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Dibromidobis(3-bromobenzyl-κC)(4,7-diphenyl-1,10-phenanthroline-$\kappa^2 N,N'$)tin(IV)

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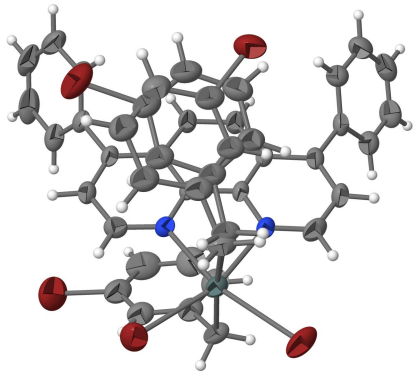
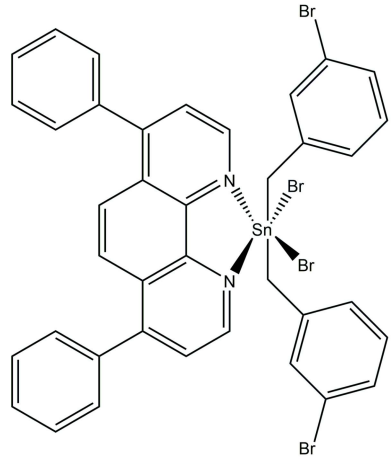
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $[SnBr_2(C_7H_6Br)_2(C_{24}H_{16}N_2)]$, the Sn atom is coordinated to a 4,7-diphenyl-1,10-phenanthroline, two 3-bromobenzyl and two bromide ligands, leading to a six-coordinate $C_2Br_2N_2$ donor set. The bromobenzyl ligands are *trans* to each other, while the Br anions are in a *cis* arrangement. One of the two 3-bromobenzyl ligands is disordered over two similar conformations, with occupancies of 0.7078 (18) and 0.2922 (18). In the crystal, molecules are linked into centrosymmetric dimers by Br···Br halogen bonds [3.5972 (12) Å], which are linked into a supramolecular layer in the *ac* plane by weak intermolecular C—H···Br interactions.

3D view



Chemical scheme



Structure description

Organotin compounds are mostly known for their biocidal effects and have been used for multiple applications, being utilized as wood preservatives, acaricides, disinfectants, bactericides, fungicides, molluscicides, PVC stabilizers and marine antifouling products (Snoeij *et al.*, 1987). In addition, much recent interest has focused on the potential applications of organotin compounds for their cytotoxicity and antitumour activities against various cell lines (Yadav *et al.*, 2015; Varela-Ramirez *et al.*, 2011). Metal complexes of 1,10-phenanthroline have also been found to show excellent biological activity, playing several roles, displaying both antimicrobial and antifungal activities (McCann *et al.*, 2012*a*) and anticancer potential (McCann *et al.*, 2012*b*). Several studies show that this ligand and a number of its complexes are effective against various strains of microorganisms (Josa Parada *et al.*, 2017). Both diorgano- and triorganotin compounds

Table 1
Selected geometric parameters (Å, °).

Sn1—C25	2.211 (4)	Sn1—N2	2.353 (3)
Sn1—C32	2.218 (13)	Sn1—Br2	2.6355 (6)
Sn1—N1	2.320 (3)	Sn1—Br1	2.7059 (5)
C25—Sn1—C32	174.0 (3)	N1—Sn1—Br2	91.31 (8)
C25—Sn1—N1	91.65 (13)	N2—Sn1—Br2	161.60 (8)
C32—Sn1—N1	89.8 (2)	C25—Sn1—Br1	88.35 (10)
C25—Sn1—N2	88.03 (15)	C32—Sn1—Br1	88.7 (2)
C32—Sn1—N2	87.0 (2)	N1—Sn1—Br1	164.19 (8)
N1—Sn1—N2	70.32 (11)	N2—Sn1—Br1	93.89 (8)
C25—Sn1—Br2	91.60 (13)	Br2—Sn1—Br1	104.49 (2)
C32—Sn1—Br2	94.2 (2)		

have been confirmed to show cytotoxicity against various cancer cell lines (Yadav *et al.*, 2015).

In light of these biological activities for both organotin compounds and metal complexes of phenanthroline derivatives, and the lack of such examples in the literature where both Sn and 4,7-diphenyl-1,10-phenanthroline were combined [the Cambridge Structural Database (CSD; Groom *et al.*, 2016) gave two hits: (4,7-diphenyl-1,10-phenanthroline)dimethylbis(isothiocyanato)tin(IV) (Najafi *et al.*, 2011) and di-*n*-butyl-dichlorido(4,7-diphenylphenanthroline)tin(IV) (Hu *et al.*, 1989)], it was decided to synthesize and structurally characterize the title compound, (I). Its biological activity will be reported elsewhere.

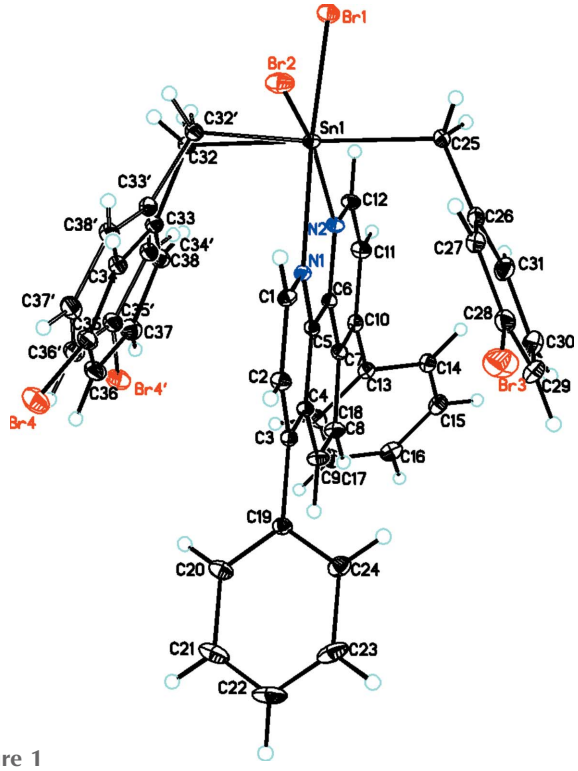


Figure 1
The molecular structure of (I), showing the folding of the 3-bromobenzyl rings in order to form π–π interactions with the 4,7-diphenyl-1,10-phenanthroline ligand. Displacement ellipsoids are drawn at the 30% probability level.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···Br2	0.93	2.78	3.477 (4)	133
C12—H12*A*···Br1	0.93	2.97	3.656 (5)	132
C36—H36*A*···Br2^{i}	0.93	3.00	3.883 (3)	159

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

In (I), the Sn atom is coordinated by a 4,7-diphenyl-1,10-phenanthroline, two 3-bromobenzyl and two bromide ligands, leading to a six-coordinate $C_2Br_2N_2$ donor set (see Fig. 1). The bromobenzyl ligands are *trans* to each other, while the Br anions are in a *cis* arrangement. The geometry about the Sn atom is distorted octahedral due in part to the small bite distance of the 4,7-diphenyl-1,10-phenanthroline ligand. The *cis* angles range from 70.32 (11) to 94.2 (2)° and the *trans* angles range from 174.0 (3) to 161.60 (8)° (Table 1). One of the interesting aspects of the structure is the conformation adopted by the 3-bromobenzyl ligands. As indicated above, these are arranged in a *trans* fashion in the Sn coordination sphere. However, they are not arranged in the normal way to minimize steric repulsion, but rather are both tilted away from the SnN_2Br_2 plane, with a dihedral angle of 40.1 (2)° between them. The reason for this appears to be so that they can form intramolecular π–π interactions with the central phenanthroline moiety [$Cg\cdots Cg$ = 3.584 (2) and 3.694 (3) Å]. The 3-bromobenzyl rings and the phenanthroline ring are not mutually parallel, but make dihedral angles of 24.4 (2) and 21.7 (3)°. These values are about the closest these rings can

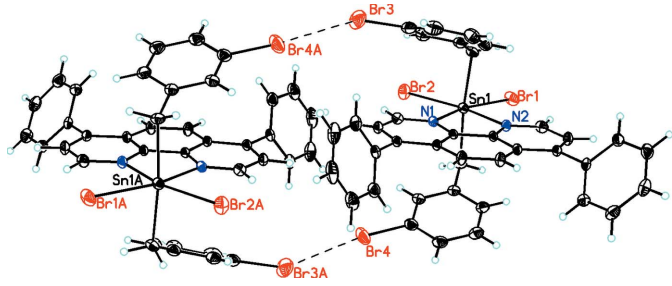


Figure 2
Diagram of (I) (major component only), showing the formation of $R_2^2(22)$ rings due to the formation of intermolecular Br···Br interactions (shown as dashed lines).

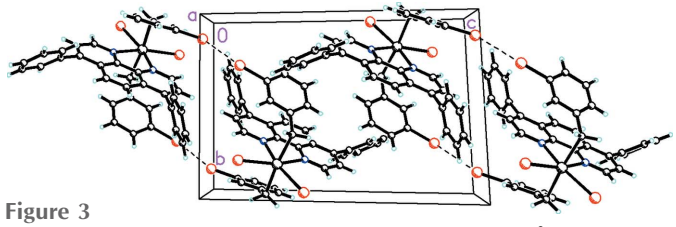


Figure 3
Packing diagram for (I), showing both the formation of $R_2^2(22)$ rings due to the formation of intermolecular Br···Br interactions, as well as the C—H···Br interactions linking these dimers into a two-dimensional layer (all interactions are shown as dashed lines).

Table 3
Experimental details.

Crystal data	
Chemical formula	$[SnBr_2(C_7H_6Br)_2(C_{24}H_{16}N_2)]$
M_r	950.95
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	296
a, b, c (Å)	10.1328 (3), 11.2430 (3), 16.7726 (4)
α, β, γ (°)	83.216 (2), 72.639 (2), 71.787 (1)
V (Å^3)	1731.72 (8)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.38
Crystal size (mm)	0.10 × 0.10 × 0.05
Data collection	
Diffractometer	Bruker Kappa APEX3 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.588, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	77114, 10637, 6920
R_{int}	0.056
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.719
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.050, 0.123, 1.04
No. of reflections	10637
No. of parameters	444
No. of restraints	342
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.14, −1.47

Computer programs: *APEX3* (Bruker, 2016), *SAINT* (Bruker, 2016), *XPREP* (Bruker, 2016), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*) and *ORTEP-3* (Farrugia, 2012).

approach each other while maintaining a tetrahedral (sp^3) angle at the benzyl C atoms.

As far as comparisons with related structures are concerned, there is only one other structure which bears some resemblance to (I), namely dibromobis(pentafluoroethyl)(1,10-phenanthroline)tin(IV), (II) (Klosener *et al.*, 2017). The phenanthroline bite angle for (II) is 72.40 (9)°, which is slightly wider that the value found for (I) of 70.32 (11)°

In the crystal, molecules are linked into centrosymmetric dimers (Fig. 2) by Br···Br halogen bonds [Br3···Br4 = 3.5972 (12) Å] and the dimers are linked into a supramolecular layer in the *ac* plane by weak intermolecular C—H···Br interactions (Table 2 and Fig. 3).

Synthesis and crystallization

3-Bromobenzyl bromide, tin powder and 4,7-diphenyl-1,10-phenanthroline were purchased from Sigma–Aldrich and used without further purification. All solvents were dried according to standard procedures.

Synthesis of bis (3-bromobenzyl) tin dibromide. Tin powder (2 g, 16.8 mmol) and 3-bromobenzyl bromide (4.21 g, 16.8 mmol) in toluene (60 ml) were refluxed at 110 °C for 3 h. The crystallized products were extracted under vacuum, purified with chloroform and used for the synthesis of the complex.

Synthesis of dibromidobis(3-bromobenzyl)(4,7-diphenyl-1,10-phenanthroline)tin(IV), (I). Bis(3-bromobenzyl)tin dibromide (0.46 g, 0.752 mmol) in methanol (50 ml) was reacted with 4,7-diphenyl-1,10-phenanthroline (0.25 g, 0.752 mmol) at room temperature for 24 h. The yellow product was recrystallized by the vapour-diffusion method using chloroform as solvent and petroleum ether as anti-solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. One of the two 3-bromobenzyl ligands is disordered over two similar conformations, with occupancies of 0.7078 (18) and 0.2929 (18), and were constrained to have similar geometries using the SAME command in *SHELXL2018* (Sheldrick, 2015*b*). H atoms were idealized using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C)$. The maximum and minimum residual electron-density peaks of 1.14 and −1.47 Å^{-3}, respectively, were located 0.71 and 0.77 Å from the C12 and Br3 atoms.

Acknowledgements

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full crystallographic data

IUCrData (2019). **4**, x190336 [https://doi.org/10.1107/S2414314619003365]

Dibromidobis(3-bromobenzyl-κC)(4,7-diphenyl-1,10-phenanthroline-$\kappa^2 N,N'$)tin(IV)

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Crystal data

$[SnBr_2(C_7H_6Br)_2(C_{24}H_{16}N_2)]$
M_r = 950.95
Triclinic, $P\overline{1}$
a = 10.1328 (3) Å
b = 11.2430 (3) Å
c = 16.7726 (4) Å
α = 83.216 (2)°
β = 72.639 (2)°
γ = 71.787 (1)°
V = 1731.72 (8) Å^3
Z = 2
$F(000)$ = 920
D_x = 1.824 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9823 reflections
θ = 3.0–28.6°
μ = 5.38 mm^{-1}
T = 296 K
Block, yellow
0.10 × 0.10 × 0.05 mm

Data collection

Bruker Kappa APEX3 CMOS diffractometer
ω and φ scan
Absorption correction: multi-scan (SADABS; Bruker, 2016)
T_{min} = 0.588, T_{max} = 0.746
77114 measured reflections
10637 independent reflections
6920 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
θ_{max} = 30.7°, θ_{min} = 3.2°
h = −14→14
k = −16→16
l = −23→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.123
S = 1.04
10637 reflections
444 parameters
342 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
$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 5.1192P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.14 e Å^{-3}
$\Delta\rho_{min}$ = −1.47 e Å^{-3}
Extinction correction: SHELXL2018 (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0039 (4)

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Sn1	0.38752 (3)	0.17331 (3)	0.72938 (2)	0.03379 (10)	
Br1	0.33777 (7)	0.02517 (5)	0.63249 (4)	0.06410 (18)	
Br2	0.16984 (6)	0.19942 (6)	0.86610 (4)	0.06052 (16)	
N1	0.4864 (4)	0.2968 (3)	0.7817 (2)	0.0308 (7)	
N2	0.5998 (4)	0.1939 (3)	0.6302 (2)	0.0341 (7)	
C1	0.4282 (5)	0.3489 (4)	0.8548 (3)	0.0366 (9)	
H1A	0.341361	0.336726	0.887668	0.044*	
C2	0.4896 (5)	0.4216 (4)	0.8856 (3)	0.0371 (9)	
H2A	0.442692	0.458385	0.937283	0.045*	
C3	0.6184 (4)	0.4389 (4)	0.8402 (2)	0.0319 (8)	
C4	0.6838 (4)	0.3835 (3)	0.7609 (2)	0.0298 (8)	
C5	0.6128 (4)	0.3139 (3)	0.7340 (2)	0.0281 (7)	
C6	0.6732 (4)	0.2596 (3)	0.6529 (2)	0.0286 (8)	
C7	0.8030 (4)	0.2756 (4)	0.6007 (2)	0.0328 (8)	
C8	0.8698 (5)	0.3509 (4)	0.6294 (3)	0.0410 (10)	
H8A	0.953686	0.365947	0.594406	0.049*	
C9	0.8143 (5)	0.4001 (4)	0.7055 (3)	0.0395 (10)	
H9A	0.862230	0.446305	0.722592	0.047*	
C10	0.8584 (4)	0.2214 (4)	0.5210 (2)	0.0347 (9)	
C11	0.7795 (5)	0.1564 (4)	0.4997 (3)	0.0426 (10)	
H11A	0.811934	0.120607	0.447548	0.051*	
C12	0.6517 (5)	0.1440 (4)	0.5558 (3)	0.0451 (11)	
H12A	0.600943	0.098914	0.540185	0.054*	
C13	0.9940 (5)	0.2357 (4)	0.4614 (2)	0.0357 (9)	
C14	0.9906 (5)	0.2837 (4)	0.3814 (3)	0.0440 (10)	
H14A	0.905237	0.304162	0.365872	0.053*	
C15	1.1139 (6)	0.3008 (5)	0.3255 (3)	0.0537 (12)	
H15A	1.111680	0.333651	0.272256	0.064*	
C16	1.2389 (6)	0.2699 (5)	0.3477 (3)	0.0570 (14)	
H16A	1.321496	0.283353	0.309874	0.068*	
C17	1.2442 (5)	0.2190 (5)	0.4256 (4)	0.0565 (13)	
H17A	1.330992	0.195671	0.439754	0.068*	
C18	1.1215 (5)	0.2023 (5)	0.4826 (3)	0.0469 (11)	
H18A	1.125085	0.168349	0.535556	0.056*	
C19	0.6850 (5)	0.5157 (4)	0.8721 (2)	0.0359 (9)	
C20	0.8143 (6)	0.4632 (5)	0.8906 (3)	0.0525 (12)	
H20A	0.862273	0.378558	0.881796	0.063*	
C21	0.8736 (7)	0.5360 (7)	0.9224 (4)	0.0700 (18)	
H21A	0.960660	0.499760	0.935713	0.084*	

C22	0.8050 (8)	0.6607 (7)	0.9343 (4)	0.077 (2)	
H22A	0.845981	0.709600	0.954680	0.092*	
C23	0.6777 (8)	0.7127 (6)	0.9163 (4)	0.0697 (18)	
H23A	0.631127	0.797693	0.924707	0.084*	
C24	0.6150 (6)	0.6415 (4)	0.8855 (3)	0.0481 (11)	
H24A	0.526526	0.678099	0.873946	0.058*	
Br3	0.17356 (10)	0.71660 (8)	0.85740 (6)	0.0998 (3)	
C25	0.2648 (5)	0.3378 (4)	0.6683 (3)	0.0419 (10)	
H25A	0.286528	0.321174	0.609603	0.050*	
H25B	0.162171	0.349458	0.693184	0.050*	
C26	0.2978 (4)	0.4559 (2)	0.67555 (18)	0.0470 (11)	
C27	0.2270 (3)	0.5234 (3)	0.74818 (16)	0.0504 (12)	
H27A	0.157510	0.496840	0.790011	0.060*	
C28	0.2602 (4)	0.6307 (3)	0.75830 (17)	0.0594 (14)	
C29	0.3642 (4)	0.6704 (3)	0.6958 (2)	0.0749 (19)	
H29A	0.386364	0.742139	0.702556	0.090*	
C30	0.4349 (4)	0.6028 (3)	0.62315 (19)	0.0682 (16)	
H30A	0.504435	0.629389	0.581319	0.082*	
C31	0.4017 (4)	0.4956 (3)	0.61303 (16)	0.0599 (14)	
H31A	0.449046	0.450363	0.564427	0.072*	
Br4	0.74161 (13)	0.12905 (11)	0.99659 (6)	0.0867 (4)	0.7078 (18)
C32	0.5264 (7)	0.0032 (13)	0.7775 (6)	0.0418 (14)	0.7078 (18)
H32A	0.467748	−0.025946	0.828296	0.050*	0.7078 (18)
H32D	0.559912	−0.061825	0.736771	0.050*	0.7078 (18)
C33	0.6549 (4)	0.0197 (5)	0.7958 (2)	0.0411 (12)	0.7078 (18)
C34	0.6406 (3)	0.0586 (5)	0.8744 (2)	0.0452 (13)	0.7078 (18)
H34A	0.552033	0.073368	0.914914	0.054*	0.7078 (18)
C35	0.7588 (4)	0.0755 (5)	0.8924 (2)	0.0522 (14)	0.7078 (18)
C36	0.8912 (4)	0.0534 (5)	0.8319 (3)	0.0576 (15)	0.7078 (18)
H36A	0.970292	0.064717	0.843903	0.069*	0.7078 (18)
C37	0.9055 (4)	0.0145 (5)	0.7533 (2)	0.0583 (16)	0.7078 (18)
H37A	0.994127	−0.000251	0.712761	0.070*	0.7078 (18)
C38	0.7874 (4)	−0.0024 (5)	0.73526 (19)	0.0489 (14)	0.7078 (18)
H38A	0.796916	−0.028410	0.682694	0.059*	0.7078 (18)
Br4′	1.0330 (2)	0.0096 (2)	0.73285 (14)	0.0682 (7)	0.2922 (18)
C32′	0.4920 (14)	0.010 (4)	0.7812 (12)	0.045 (3)	0.2922 (18)
H32B	0.420210	−0.019752	0.823919	0.054*	0.2922 (18)
H32C	0.537565	−0.051949	0.738235	0.054*	0.2922 (18)
C33′	0.6043 (6)	0.0184 (14)	0.8195 (6)	0.045 (2)	0.2922 (18)
C34′	0.7443 (7)	0.0041 (13)	0.7687 (5)	0.045 (2)	0.2922 (18)
H34B	0.768330	−0.016692	0.713079	0.054*	0.2922 (18)
C35′	0.8483 (5)	0.0208 (12)	0.8011 (4)	0.050 (2)	0.2922 (18)
C36′	0.8124 (7)	0.0519 (13)	0.8843 (4)	0.052 (2)	0.2922 (18)
H36B	0.881969	0.063077	0.905934	0.063*	0.2922 (18)
C37′	0.6724 (7)	0.0662 (13)	0.9350 (4)	0.057 (2)	0.2922 (18)
H37B	0.648295	0.086977	0.990655	0.069*	0.2922 (18)
C38′	0.5683 (6)	0.0495 (13)	0.9026 (5)	0.051 (2)	0.2922 (18)
H38B	0.474636	0.059043	0.936589	0.061*	0.2922 (18)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sn1	0.03763 (16)	0.03340 (15)	0.03712 (16)	−0.01548 (11)	−0.01446 (12)	−0.00210 (11)
Br1	0.0924 (4)	0.0533 (3)	0.0721 (4)	−0.0312 (3)	−0.0480 (3)	−0.0061 (3)
Br2	0.0514 (3)	0.0794 (4)	0.0558 (3)	−0.0348 (3)	−0.0020 (2)	−0.0114 (3)
N1	0.0349 (17)	0.0314 (17)	0.0296 (16)	−0.0130 (14)	−0.0109 (14)	−0.0003 (13)
N2	0.0368 (18)	0.0363 (18)	0.0328 (17)	−0.0127 (15)	−0.0096 (14)	−0.0088 (14)
C1	0.035 (2)	0.039 (2)	0.039 (2)	−0.0182 (18)	−0.0082 (18)	0.0038 (17)
C2	0.039 (2)	0.043 (2)	0.030 (2)	−0.0129 (18)	−0.0060 (17)	−0.0088 (17)
C3	0.039 (2)	0.0291 (19)	0.0292 (19)	−0.0091 (16)	−0.0122 (16)	−0.0048 (15)
C4	0.035 (2)	0.0280 (18)	0.0278 (19)	−0.0086 (15)	−0.0092 (15)	−0.0062 (15)
C5	0.0321 (19)	0.0286 (18)	0.0253 (18)	−0.0079 (15)	−0.0099 (15)	−0.0039 (14)
C6	0.036 (2)	0.0269 (18)	0.0247 (18)	−0.0088 (15)	−0.0098 (15)	−0.0044 (14)
C7	0.038 (2)	0.034 (2)	0.0267 (19)	−0.0104 (17)	−0.0086 (16)	−0.0049 (15)
C8	0.042 (2)	0.049 (3)	0.034 (2)	−0.023 (2)	−0.0020 (18)	−0.0083 (19)
C9	0.042 (2)	0.045 (2)	0.036 (2)	−0.023 (2)	−0.0018 (18)	−0.0116 (18)
C10	0.038 (2)	0.034 (2)	0.028 (2)	−0.0054 (17)	−0.0073 (17)	−0.0040 (16)
C11	0.046 (2)	0.051 (3)	0.032 (2)	−0.016 (2)	−0.0057 (19)	−0.0146 (19)
C12	0.055 (3)	0.038 (2)	0.054 (3)	−0.017 (2)	−0.027 (2)	−0.008 (2)
C13	0.041 (2)	0.035 (2)	0.028 (2)	−0.0105 (17)	−0.0029 (17)	−0.0089 (16)
C14	0.049 (3)	0.042 (2)	0.038 (2)	−0.011 (2)	−0.010 (2)	−0.0022 (19)
C15	0.064 (3)	0.051 (3)	0.040 (3)	−0.020 (2)	−0.003 (2)	0.003 (2)
C16	0.054 (3)	0.055 (3)	0.053 (3)	−0.022 (2)	0.009 (2)	−0.013 (2)
C17	0.039 (3)	0.060 (3)	0.067 (4)	−0.011 (2)	−0.009 (2)	−0.016 (3)
C18	0.041 (2)	0.052 (3)	0.045 (3)	−0.008 (2)	−0.014 (2)	−0.005 (2)
C19	0.045 (2)	0.042 (2)	0.0265 (19)	−0.0201 (19)	−0.0087 (17)	−0.0046 (16)
C20	0.051 (3)	0.067 (3)	0.047 (3)	−0.020 (2)	−0.017 (2)	−0.016 (2)
C21	0.060 (3)	0.116 (5)	0.053 (3)	−0.044 (4)	−0.017 (3)	−0.020 (3)
C22	0.092 (5)	0.114 (6)	0.050 (3)	−0.075 (5)	−0.002 (3)	−0.027 (3)
C23	0.107 (5)	0.057 (3)	0.052 (3)	−0.052 (3)	0.002 (3)	−0.017 (3)
C24	0.065 (3)	0.043 (3)	0.038 (2)	−0.023 (2)	−0.008 (2)	−0.0061 (19)
Br3	0.1022 (6)	0.0841 (5)	0.1170 (7)	−0.0153 (4)	−0.0318 (5)	−0.0468 (5)
C25	0.051 (3)	0.038 (2)	0.047 (3)	−0.016 (2)	−0.028 (2)	0.0059 (19)
C26	0.054 (3)	0.039 (2)	0.050 (3)	−0.008 (2)	−0.025 (2)	0.006 (2)
C27	0.055 (3)	0.041 (3)	0.060 (3)	−0.014 (2)	−0.027 (2)	0.006 (2)
C28	0.065 (3)	0.044 (3)	0.075 (4)	−0.006 (2)	−0.038 (3)	−0.003 (3)
C29	0.088 (5)	0.042 (3)	0.108 (5)	−0.028 (3)	−0.046 (4)	0.019 (3)
C30	0.083 (4)	0.061 (4)	0.061 (4)	−0.027 (3)	−0.023 (3)	0.020 (3)
C31	0.076 (4)	0.054 (3)	0.053 (3)	−0.025 (3)	−0.021 (3)	0.013 (2)
Br4	0.1113 (9)	0.1036 (8)	0.0660 (6)	−0.0356 (6)	−0.0479 (6)	−0.0095 (5)
C32	0.039 (3)	0.032 (3)	0.060 (3)	−0.008 (4)	−0.026 (3)	0.000 (3)
C33	0.043 (3)	0.032 (2)	0.054 (3)	−0.012 (2)	−0.022 (2)	0.000 (2)
C34	0.046 (3)	0.042 (3)	0.054 (3)	−0.012 (2)	−0.024 (2)	0.003 (2)
C35	0.055 (3)	0.050 (3)	0.060 (3)	−0.013 (3)	−0.030 (3)	−0.004 (3)
C36	0.046 (3)	0.059 (3)	0.075 (4)	−0.013 (3)	−0.030 (3)	−0.003 (3)
C37	0.041 (3)	0.060 (3)	0.071 (4)	−0.009 (3)	−0.016 (3)	−0.005 (3)
C38	0.044 (3)	0.043 (3)	0.061 (3)	−0.007 (3)	−0.021 (3)	−0.006 (3)

Br4′	0.0440 (11)	0.0825 (15)	0.0820 (15)	−0.0203 (10)	−0.0192 (9)	−0.0073 (11)
C32′	0.043 (5)	0.036 (5)	0.062 (5)	−0.011 (6)	−0.025 (5)	0.000 (5)
C33′	0.044 (4)	0.036 (4)	0.057 (4)	−0.009 (4)	−0.022 (3)	0.002 (4)
C34′	0.043 (4)	0.041 (4)	0.056 (4)	−0.009 (4)	−0.023 (4)	0.000 (4)
C35′	0.046 (4)	0.047 (4)	0.063 (4)	−0.011 (4)	−0.025 (3)	−0.001 (4)
C36′	0.050 (4)	0.051 (4)	0.062 (4)	−0.013 (4)	−0.026 (4)	−0.004 (4)
C37′	0.057 (5)	0.058 (5)	0.059 (5)	−0.010 (4)	−0.027 (4)	−0.003 (4)
C38′	0.049 (4)	0.048 (4)	0.057 (4)	−0.011 (4)	−0.023 (4)	0.000 (4)

Geometric parameters (Å, º)

Sn1—C32′	2.05 (4)	C22—C23	1.347 (10)
Sn1—C25	2.211 (4)	C22—H22A	0.9300
Sn1—C32	2.218 (13)	C23—C24	1.387 (7)
Sn1—N1	2.320 (3)	C23—H23A	0.9300
Sn1—N2	2.353 (3)	C24—H24A	0.9300
Sn1—Br2	2.6355 (6)	Br3—Br4^{i}	3.5972 (12)
Sn1—Br1	2.7059 (5)	Br3—C28	1.856 (2)
N1—C1	1.310 (5)	C25—C26	1.493 (4)
N1—C5	1.350 (5)	C25—H25A	0.9700
N2—C12	1.317 (6)	C25—H25B	0.9700
N2—C6	1.351 (5)	C26—C27	1.3900
C1—C2	1.390 (6)	C26—C31	1.3900
C1—H1A	0.9300	C27—C28	1.3900
C2—C3	1.360 (6)	C27—H27A	0.9300
C2—H2A	0.9300	C28—C29	1.3900
C3—C4	1.417 (5)	C29—C30	1.3900
C3—C19	1.477 (5)	C29—H29A	0.9300
C4—C5	1.401 (5)	C30—C31	1.3900
C4—C9	1.424 (6)	C30—H30A	0.9300
C5—C6	1.435 (5)	C31—H31A	0.9300
C6—C7	1.398 (6)	Br4—C35	1.857 (2)
C7—C10	1.415 (5)	C32—C33	1.492 (4)
C7—C8	1.434 (6)	C32—H32A	0.9700
C8—C9	1.339 (6)	C32—H32D	0.9700
C8—H8A	0.9300	C33—C34	1.3900
C9—H9A	0.9300	C33—C38	1.3900
C10—C11	1.377 (6)	C34—C35	1.3900
C10—C13	1.481 (6)	C34—H34A	0.9300
C11—C12	1.392 (7)	C35—C36	1.3900
C11—H11A	0.9300	C36—C37	1.3900
C12—H12A	0.9300	C36—H36A	0.9300
C13—C18	1.370 (6)	C37—C38	1.3900
C13—C14	1.393 (6)	C37—H37A	0.9300
C14—C15	1.373 (7)	C38—H38A	0.9300
C14—H14A	0.9300	Br4′—C35′	1.854 (3)
C15—C16	1.356 (8)	C32′—C33′	1.493 (4)
C15—H15A	0.9300	C32′—H32B	0.9700

C16—C17	1.372 (8)	C32′—H32C	0.9700
C16—H16A	0.9300	C33′—C34′	1.3900
C17—C18	1.375 (7)	C33′—C38′	1.3900
C17—H17A	0.9300	C34′—C35′	1.3900
C18—H18A	0.9300	C34′—H34B	0.9300
C19—C20	1.370 (7)	C35′—C36′	1.3900
C19—C24	1.380 (6)	C36′—C37′	1.3900
C20—C21	1.385 (7)	C36′—H36B	0.9300
C20—H20A	0.9300	C37′—C38′	1.3900
C21—C22	1.365 (10)	C37′—H37B	0.9300
C21—H21A	0.9300	C38′—H38B	0.9300

C32′—Sn1—C25	174.2 (5)	C21—C20—H20A	120.0
C25—Sn1—C32	174.0 (3)	C22—C21—C20	120.3 (6)
C32′—Sn1—N1	94.2 (5)	C22—C21—H21A	119.9
C25—Sn1—N1	91.65 (13)	C20—C21—H21A	119.9
C32—Sn1—N1	89.8 (2)	C23—C22—C21	119.9 (5)
C32′—Sn1—N2	94.0 (4)	C23—C22—H22A	120.1
C25—Sn1—N2	88.03 (15)	C21—C22—H22A	120.1
C32—Sn1—N2	87.0 (2)	C22—C23—C24	120.9 (6)
N1—Sn1—N2	70.32 (11)	C22—C23—H23A	119.5
C32′—Sn1—Br2	88.2 (4)	C24—C23—H23A	119.5
C25—Sn1—Br2	91.60 (13)	C19—C24—C23	119.5 (5)
C32—Sn1—Br2	94.2 (2)	C19—C24—H24A	120.3
N1—Sn1—Br2	91.31 (8)	C23—C24—H24A	120.3
N2—Sn1—Br2	161.60 (8)	C26—C25—Sn1	113.4 (3)
C32′—Sn1—Br1	86.1 (5)	C26—C25—H25A	108.9
C25—Sn1—Br1	88.35 (10)	Sn1—C25—H25A	108.9
C32—Sn1—Br1	88.7 (2)	C26—C25—H25B	108.9
N1—Sn1—Br1	164.19 (8)	Sn1—C25—H25B	108.9
N2—Sn1—Br1	93.89 (8)	H25A—C25—H25B	107.7
Br2—Sn1—Br1	104.49 (2)	C27—C26—C31	120.0
C1—N1—C5	118.5 (3)	C27—C26—C25	118.7 (3)
C1—N1—Sn1	124.0 (3)	C31—C26—C25	121.3 (3)
C5—N1—Sn1	117.5 (2)	C28—C27—C26	120.0
C12—N2—C6	118.9 (4)	C28—C27—H27A	120.0
C12—N2—Sn1	124.4 (3)	C26—C27—H27A	120.0
C6—N2—Sn1	116.7 (2)	C29—C28—C27	120.0
N1—C1—C2	123.3 (4)	C29—C28—Br3	119.64 (18)
N1—C1—H1A	118.4	C27—C28—Br3	120.28 (18)
C2—C1—H1A	118.4	C28—C29—C30	120.0
C3—C2—C1	120.0 (4)	C28—C29—H29A	120.0
C3—C2—H2A	120.0	C30—C29—H29A	120.0
C1—C2—H2A	120.0	C31—C30—C29	120.0
C2—C3—C4	117.8 (4)	C31—C30—H30A	120.0
C2—C3—C19	120.7 (4)	C29—C30—H30A	120.0
C4—C3—C19	121.5 (4)	C30—C31—C26	120.0
C5—C4—C3	118.3 (4)	C30—C31—H31A	120.0

C5—C4—C9	118.3 (3)	C26—C31—H31A	120.0
C3—C4—C9	123.3 (3)	C33—C32—Sn1	115.4 (8)
N1—C5—C4	122.0 (3)	C33—C32—H32A	108.4
N1—C5—C6	118.0 (3)	Sn1—C32—H32A	108.4
C4—C5—C6	120.0 (3)	C33—C32—H32D	108.4
N2—C6—C7	122.3 (3)	Sn1—C32—H32D	108.4
N2—C6—C5	117.4 (3)	H32A—C32—H32D	107.5
C7—C6—C5	120.3 (3)	C34—C33—C38	120.0
C6—C7—C10	118.5 (4)	C34—C33—C32	119.2 (3)
C6—C7—C8	118.0 (3)	C38—C33—C32	120.8 (3)
C10—C7—C8	123.5 (4)	C33—C34—C35	120.0
C9—C8—C7	121.6 (4)	C33—C34—H34A	120.0
C9—C8—H8A	119.2	C35—C34—H34A	120.0
C7—C8—H8A	119.2	C36—C35—C34	120.0
C8—C9—C4	121.8 (4)	C36—C35—Br4	119.3 (2)
C8—C9—H9A	119.1	C34—C35—Br4	120.7 (2)
C4—C9—H9A	119.1	C37—C36—C35	120.0
C11—C10—C7	117.5 (4)	C37—C36—H36A	120.0
C11—C10—C13	120.7 (4)	C35—C36—H36A	120.0
C7—C10—C13	121.8 (4)	C36—C37—C38	120.0
C10—C11—C12	120.4 (4)	C36—C37—H37A	120.0
C10—C11—H11A	119.8	C38—C37—H37A	120.0
C12—C11—H11A	119.8	C37—C38—C33	120.0
N2—C12—C11	122.4 (4)	C37—C38—H38A	120.0
N2—C12—H12A	118.8	C33—C38—H38A	120.0
C11—C12—H12A	118.8	C33′—C32′—Sn1	116 (2)
C18—C13—C14	119.6 (4)	C33′—C32′—H32B	108.3
C18—C13—C10	122.0 (4)	Sn1—C32′—H32B	108.3
C14—C13—C10	118.4 (4)	C33′—C32′—H32C	108.3
C15—C14—C13	119.7 (5)	Sn1—C32′—H32C	108.3
C15—C14—H14A	120.2	H32B—C32′—H32C	107.4
C13—C14—H14A	120.2	C34′—C33′—C38′	120.0
C16—C15—C14	120.3 (5)	C34′—C33′—C32′	118.7 (4)
C16—C15—H15A	119.8	C38′—C33′—C32′	121.1 (4)
C14—C15—H15A	119.8	C33′—C34′—C35′	120.0
C15—C16—C17	120.3 (5)	C33′—C34′—H34B	120.0
C15—C16—H16A	119.8	C35′—C34′—H34B	120.0
C17—C16—H16A	119.8	C36′—C35′—C34′	120.0
C16—C17—C18	120.2 (5)	C36′—C35′—Br4′	119.5 (3)
C16—C17—H17A	119.9	C34′—C35′—Br4′	120.4 (3)
C18—C17—H17A	119.9	C37′—C36′—C35′	120.0
C13—C18—C17	119.9 (5)	C37′—C36′—H36B	120.0
C13—C18—H18A	120.1	C35′—C36′—H36B	120.0
C17—C18—H18A	120.1	C36′—C37′—C38′	120.0
C20—C19—C24	119.4 (4)	C36′—C37′—H37B	120.0
C20—C19—C3	120.8 (4)	C38′—C37′—H37B	120.0
C24—C19—C3	119.8 (4)	C37′—C38′—C33′	120.0
C19—C20—C21	120.1 (5)	C37′—C38′—H38B	120.0

C19—C20—H20A	120.0	C33′—C38′—H38B	120.0
C5—N1—C1—C2	0.3 (6)	C14—C13—C18—C17	1.5 (7)
Sn1—N1—C1—C2	179.3 (3)	C10—C13—C18—C17	−179.1 (4)
N1—C1—C2—C3	−1.6 (7)	C16—C17—C18—C13	0.5 (8)
C1—C2—C3—C4	1.5 (6)	C2—C3—C19—C20	115.5 (5)
C1—C2—C3—C19	−179.9 (4)	C4—C3—C19—C20	−66.0 (6)
C2—C3—C4—C5	−0.2 (6)	C2—C3—C19—C24	−63.0 (6)
C19—C3—C4—C5	−178.7 (4)	C4—C3—C19—C24	115.5 (5)
C2—C3—C4—C9	176.5 (4)	C24—C19—C20—C21	0.0 (7)
C19—C3—C4—C9	−2.0 (6)	C3—C19—C20—C21	−178.5 (5)
C1—N1—C5—C4	1.1 (6)	C19—C20—C21—C22	−1.0 (9)
Sn1—N1—C5—C4	−178.0 (3)	C20—C21—C22—C23	1.1 (9)
C1—N1—C5—C6	−178.1 (4)	C21—C22—C23—C24	−0.2 (9)
Sn1—N1—C5—C6	2.8 (4)	C20—C19—C24—C23	0.9 (7)
C3—C4—C5—N1	−1.2 (6)	C3—C19—C24—C23	179.4 (4)
C9—C4—C5—N1	−178.1 (4)	C22—C23—C24—C19	−0.8 (8)
C3—C4—C5—C6	178.0 (4)	Sn1—C25—C26—C27	−82.9 (3)
C9—C4—C5—C6	1.1 (6)	Sn1—C25—C26—C31	94.2 (3)
C12—N2—C6—C7	−0.6 (6)	C31—C26—C27—C28	0.0
Sn1—N2—C6—C7	178.2 (3)	C25—C26—C27—C28	177.1 (3)
C12—N2—C6—C5	179.3 (4)	C26—C27—C28—C29	0.0
Sn1—N2—C6—C5	−2.0 (5)	C26—C27—C28—Br3	−176.7 (3)
N1—C5—C6—N2	−0.6 (5)	C27—C28—C29—C30	0.0
C4—C5—C6—N2	−179.8 (4)	Br3—C28—C29—C30	176.7 (3)
N1—C5—C6—C7	179.3 (3)	C28—C29—C30—C31	0.0
C4—C5—C6—C7	0.1 (6)	C29—C30—C31—C26	0.0
N2—C6—C7—C10	0.3 (6)	C27—C26—C31—C30	0.0
C5—C6—C7—C10	−179.5 (4)	C25—C26—C31—C30	−177.1 (3)
N2—C6—C7—C8	177.7 (4)	Sn1—C32—C33—C34	88.1 (6)
C5—C6—C7—C8	−2.1 (6)	Sn1—C32—C33—C38	−91.4 (5)
C6—C7—C8—C9	3.1 (7)	C38—C33—C34—C35	0.0
C10—C7—C8—C9	−179.7 (4)	C32—C33—C34—C35	−179.5 (7)
C7—C8—C9—C4	−1.9 (7)	C33—C34—C35—C36	0.0
C5—C4—C9—C8	−0.2 (7)	C33—C34—C35—Br4	179.3 (4)
C3—C4—C9—C8	−176.9 (4)	C34—C35—C36—C37	0.0
C6—C7—C10—C11	0.5 (6)	Br4—C35—C36—C37	−179.4 (4)
C8—C7—C10—C11	−176.8 (4)	C35—C36—C37—C38	0.0
C6—C7—C10—C13	179.0 (4)	C36—C37—C38—C33	0.0
C8—C7—C10—C13	1.8 (6)	C34—C33—C38—C37	0.0
C7—C10—C11—C12	−1.0 (7)	C32—C33—C38—C37	179.4 (8)
C13—C10—C11—C12	−179.6 (4)	Sn1—C32′—C33′—C34′	−86.4 (12)
C6—N2—C12—C11	0.1 (7)	Sn1—C32′—C33′—C38′	88.6 (14)
Sn1—N2—C12—C11	−178.6 (3)	C38′—C33′—C34′—C35′	0.0
C10—C11—C12—N2	0.7 (7)	C32′—C33′—C34′—C35′	175 (2)
C11—C10—C13—C18	−126.2 (5)	C33′—C34′—C35′—C36′	0.0
C7—C10—C13—C18	55.2 (6)	C33′—C34′—C35′—Br4′	−177.0 (9)
C11—C10—C13—C14	53.2 (6)	C34′—C35′—C36′—C37′	0.0

C7—C10—C13—C14	−125.3 (4)	Br4′—C35′—C36′—C37′	177.0 (9)
C18—C13—C14—C15	−2.1 (7)	C35′—C36′—C37′—C38′	0.0
C10—C13—C14—C15	178.5 (4)	C36′—C37′—C38′—C33′	0.0
C13—C14—C15—C16	0.7 (7)	C34′—C33′—C38′—C37′	0.0
C14—C15—C16—C17	1.3 (8)	C32′—C33′—C38′—C37′	−175 (2)
C15—C16—C17—C18	−1.9 (8)		

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+2.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1*A*···Br2	0.93	2.78	3.477 (4)	133
C12—H12*A*···Br1	0.93	2.97	3.656 (5)	132
C36—H36*A*···Br2^{ii}	0.93	3.00	3.883 (3)	159

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