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Crystal structure of bis(benzoato- κ O)[5,15-diphenyl-10,20-bis(pyridin-4-yl)porphyrinato- κ^4 N,N',N'',N''']tin(IV)

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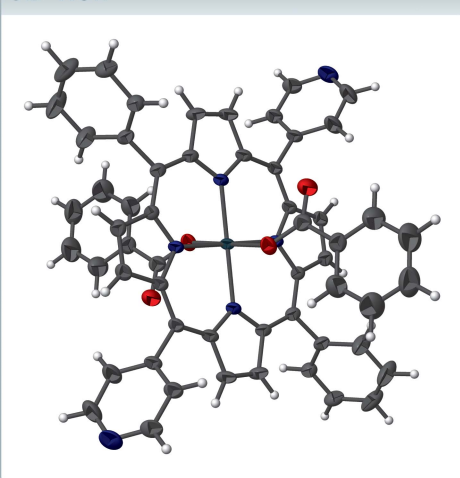
Keywords: crystal structure; Sn^{IV} porphyrin; axial bonding; N₄O₂ coordination set.

CCDC reference: 1913141

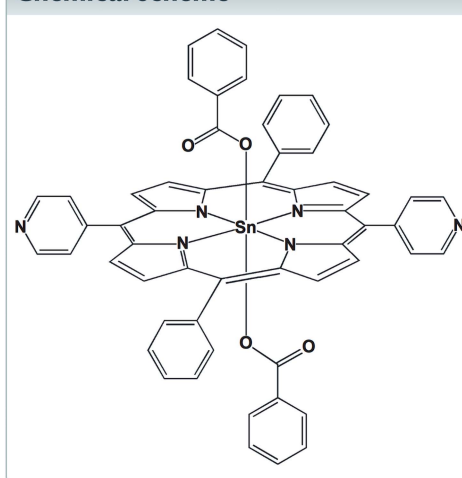
Structural data: full structural data are available from iucrdata.iucr.org

In the crystal structure of the title compound, [Sn(C₄₂H₂₆N₆)(C₇H₅O₂)₂], the Sn^{IV} ion is located on a crystallographic inversion centre and is octahedrally coordinated with an N₄O₂ set. Four N atoms of the porphyrin ring form the equatorial plane while the axial positions are occupied by two O atoms from benzoate anions. The molecular packing of the title complex involves non-classical hydrogen bonds of the types C–H···O and C–H···N, leading to a three-dimensional network structure.

3D view



Chemical scheme



Structure description

Tin(IV) porphyrin is a suitable scaffold for use as a building block in the design of supramolecular porphyrin assemblies (Kim *et al.*, 2005, 2019; Titi *et al.*, 2013a; Jo *et al.*, 2015). Tin(IV) porphyrins readily form stable complexes, with the central tin(IV) atom usually in a sixfold coordination. Next to the porphyrin core, two *trans* axial oxyanion ligands are frequently encountered as a result of the oxophilic nature of the high-valent tin(IV) atom (Arnold & Blok, 2004; Shetti *et al.*, 2012; Titi *et al.*, 2015). The latter can be accommodated in the porphyrin core without a considerable distortion from planarity of the macrocyclic ligand (Lee *et al.*, 2006; Kim *et al.*, 2008a; Li *et al.*, 2015). Structural information for these complexes are readily obtainable as these complexes are diamagnetic with NMR-active Sn nuclei. Interesting optical and luminescent properties are also important characteristics of these complexes (Jang *et al.*, 2007a,b; Kim *et al.*, 2008b, 2010; Indelli *et al.*, 2010; Yoo *et al.*, 2016). A large number of Sn^{IV} porphyrins have been synthesized through variation of the axial ligands such as hydroxide, alkoxide, carboxylate, halide, perchlorate or nitrate (Smith *et al.*, 1991; Singh & Kim, 2012; Wang *et al.*, 2016). Among these compounds, hydroxido-tin(IV) porphyrins have been developed

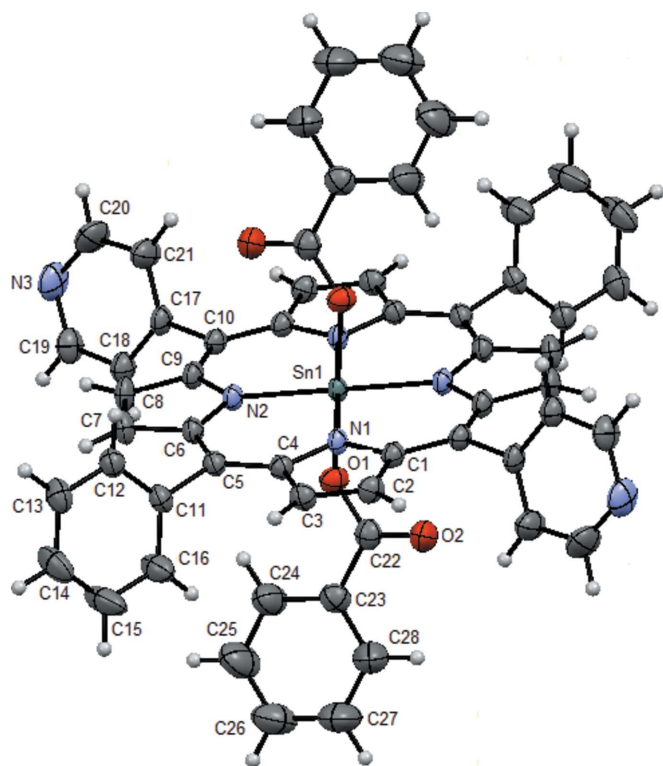


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level. Unlabelled atoms are generated by the symmetry operation $-x + 1, -y + 1, -z + 1$.

as useful precursors for the preparation of various other tin(IV) porphyrin complexes bearing preferentially oxygen donor ligands (Kim *et al.*, 2004, 2007, 2009, 2012; Singh *et al.*, 2012; Titi *et al.*, 2013*b*). The strong preference of Sn^{IV} for coordination to oxanionic ligands such as carboxylates and alkoxides can be advantageous when constructing multiporphyrin assemblies. Here we report on the synthesis and crystal structure analysis of the title compound [Sn(C₄₂H₂₆N₆)(C₇H₅O₂)₂] or [Sn(BPBPYP)(PhCOO)₂] [where BPBPYP is the 5,15-bis(phenyl)-10,20-bis(4-pyridyl) porphyrinato dianion and PhCOO is the benzoate anion].

The molecular structure of [Sn(BPBPYP)(PhCOO)₂] (Fig. 1) reveals the tin(IV) atom (site symmetry $\bar{1}$) is in an octahedral coordination environment. The equatorial plane is formed by four N atoms of the porphyrin ring while the axial positions are occupied by O atoms of two benzoate groups. Relevant bond lengths and angles are listed in Table 1. The two different types of rings of the BPBPYP system are inclined by 71.48 (7)° (phenyl ring) and by 65.81 (7)° (pyridyl ring) relative to the planar porphyrin core. As for all carboxylate examples, the coordinating interaction of the benzoate ligand with the central metal is purely unidentate, the second carboxylate oxygen being 3.3845 (19) Å away from the tin(IV) atom. The Sn1—O1 bond length [2.0794 (15) Å] is slightly longer than that in Sn(TPP)(PhCOO)₂ [2.055 (5) Å; TPP = tetraphenylporphyrin; Smith *et al.*, 1991]. The relevant torsion angle for the benzoate ring including the coordinating O1 atom, C28—C23—C22—O1 is $-170.9 (3)^\circ$.

Table 1
Selected geometric parameters (Å, °).

Sn1—O1	2.0794 (15)	Sn1—N1	2.0942 (17)
Sn1—N2	2.0874 (17)		
O1—Sn1—N2	96.88 (7)	N2—Sn1—N1	89.81 (7)
O1—Sn1—N1	89.01 (6)	C22—O1—Sn1	128.68 (15)

Table 2
Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
C12—H12A...N3 ⁱ	0.95 (1)	2.69 (1)	3.360 (3)	128 (1)
C18—H18A...O1 ⁱ	0.95 (1)	2.69 (2)	3.357 (3)	128 (1)
C13—H13A...O2 ⁱⁱ	0.95 (1)	2.72 (1)	3.411 (3)	130 (1)

Symmetry codes: (i) $x, -y + 1, z - \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y + \frac{3}{2}, -z + 1$.

The packing of the title complex (Figs. 2 and 3) involves three intermolecular non-classical hydrogen bonds of weak strength. One hydrogen bond forms between the phenyl H12A atom of one porphyrin molecule with the pyridine N3 atom of the adjacent porphyrin molecule. The other two involve phenyl H18A and H13A atoms and benzoate O1 and O2 atoms (Table 2). Moreover, there is a π – π interaction between the pyridyl ring and a neighbouring pyrrole ring, C18...C_g = 3.523 (3) Å, where C_g is the centroid of the N1/C1–C4 pyrrole ring.

Synthesis and crystallization

The title compound was prepared according to a literature procedure (Kim *et al.*, 2005). Solid benzoic acid (30 mg,

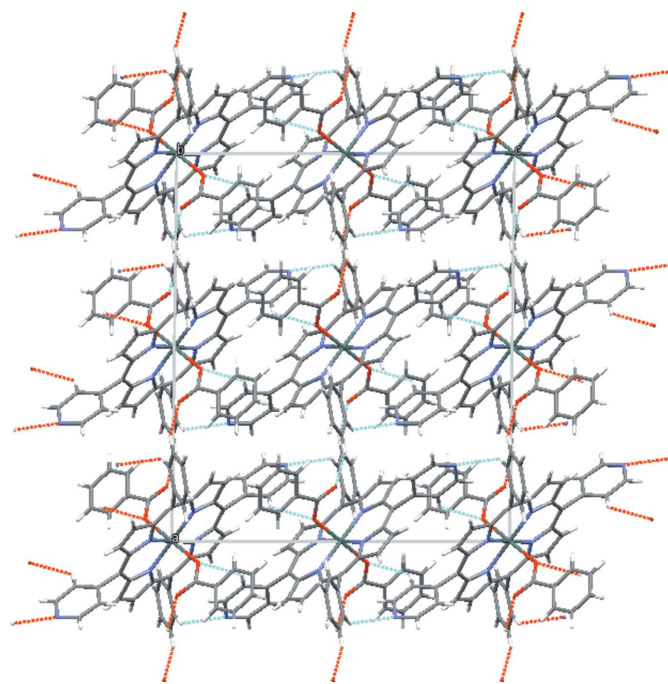


Figure 2
View of the packing of the molecular components in the title compound in a view along [010]. Red and cyan lines represent intermolecular hydrogen bonds (Table 2).

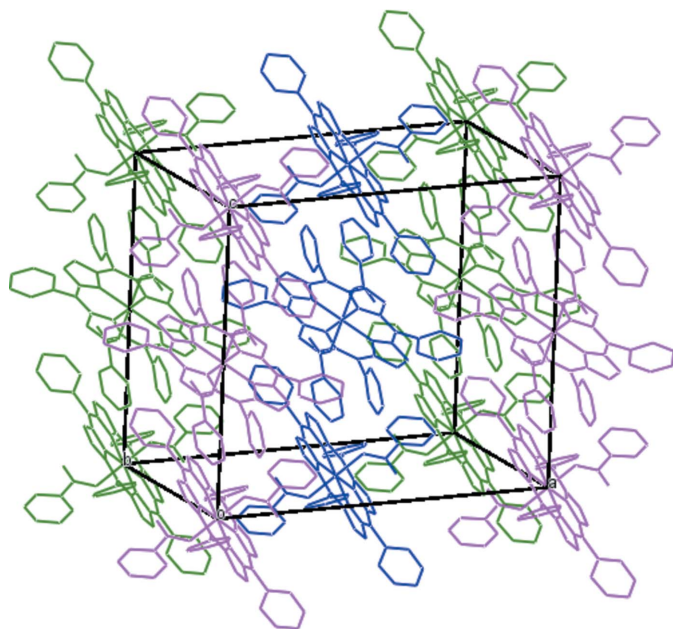


Figure 3
View of the three-dimensional packing in a view along [111]. Colour code; purple (front layer), blue (middle layer), and green (back end layer). Hydrogen atoms are omitted for clarity.

0.25 mmol) was added into a solution of $[\text{Sn}(\text{BPBPYP})(\text{OH})_2]$ (77 mg, 0.1 mmol) in THF (20 ml) and the mixture was refluxed for 12 h. The solution was filtered and evaporated to dryness *in vacuo*. The crude product was extracted with CHCl_3 and filtered through a Celite pad. The product was recrystallized from a CHCl_3/n -hexane solution ($v/v = 1:1$) to afford a violet powder (83 mg, 86%). Single crystals suitable for X-ray analysis were obtained by direct diffusion of *n*-hexane into a CHCl_3 solution of the title compound at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3.

Funding information

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Table 3

Experimental details.

Crystal data	
Chemical formula	$[\text{Sn}(\text{C}_{42}\text{H}_{26}\text{N}_6)(\text{C}_7\text{H}_5\text{O}_2)_2]$
M_r	975.60
Crystal system, space group	Monoclinic, $C2/c$
Temperature (K)	173
a, b, c (Å)	20.8021 (4), 11.4260 (2), 18.1164 (4)
β (°)	90.745 (1)
V (Å ³)	4305.63 (15)
Z	4
Radiation type	Mo $K\alpha$
μ (mm ⁻¹)	0.65
Crystal size (mm)	0.16 × 0.15 × 0.09
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (<i>SADABS</i> ; Bruker, 2014)
T_{\min} , T_{\max}	0.705, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	35578, 4972, 3804
R_{int}	0.048
$(\sin \theta/\lambda)_{\text{max}}$ (Å ⁻¹)	0.652
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.030, 0.075, 1.04
No. of reflections	4972
No. of parameters	304
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$, $\Delta\rho_{\text{min}}$ (e Å ⁻³)	0.40, -0.39

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012), *Mercury* (Macrae *et al.*, 2008) and *pubCIF* (Westrip, 2010).

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full crystallographic data

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Crystal structure of bis(benzoato- κO)[5,15-diphenyl-10,20-bis(pyridin-4-yl)porphyrinato- $\kappa^4 N, N', N'', N'''$]tin(IV)

Nirmal K. Shee, Chang-Ju Lee and Hee-Joon Kim

Bis(benzoato- κO)[5,15-diphenyl-10,20-bis(pyridin-4-yl)porphyrinato- $\kappa^4 N, N', N'', N'''$]tin(IV)

Crystal data

[Sn(C₄₂H₂₆N₆)(C₇H₅O₂)₂]

$M_r = 975.60$

Monoclinic, $C2/c$

$a = 20.8021$ (4) Å

$b = 11.4260$ (2) Å

$c = 18.1164$ (4) Å

$\beta = 90.745$ (1)°

$V = 4305.63$ (15) Å³

$Z = 4$

$F(000) = 1984$

$D_x = 1.505$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 8728 reflections

$\theta = 2.3$ – 24.8 °

$\mu = 0.65$ mm⁻¹

$T = 173$ K

Block, violet

$0.16 \times 0.15 \times 0.09$ mm

Data collection

Bruker APEXII CCD
diffractometer

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Bruker, 2014)

$T_{\min} = 0.705$, $T_{\max} = 0.746$

35578 measured reflections

4972 independent reflections

3804 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 27.6$ °, $\theta_{\min} = 2.0$ °

$h = -26 \rightarrow 26$

$k = -14 \rightarrow 14$

$l = -23 \rightarrow 23$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.030$

$wR(F^2) = 0.075$

$S = 1.04$

4972 reflections

304 parameters

0 restraints

Hydrogen site location: inferred from
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0317P)^2 + 4.0687P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.40$ e Å⁻³

$\Delta\rho_{\min} = -0.39$ e Å⁻³

Special details

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

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.5000	0.5000	0.5000	0.02250 (7)
O1	0.44403 (8)	0.41626 (14)	0.42008 (9)	0.0324 (4)
O2	0.35962 (9)	0.35219 (16)	0.48265 (11)	0.0495 (5)
N1	0.49675 (8)	0.65244 (15)	0.43588 (10)	0.0245 (4)
N2	0.42420 (8)	0.56314 (15)	0.56302 (10)	0.0253 (4)
N3	0.30373 (11)	0.2884 (2)	0.83538 (13)	0.0492 (6)
C1	0.53422 (10)	0.67472 (19)	0.37562 (12)	0.0256 (5)
C2	0.51565 (11)	0.78669 (19)	0.34642 (13)	0.0298 (5)
H2A	0.5336	0.8240	0.3046	0.036*
C3	0.46794 (11)	0.82998 (19)	0.38894 (13)	0.0299 (5)
H3A	0.4464	0.9026	0.3822	0.036*
C4	0.45597 (10)	0.74582 (18)	0.44611 (12)	0.0256 (5)
C5	0.40974 (10)	0.75569 (19)	0.50169 (12)	0.0263 (5)
C6	0.39522 (10)	0.67094 (19)	0.55466 (12)	0.0268 (5)
C7	0.34847 (11)	0.6824 (2)	0.61206 (13)	0.0328 (5)
H7A	0.3210	0.7477	0.6197	0.039*
C8	0.35058 (11)	0.5841 (2)	0.65310 (13)	0.0338 (5)
H8A	0.3245	0.5678	0.6945	0.041*
C9	0.39888 (10)	0.50826 (19)	0.62359 (12)	0.0274 (5)
C10	0.41763 (10)	0.39927 (19)	0.65170 (12)	0.0260 (5)
C11	0.37336 (11)	0.86845 (19)	0.50731 (13)	0.0292 (5)
C12	0.30815 (11)	0.8741 (2)	0.48994 (13)	0.0336 (5)
H12A	0.2871	0.8075	0.4696	0.040*
C13	0.27340 (13)	0.9755 (2)	0.50184 (15)	0.0410 (6)
H13A	0.2285	0.9776	0.4915	0.049*
C14	0.30417 (15)	1.0727 (3)	0.52860 (18)	0.0572 (8)
H14A	0.2804	1.1421	0.5379	0.069*
C15	0.36917 (16)	1.0706 (3)	0.54213 (19)	0.0637 (9)
H15A	0.3906	1.1397	0.5581	0.076*
C16	0.40391 (14)	0.9680 (2)	0.53259 (17)	0.0466 (7)
H16A	0.4487	0.9665	0.5435	0.056*
C17	0.38046 (11)	0.3568 (2)	0.71710 (13)	0.0296 (5)
C18	0.38393 (11)	0.4140 (2)	0.78459 (13)	0.0338 (5)
H18A	0.4131	0.4770	0.7920	0.041*
C19	0.34427 (12)	0.3779 (2)	0.84088 (14)	0.0394 (6)
H19A	0.3461	0.4196	0.8862	0.047*
C20	0.30314 (15)	0.2318 (3)	0.77159 (18)	0.0586 (8)
H20A	0.2760	0.1653	0.7670	0.070*
C21	0.33945 (13)	0.2629 (2)	0.71119 (16)	0.0492 (7)
H21A	0.3361	0.2201	0.6664	0.059*
C22	0.39476 (12)	0.3487 (2)	0.42894 (14)	0.0340 (5)
C23	0.38259 (12)	0.2618 (2)	0.36792 (14)	0.0374 (6)
C24	0.42668 (16)	0.2422 (3)	0.31373 (17)	0.0598 (8)
H24A	0.4654	0.2863	0.3130	0.072*
C25	0.4149 (2)	0.1576 (3)	0.25950 (19)	0.0778 (11)

H25A	0.4454	0.1462	0.2216	0.093*
C26	0.36105 (18)	0.0917 (3)	0.25978 (19)	0.0694 (10)
H26A	0.3542	0.0324	0.2238	0.083*
C27	0.31690 (19)	0.1125 (3)	0.3128 (2)	0.0793 (11)
H27A	0.2783	0.0681	0.3131	0.095*
C28	0.32706 (15)	0.1974 (3)	0.3663 (2)	0.0645 (9)
H28A	0.2951	0.2110	0.4024	0.077*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.02343 (11)	0.02357 (11)	0.02071 (12)	0.00149 (9)	0.00881 (8)	0.00118 (9)
O1	0.0359 (9)	0.0332 (9)	0.0281 (9)	-0.0071 (7)	0.0024 (7)	0.0017 (7)
O2	0.0420 (11)	0.0505 (11)	0.0563 (13)	-0.0084 (9)	0.0170 (10)	-0.0137 (10)
N1	0.0241 (9)	0.0268 (9)	0.0227 (10)	0.0013 (7)	0.0087 (8)	0.0014 (8)
N2	0.0250 (10)	0.0272 (10)	0.0241 (10)	0.0004 (8)	0.0098 (8)	0.0006 (8)
N3	0.0519 (14)	0.0578 (15)	0.0384 (14)	-0.0046 (12)	0.0197 (11)	0.0095 (12)
C1	0.0253 (11)	0.0301 (12)	0.0214 (11)	-0.0026 (9)	0.0043 (9)	0.0005 (9)
C2	0.0335 (13)	0.0307 (12)	0.0251 (12)	-0.0036 (10)	0.0051 (10)	0.0048 (10)
C3	0.0331 (13)	0.0263 (11)	0.0304 (13)	0.0010 (10)	0.0022 (10)	0.0021 (10)
C4	0.0259 (11)	0.0237 (11)	0.0274 (12)	0.0014 (9)	0.0032 (9)	-0.0001 (9)
C5	0.0259 (11)	0.0279 (11)	0.0252 (12)	0.0021 (9)	0.0022 (9)	-0.0034 (9)
C6	0.0262 (11)	0.0300 (12)	0.0244 (12)	0.0023 (9)	0.0068 (9)	-0.0025 (9)
C7	0.0312 (13)	0.0393 (13)	0.0281 (13)	0.0102 (10)	0.0098 (10)	-0.0014 (10)
C8	0.0294 (12)	0.0440 (14)	0.0283 (13)	0.0061 (11)	0.0136 (10)	0.0029 (11)
C9	0.0247 (11)	0.0346 (12)	0.0231 (11)	-0.0009 (10)	0.0086 (9)	-0.0005 (10)
C10	0.0262 (11)	0.0302 (12)	0.0216 (11)	-0.0039 (9)	0.0066 (9)	0.0002 (9)
C11	0.0341 (13)	0.0276 (12)	0.0260 (12)	0.0052 (10)	0.0056 (10)	-0.0022 (9)
C12	0.0342 (13)	0.0321 (12)	0.0346 (14)	0.0018 (10)	0.0056 (11)	-0.0016 (10)
C13	0.0384 (14)	0.0433 (16)	0.0414 (16)	0.0135 (11)	0.0024 (12)	-0.0026 (11)
C14	0.065 (2)	0.0432 (17)	0.064 (2)	0.0247 (15)	-0.0122 (16)	-0.0192 (15)
C15	0.068 (2)	0.0367 (16)	0.086 (3)	0.0102 (15)	-0.0248 (18)	-0.0261 (16)
C16	0.0427 (16)	0.0372 (14)	0.0597 (19)	0.0074 (12)	-0.0135 (14)	-0.0143 (13)
C17	0.0279 (12)	0.0351 (13)	0.0262 (12)	-0.0002 (10)	0.0109 (10)	0.0019 (10)
C18	0.0335 (13)	0.0387 (13)	0.0294 (13)	-0.0002 (11)	0.0084 (10)	0.0023 (11)
C19	0.0436 (15)	0.0493 (16)	0.0255 (13)	0.0026 (12)	0.0099 (11)	0.0046 (11)
C20	0.0584 (19)	0.0545 (18)	0.064 (2)	-0.0252 (15)	0.0254 (16)	0.0005 (16)
C21	0.0535 (17)	0.0533 (17)	0.0414 (16)	-0.0213 (14)	0.0208 (14)	-0.0102 (13)
C22	0.0335 (13)	0.0330 (13)	0.0357 (14)	0.0046 (11)	0.0025 (11)	0.0034 (11)
C23	0.0444 (15)	0.0317 (13)	0.0362 (14)	-0.0012 (11)	0.0030 (12)	0.0021 (11)
C24	0.070 (2)	0.0571 (19)	0.0525 (19)	-0.0200 (16)	0.0203 (17)	-0.0149 (15)
C25	0.105 (3)	0.073 (2)	0.057 (2)	-0.023 (2)	0.027 (2)	-0.0246 (18)
C26	0.095 (3)	0.0534 (19)	0.060 (2)	-0.0219 (19)	0.002 (2)	-0.0125 (17)
C27	0.079 (3)	0.071 (2)	0.089 (3)	-0.032 (2)	0.007 (2)	-0.030 (2)
C28	0.0524 (19)	0.064 (2)	0.078 (2)	-0.0141 (16)	0.0102 (17)	-0.0252 (18)

Geometric parameters (Å, °)

Sn1—O1 ⁱ	2.0794 (15)	C11—C16	1.378 (3)
Sn1—O1	2.0794 (15)	C11—C12	1.390 (3)
Sn1—N2	2.0874 (17)	C12—C13	1.384 (3)
Sn1—N2 ⁱ	2.0874 (17)	C12—H12A	0.9500
Sn1—N1 ⁱ	2.0941 (17)	C13—C14	1.368 (4)
Sn1—N1	2.0942 (17)	C13—H13A	0.9500
O1—C22	1.294 (3)	C14—C15	1.371 (4)
O2—C22	1.225 (3)	C14—H14A	0.9500
N1—C1	1.373 (3)	C15—C16	1.389 (4)
N1—C4	1.377 (3)	C15—H15A	0.9500
N2—C9	1.375 (3)	C16—H16A	0.9500
N2—C6	1.379 (3)	C17—C21	1.374 (3)
N3—C20	1.325 (4)	C17—C18	1.387 (3)
N3—C19	1.328 (3)	C18—C19	1.383 (3)
C1—C10 ⁱ	1.406 (3)	C18—H18A	0.9500
C1—C2	1.435 (3)	C19—H19A	0.9500
C2—C3	1.358 (3)	C20—C21	1.384 (4)
C2—H2A	0.9500	C20—H20A	0.9500
C3—C4	1.437 (3)	C21—H21A	0.9500
C3—H3A	0.9500	C22—C23	1.505 (3)
C4—C5	1.406 (3)	C23—C28	1.370 (4)
C5—C6	1.399 (3)	C23—C24	1.370 (4)
C5—C11	1.498 (3)	C24—C25	1.398 (4)
C6—C7	1.439 (3)	C24—H24A	0.9500
C7—C8	1.348 (3)	C25—C26	1.349 (5)
C7—H7A	0.9500	C25—H25A	0.9500
C8—C9	1.435 (3)	C26—C27	1.358 (5)
C8—H8A	0.9500	C26—H26A	0.9500
C9—C10	1.399 (3)	C27—C28	1.386 (4)
C10—C1 ⁱ	1.406 (3)	C27—H27A	0.9500
C10—C17	1.504 (3)	C28—H28A	0.9500
O1 ⁱ —Sn1—O1	180.0	C16—C11—C5	120.1 (2)
O1 ⁱ —Sn1—N2	83.12 (7)	C12—C11—C5	121.1 (2)
O1—Sn1—N2	96.88 (7)	C13—C12—C11	120.9 (2)
O1 ⁱ —Sn1—N2 ⁱ	96.88 (7)	C13—C12—H12A	119.5
O1—Sn1—N2 ⁱ	83.12 (7)	C11—C12—H12A	119.5
N2—Sn1—N2 ⁱ	180.00 (8)	C14—C13—C12	119.5 (3)
O1 ⁱ —Sn1—N1 ⁱ	89.01 (6)	C14—C13—H13A	120.3
O1—Sn1—N1 ⁱ	90.99 (6)	C12—C13—H13A	120.3
N2—Sn1—N1 ⁱ	90.19 (7)	C13—C14—C15	120.3 (3)
N2 ⁱ —Sn1—N1 ⁱ	89.81 (7)	C13—C14—H14A	119.8
O1 ⁱ —Sn1—N1	90.99 (6)	C15—C14—H14A	119.8
O1—Sn1—N1	89.01 (6)	C14—C15—C16	120.4 (3)
N2—Sn1—N1	89.81 (7)	C14—C15—H15A	119.8
N2 ⁱ —Sn1—N1	90.19 (7)	C16—C15—H15A	119.8

N1 ⁱ —Sn1—N1	180.0	C11—C16—C15	120.0 (3)
C22—O1—Sn1	128.68 (15)	C11—C16—H16A	120.0
C1—N1—C4	108.68 (18)	C15—C16—H16A	120.0
C1—N1—Sn1	125.49 (14)	C21—C17—C18	117.5 (2)
C4—N1—Sn1	125.82 (14)	C21—C17—C10	121.0 (2)
C9—N2—C6	108.88 (17)	C18—C17—C10	121.4 (2)
C9—N2—Sn1	125.37 (14)	C19—C18—C17	119.0 (2)
C6—N2—Sn1	125.52 (14)	C19—C18—H18A	120.5
C20—N3—C19	116.1 (2)	C17—C18—H18A	120.5
N1—C1—C10 ⁱ	125.6 (2)	N3—C19—C18	123.9 (2)
N1—C1—C2	107.78 (19)	N3—C19—H19A	118.0
C10 ⁱ —C1—C2	126.6 (2)	C18—C19—H19A	118.0
C3—C2—C1	108.1 (2)	N3—C20—C21	124.4 (3)
C3—C2—H2A	125.9	N3—C20—H20A	117.8
C1—C2—H2A	125.9	C21—C20—H20A	117.8
C2—C3—C4	107.4 (2)	C17—C21—C20	118.9 (3)
C2—C3—H3A	126.3	C17—C21—H21A	120.5
C4—C3—H3A	126.3	C20—C21—H21A	120.5
N1—C4—C5	125.9 (2)	O2—C22—O1	124.1 (2)
N1—C4—C3	107.97 (19)	O2—C22—C23	120.5 (2)
C5—C4—C3	126.1 (2)	O1—C22—C23	115.3 (2)
C6—C5—C4	126.3 (2)	C28—C23—C24	118.0 (3)
C6—C5—C11	115.77 (19)	C28—C23—C22	120.2 (2)
C4—C5—C11	117.94 (19)	C24—C23—C22	121.7 (2)
N2—C6—C5	126.6 (2)	C23—C24—C25	120.2 (3)
N2—C6—C7	107.51 (19)	C23—C24—H24A	119.9
C5—C6—C7	125.9 (2)	C25—C24—H24A	119.9
C8—C7—C6	107.8 (2)	C26—C25—C24	121.4 (3)
C8—C7—H7A	126.1	C26—C25—H25A	119.3
C6—C7—H7A	126.1	C24—C25—H25A	119.3
C7—C8—C9	108.4 (2)	C25—C26—C27	118.3 (3)
C7—C8—H8A	125.8	C25—C26—H26A	120.9
C9—C8—H8A	125.8	C27—C26—H26A	120.9
N2—C9—C10	126.1 (2)	C26—C27—C28	121.3 (3)
N2—C9—C8	107.41 (19)	C26—C27—H27A	119.4
C10—C9—C8	126.5 (2)	C28—C27—H27A	119.4
C9—C10—C1 ⁱ	127.1 (2)	C23—C28—C27	120.8 (3)
C9—C10—C17	115.50 (19)	C23—C28—H28A	119.6
C1 ⁱ —C10—C17	117.33 (19)	C27—C28—H28A	119.6
C16—C11—C12	118.7 (2)		

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

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12A \cdots N3 ⁱⁱ	0.95 (1)	2.69 (1)	3.360 (3)	128 (1)

C18—H18A···O1 ⁱⁱ	0.95 (1)	2.69 (2)	3.357 (3)	128 (1)
C13—H13A···O2 ⁱⁱⁱ	0.95 (1)	2.72 (1)	3.411 (3)	130 (1)

Symmetry codes: (ii) $x, -y+1, z-1/2$; (iii) $-x+1/2, -y+3/2, -z+1$.