0118 (14) | 0.0142 (15) | 0.0217 (16) | −0.0041 (11) | −0.0051 (12) | −0.0011 (12) |
| C7 | 0.0144 (14) | 0.0132 (15) | 0.0188 (15) | −0.0019 (11) | −0.0089 (12) | 0.0025 (12) |
| C8 | 0.0149 (15) | 0.0174 (16) | 0.0218 (16) | −0.0056 (11) | −0.0040 (13) | −0.0006 (13) |
| C9 | 0.0226 (17) | 0.0192 (17) | 0.0300 (19) | −0.0075 (13) | −0.0078 (15) | −0.0041 (15) |
| C10 | 0.033 (2) | 0.0203 (18) | 0.034 (2) | −0.0134 (15) | −0.0121 (17) | 0.0024 (16) |
| C11 | 0.066 (4) | 0.041 (3) | 0.047 (3) | −0.034 (3) | −0.031 (3) | 0.004 (2) |
| C12 | 0.0168 (15) | 0.0209 (17) | 0.0175 (15) | −0.0020 (12) | −0.0073 (12) | −0.0038 (13) |
| C13 | 0.0201 (17) | 0.033 (2) | 0.0234 (18) | −0.0076 (14) | −0.0060 (14) | −0.0104 (16) |
| C14 | 0.035 (2) | 0.033 (2) | 0.0184 (17) | −0.0131 (16) | −0.0098 (16) | −0.0030 (15) |
| C15 | 0.043 (3) | 0.035 (2) | 0.026 (2) | −0.0060 (18) | −0.0123 (19) | −0.0121 (18) |
| C16 | 0.0147 (14) | 0.0166 (15) | 0.0148 (14) | −0.0032 (11) | −0.0048 (12) | 0.0011 (12) |
| C17 | 0.0132 (14) | 0.0192 (16) | 0.0143 (14) | −0.0013 (11) | −0.0035 (12) | 0.0003 (12) |
| C18 | 0.0118 (13) | 0.0148 (15) | 0.0173 (15) | −0.0048 (11) | −0.0034 (12) | −0.0007 (12) |
| C19 | 0.0121 (13) | 0.0130 (14) | 0.0159 (14) | −0.0039 (10) | −0.0060 (11) | −0.0007 (11) |
| C20 | 0.0124 (13) | 0.0141 (14) | 0.0122 (13) | −0.0048 (10) | −0.0026 (11) | −0.0014 (11) |
| C21 | 0.0102 (13) | 0.0144 (14) | 0.0117 (13) | −0.0014 (10) | −0.0012 (11) | −0.0026 (11) |
| C22 | 0.0132 (14) | 0.0122 (14) | 0.0168 (14) | −0.0028 (10) | −0.0061 (11) | −0.0038 (12) |
| C23 | 0.0211 (16) | 0.0192 (16) | 0.0171 (15) | −0.0079 (12) | −0.0042 (13) | −0.0024 (13) |
| C24 | 0.0202 (16) | 0.0174 (16) | 0.0195 (16) | −0.0063 (12) | −0.0090 (13) | −0.0020 (13) |
| C25 | 0.0188 (16) | 0.0197 (17) | 0.0275 (18) | −0.0053 (12) | −0.0076 (14) | −0.0073 (14) |
| C26 | 0.026 (2) | 0.035 (2) | 0.034 (2) | −0.0072 (15) | −0.0130 (17) | −0.0120 (18) |
| C27 | 0.0165 (15) | 0.0186 (16) | 0.0169 (15) | −0.0079 (12) | −0.0040 (12) | −0.0006 (12) |
| C28 | 0.0233 (17) | 0.0228 (17) | 0.0164 (15) | −0.0126 (13) | −0.0053 (13) | 0.0007 (13) |
| C29 | 0.0185 (16) | 0.0252 (18) | 0.0259 (18) | −0.0125 (13) | −0.0081 (14) | 0.0020 (14) |
| C30 | 0.0252 (19) | 0.029 (2) | 0.033 (2) | −0.0119 (15) | −0.0110 (16) | −0.0075 (17) |

*Geometric parameters (Å, º)*

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|---|---|---|---|
| Sn1—O9 | 2.022 (2) | C11—H11C | 0.9600 |
| Sn1—C8 | 2.117 (4) | C12—C13 | 1.520 (5) |
| Sn1—C12 | 2.125 (3) | C12—H12A | 0.9700 |
| Sn1—O3 | 2.200 (2) | C12—H12B | 0.9700 |
| Sn1—O8 | 2.243 (2) | C13—C14 | 1.504 (5) |
| Sn2—O9$^{i}$ | 2.044 (2) | C13—H13A | 0.9700 |
| Sn2—C23 | 2.121 (3) | C13—H13B | 0.9700 |
| Sn2—C27 | 2.133 (3) | C14—C15 | 1.517 (6) |
| Sn2—O9 | 2.163 (2) | C14—H14A | 0.9700 |
| Sn2—O7 | 2.249 (2) | C14—H14B | 0.9700 |
| Sn2—Sn2$^{i}$ | 3.2982 (4) | C15—H15A | 0.9600 |
| O1—N2 | 1.255 (5) | C15—H15B | 0.9600 |
| O2—N2 | 1.228 (5) | C15—H15C | 0.9600 |
| O3—C7 | 1.301 (4) | C16—C17 | 1.360 (4) |
| O4—C7 | 1.229 (4) | C16—C21 | 1.415 (4) |

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| O5—N4 | 1.251 (4) | C16—H16A | 0.9300 |
| O6—N4 | 1.238 (4) | C17—C18 | 1.425 (5) |
| O7—C22 | 1.260 (4) | C17—H17A | 0.9300 |
| O8—C22$^{i}$ | 1.260 (4) | C18—C19 | 1.415 (5) |
| O9—Sn2$^{i}$ | 2.044 (2) | C19—C20 | 1.409 (4) |
| N1—C3 | 1.357 (5) | C20—C21 | 1.369 (5) |
| N1—H1N1 | 0.9127 | C20—H20A | 0.9300 |
| N1—H2N1 | 1.0326 | C21—C22 | 1.499 (4) |
| N2—C4 | 1.439 (5) | C22—O8$^{i}$ | 1.260 (4) |
| N3—C18 | 1.348 (4) | C23—C24 | 1.527 (5) |
| N3—H1N3 | 0.8828 | C23—H23A | 0.9700 |
| N3—H2N3 | 0.8795 | C23—H23B | 0.9700 |
| N4—C19 | 1.439 (4) | C24—C25 | 1.527 (5) |
| C1—C2 | 1.363 (5) | C24—H24A | 0.9700 |
| C1—C6 | 1.404 (5) | C24—H24B | 0.9700 |
| C1—H1A | 0.9300 | C25—C26 | 1.518 (6) |
| C2—C3 | 1.413 (6) | C25—H25A | 0.9700 |
| C2—H2A | 0.9300 | C25—H25B | 0.9700 |
| C3—C4 | 1.408 (5) | C26—H26A | 0.9600 |
| C4—C5 | 1.408 (5) | C26—H26B | 0.9600 |
| C5—C6 | 1.371 (5) | C26—H26C | 0.9600 |
| C5—H5A | 0.9300 | C27—C28 | 1.526 (5) |
| C6—C7 | 1.500 (5) | C27—H27A | 0.9700 |
| C8—C9 | 1.533 (5) | C27—H27B | 0.9700 |
| C8—H8A | 0.9700 | C28—C29 | 1.521 (5) |
| C8—H8B | 0.9700 | C28—H28A | 0.9700 |
| C9—C10 | 1.543 (6) | C28—H28B | 0.9700 |
| C9—H9A | 0.9700 | C29—C30 | 1.517 (5) |
| C9—H9B | 0.9700 | C29—H29A | 0.9700 |
| C10—C11 | 1.528 (7) | C29—H29B | 0.9700 |
| C10—H10A | 0.9700 | C30—H30A | 0.9600 |
| C10—H10B | 0.9700 | C30—H30B | 0.9600 |
| C11—H11A | 0.9600 | C30—H30C | 0.9600 |
| C11—H11B | 0.9600 | | |

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|---|---|---|---|
| O9—Sn1—C8 | 110.89 (12) | C13—C12—H12B | 108.1 |
| O9—Sn1—C12 | 113.25 (12) | Sn1—C12—H12B | 108.1 |
| C8—Sn1—C12 | 135.33 (14) | H12A—C12—H12B | 107.3 |
| O9—Sn1—O3 | 78.94 (9) | C14—C13—C12 | 114.5 (3) |
| C8—Sn1—O3 | 100.88 (11) | C14—C13—H13A | 108.6 |
| C12—Sn1—O3 | 93.91 (11) | C12—C13—H13A | 108.6 |
| O9—Sn1—O8 | 89.41 (9) | C14—C13—H13B | 108.6 |
| C8—Sn1—O8 | 84.97 (12) | C12—C13—H13B | 108.6 |
| C12—Sn1—O8 | 88.89 (11) | H13A—C13—H13B | 107.6 |
| O3—Sn1—O8 | 168.19 (9) | C13—C14—C15 | 112.6 (4) |
| O9$^{i}$—Sn2—C23 | 104.84 (12) | C13—C14—H14A | 109.1 |
| O9$^{i}$—Sn2—C27 | 108.28 (12) | C15—C14—H14A | 109.1 |
| C23—Sn2—C27 | 146.36 (14) | C13—C14—H14B | 109.1 |

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| O9$^{i}$—Sn2—O9 | 76.78 (9) | C15—C14—H14B | 109.1 |
| C23—Sn2—O9 | 95.98 (11) | H14A—C14—H14B | 107.8 |
| C27—Sn2—O9 | 97.07 (11) | C14—C15—H15A | 109.5 |
| O9$^{i}$—Sn2—O7 | 92.75 (9) | C14—C15—H15B | 109.5 |
| C23—Sn2—O7 | 87.89 (12) | H15A—C15—H15B | 109.5 |
| C27—Sn2—O7 | 84.87 (11) | C14—C15—H15C | 109.5 |
| O9—Sn2—O7 | 169.46 (9) | H15A—C15—H15C | 109.5 |
| O9$^{i}$—Sn2—Sn2$^{i}$ | 39.68 (6) | H15B—C15—H15C | 109.5 |
| C23—Sn2—Sn2$^{i}$ | 103.12 (10) | C17—C16—C21 | 121.3 (3) |
| C27—Sn2—Sn2$^{i}$ | 105.97 (10) | C17—C16—H16A | 119.4 |
| O9—Sn2—Sn2$^{i}$ | 37.10 (6) | C21—C16—H16A | 119.4 |
| O7—Sn2—Sn2$^{i}$ | 132.42 (6) | C16—C17—C18 | 121.9 (3) |
| C7—O3—Sn1 | 116.89 (19) | C16—C17—H17A | 119.1 |
| C22—O7—Sn2 | 133.4 (2) | C18—C17—H17A | 119.1 |
| C22$^{i}$—O8—Sn1 | 139.1 (2) | N3—C18—C19 | 125.8 (3) |
| Sn1—O9—Sn2$^{i}$ | 137.06 (11) | N3—C18—C17 | 117.9 (3) |
| Sn1—O9—Sn2 | 119.61 (11) | C19—C18—C17 | 116.3 (3) |
| Sn2$^{i}$—O9—Sn2 | 103.22 (9) | C20—C19—C18 | 120.9 (3) |
| C3—N1—H1N1 | 121.9 | C20—C19—N4 | 116.6 (3) |
| C3—N1—H2N1 | 112.1 | C18—C19—N4 | 122.5 (3) |
| H1N1—N1—H2N1 | 125.5 | C21—C20—C19 | 121.3 (3) |
| O2—N2—O1 | 121.7 (4) | C21—C20—H20A | 119.4 |
| O2—N2—C4 | 119.9 (3) | C19—C20—H20A | 119.4 |
| O1—N2—C4 | 118.4 (4) | C20—C21—C16 | 118.3 (3) |
| C18—N3—H1N3 | 111.7 | C20—C21—C22 | 121.0 (3) |
| C18—N3—H2N3 | 118.7 | C16—C21—C22 | 120.7 (3) |
| H1N3—N3—H2N3 | 128.4 | O7—C22—O8$^{i}$ | 126.0 (3) |
| O6—N4—O5 | 121.8 (3) | O7—C22—C21 | 117.0 (3) |
| O6—N4—C19 | 119.5 (3) | O8$^{i}$—C22—C21 | 117.0 (3) |
| O5—N4—C19 | 118.7 (3) | C24—C23—Sn2 | 114.1 (2) |
| C2—C1—C6 | 122.2 (4) | C24—C23—H23A | 108.7 |
| C2—C1—H1A | 118.9 | Sn2—C23—H23A | 108.7 |
| C6—C1—H1A | 118.9 | C24—C23—H23B | 108.7 |
| C1—C2—C3 | 121.5 (3) | Sn2—C23—H23B | 108.7 |
| C1—C2—H2A | 119.3 | H23A—C23—H23B | 107.6 |
| C3—C2—H2A | 119.3 | C25—C24—C23 | 113.0 (3) |
| N1—C3—C4 | 124.9 (4) | C25—C24—H24A | 109.0 |
| N1—C3—C2 | 118.9 (4) | C23—C24—H24A | 109.0 |
| C4—C3—C2 | 116.2 (3) | C25—C24—H24B | 109.0 |
| C3—C4—C5 | 121.4 (4) | C23—C24—H24B | 109.0 |
| C3—C4—N2 | 122.7 (3) | H24A—C24—H24B | 107.8 |
| C5—C4—N2 | 115.9 (3) | C26—C25—C24 | 112.3 (3) |
| C6—C5—C4 | 121.0 (3) | C26—C25—H25A | 109.1 |
| C6—C5—H5A | 119.5 | C24—C25—H25A | 109.1 |
| C4—C5—H5A | 119.5 | C26—C25—H25B | 109.1 |
| C5—C6—C1 | 117.7 (3) | C24—C25—H25B | 109.1 |
| C5—C6—C7 | 119.6 (3) | H25A—C25—H25B | 107.9 |
| C1—C6—C7 | 122.7 (3) | C25—C26—H26A | 109.5 |

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| O4—C7—O3 | 122.2 (3) | C25—C26—H26B | 109.5 |
| O4—C7—C6 | 121.6 (3) | H26A—C26—H26B | 109.5 |
| O3—C7—C6 | 116.2 (3) | C25—C26—H26C | 109.5 |
| C9—C8—Sn1 | 118.1 (2) | H26A—C26—H26C | 109.5 |
| C9—C8—H8A | 107.8 | H26B—C26—H26C | 109.5 |
| Sn1—C8—H8A | 107.8 | C28—C27—Sn2 | 115.0 (2) |
| C9—C8—H8B | 107.8 | C28—C27—H27A | 108.5 |
| Sn1—C8—H8B | 107.8 | Sn2—C27—H27A | 108.5 |
| H8A—C8—H8B | 107.1 | C28—C27—H27B | 108.5 |
| C8—C9—C10 | 112.1 (3) | Sn2—C27—H27B | 108.5 |
| C8—C9—H9A | 109.2 | H27A—C27—H27B | 107.5 |
| C10—C9—H9A | 109.2 | C29—C28—C27 | 112.5 (3) |
| C8—C9—H9B | 109.2 | C29—C28—H28A | 109.1 |
| C10—C9—H9B | 109.2 | C27—C28—H28A | 109.1 |
| H9A—C9—H9B | 107.9 | C29—C28—H28B | 109.1 |
| C11—C10—C9 | 113.5 (4) | C27—C28—H28B | 109.1 |
| C11—C10—H10A | 108.9 | H28A—C28—H28B | 107.8 |
| C9—C10—H10A | 108.9 | C30—C29—C28 | 114.2 (3) |
| C11—C10—H10B | 108.9 | C30—C29—H29A | 108.7 |
| C9—C10—H10B | 108.9 | C28—C29—H29A | 108.7 |
| H10A—C10—H10B | 107.7 | C30—C29—H29B | 108.7 |
| C10—C11—H11A | 109.5 | C28—C29—H29B | 108.7 |
| C10—C11—H11B | 109.5 | H29A—C29—H29B | 107.6 |
| H11A—C11—H11B | 109.5 | C29—C30—H30A | 109.5 |
| C10—C11—H11C | 109.5 | C29—C30—H30B | 109.5 |
| H11A—C11—H11C | 109.5 | H30A—C30—H30B | 109.5 |
| H11B—C11—H11C | 109.5 | C29—C30—H30C | 109.5 |
| C13—C12—Sn1 | 116.8 (2) | H30A—C30—H30C | 109.5 |
| C13—C12—H12A | 108.1 | H30B—C30—H30C | 109.5 |
| Sn1—C12—H12A | 108.1 | | |

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| O9—Sn1—O3—C7 | 173.3 (3) | C5—C6—C7—O3 | 164.7 (3) |
| C8—Sn1—O3—C7 | −77.3 (3) | C1—C6—C7—O3 | −15.1 (5) |
| C12—Sn1—O3—C7 | 60.4 (3) | O9—Sn1—C8—C9 | 83.0 (3) |
| O8—Sn1—O3—C7 | 163.8 (4) | C12—Sn1—C8—C9 | −106.3 (3) |
| O9$^{i}$—Sn2—O7—C22 | −11.5 (3) | O3—Sn1—C8—C9 | 0.8 (3) |
| C23—Sn2—O7—C22 | 93.3 (3) | O8—Sn1—C8—C9 | 170.4 (3) |
| C27—Sn2—O7—C22 | −119.6 (3) | Sn1—C8—C9—C10 | −166.9 (3) |
| O9—Sn2—O7—C22 | −18.5 (7) | C8—C9—C10—C11 | 66.1 (5) |
| Sn2$^{i}$—Sn2—O7—C22 | −12.6 (4) | O9—Sn1—C12—C13 | 121.2 (3) |
| O9—Sn1—O8—C22$^{i}$ | 17.1 (4) | C8—Sn1—C12—C13 | −49.4 (4) |
| C8—Sn1—O8—C22$^{i}$ | −94.0 (4) | O3—Sn1—C12—C13 | −159.2 (3) |
| C12—Sn1—O8—C22$^{i}$ | 130.3 (4) | O8—Sn1—C12—C13 | 32.3 (3) |
| O3—Sn1—O8—C22$^{i}$ | 26.4 (7) | Sn1—C12—C13—C14 | −179.8 (3) |
| C8—Sn1—O9—Sn2$^{i}$ | 82.2 (2) | C12—C13—C14—C15 | −179.6 (4) |
| C12—Sn1—O9—Sn2$^{i}$ | −90.8 (2) | C21—C16—C17—C18 | −1.4 (5) |
| O3—Sn1—O9—Sn2$^{i}$ | 179.71 (19) | C16—C17—C18—N3 | 179.4 (3) |
| O8—Sn1—O9—Sn2$^{i}$ | −2.23 (18) | C16—C17—C18—C19 | 0.4 (5) |

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| C8—Sn1—O9—Sn2 | −102.47 (15) | N3—C18—C19—C20 | −178.5 (3) |
| C12—Sn1—O9—Sn2 | 84.59 (15) | C17—C18—C19—C20 | 0.4 (5) |
| O3—Sn1—O9—Sn2 | −4.93 (11) | N3—C18—C19—N4 | 2.1 (5) |
| O8—Sn1—O9—Sn2 | 173.13 (13) | C17—C18—C19—N4 | −179.1 (3) |
| O9$^{i}$—Sn2—O9—Sn1 | −176.76 (19) | O6—N4—C19—C20 | 2.5 (5) |
| C23—Sn2—O9—Sn1 | 79.36 (15) | O5—N4—C19—C20 | −178.9 (3) |
| C27—Sn2—O9—Sn1 | −69.56 (15) | O6—N4—C19—C18 | −178.0 (3) |
| O7—Sn2—O9—Sn1 | −169.5 (4) | O5—N4—C19—C18 | 0.6 (5) |
| Sn2$^{i}$—Sn2—O9—Sn1 | −176.76 (19) | C18—C19—C20—C21 | −0.3 (5) |
| O9$^{i}$—Sn2—O9—Sn2$^{i}$ | 0.001 (2) | N4—C19—C20—C21 | 179.2 (3) |
| C23—Sn2—O9—Sn2$^{i}$ | −103.88 (13) | C19—C20—C21—C16 | −0.6 (5) |
| C27—Sn2—O9—Sn2$^{i}$ | 107.20 (13) | C19—C20—C21—C22 | 179.9 (3) |
| O7—Sn2—O9—Sn2$^{i}$ | 7.2 (5) | C17—C16—C21—C20 | 1.4 (5) |
| C6—C1—C2—C3 | −0.1 (6) | C17—C16—C21—C22 | −179.0 (3) |
| C1—C2—C3—N1 | −179.8 (4) | Sn2—O7—C22—O8$^{i}$ | 3.3 (5) |
| C1—C2—C3—C4 | 1.1 (5) | Sn2—O7—C22—C21 | −178.0 (2) |
| N1—C3—C4—C5 | 179.8 (4) | C20—C21—C22—O7 | −4.1 (5) |
| C2—C3—C4—C5 | −1.3 (5) | C16—C21—C22—O7 | 176.3 (3) |
| N1—C3—C4—N2 | −1.7 (6) | C20—C21—C22—O8$^{i}$ | 174.7 (3) |
| C2—C3—C4—N2 | 177.3 (3) | C16—C21—C22—O8$^{i}$ | −4.9 (5) |
| O2—N2—C4—C3 | −175.4 (4) | O9$^{i}$—Sn2—C23—C24 | 27.4 (3) |
| O1—N2—C4—C3 | 3.5 (6) | C27—Sn2—C23—C24 | −142.4 (2) |
| O2—N2—C4—C5 | 3.2 (6) | O9—Sn2—C23—C24 | 105.2 (2) |
| O1—N2—C4—C5 | −177.9 (4) | O7—Sn2—C23—C24 | −64.9 (3) |
| C3—C4—C5—C6 | 0.4 (5) | Sn2$^{i}$—Sn2—C23—C24 | 68.3 (3) |
| N2—C4—C5—C6 | −178.2 (3) | Sn2—C23—C24—C25 | 178.1 (2) |
| C4—C5—C6—C1 | 0.7 (5) | C23—C24—C25—C26 | −173.1 (3) |
| C4—C5—C6—C7 | −179.1 (3) | O9$^{i}$—Sn2—C27—C28 | −28.8 (3) |
| C2—C1—C6—C5 | −0.8 (5) | C23—Sn2—C27—C28 | 140.8 (3) |
| C2—C1—C6—C7 | 179.0 (3) | O9—Sn2—C27—C28 | −107.1 (2) |
| Sn1—O3—C7—O4 | 12.7 (4) | O7—Sn2—C27—C28 | 62.5 (2) |
| Sn1—O3—C7—C6 | −164.9 (2) | Sn2$^{i}$—Sn2—C27—C28 | −70.3 (2) |
| C5—C6—C7—O4 | −12.8 (5) | Sn2—C27—C28—C29 | −177.6 (2) |
| C1—C6—C7—O4 | 167.4 (3) | C27—C28—C29—C30 | −68.9 (4) |

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

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the C16–C21 phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*1···O6 | 0.91 | 2.59 | 3.422 (4) | 153 |
| N1—H2*N*1···O1 | 1.03 | 1.83 | 2.644 (5) | 133 |
| N3—H1*N*3···O4$^{ii}$ | 0.88 | 2.04 | 2.910 (4) | 167 |
| N3—H2*N*3···O5 | 0.88 | 2.06 | 2.669 (4) | 125 |
| C17—H17*A*···O4$^{ii}$ | 0.93 | 2.51 | 3.246 (5) | 137 |
| C30—H30*A*···*Cg*1$^{iii}$ | 0.96 | 2.80 | 3.584 (5) | 139 |

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