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Bis[2-(cycloheptyliminomethyl)pyridine-κ^2N,N']silver(I) tetraphenylborate

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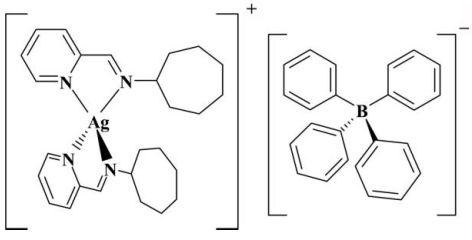
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; disorder in main residue; R factor = 0.030; wR factor = 0.079; data-to-parameter ratio = 21.9.

In the title complex, $[Ag(C_{26}H_{36}N_4)_2](C_{24}H_{20}B)$, the Ag^I atom has a distorted tetrahedral coordination. The organic ligand is bidentate, coordinating the Ag^I atom *via* two imine N atoms. One of the cycloheptyl groups and the Ag atom are disordered over two sites, with occupancy factors of *ca* 0.87 and 0.13. In this arrangement, the closest methylene group is more remote and the Ag atom also moves out by 0.405 (5) Å toward an alternative position.

Related literature

For related literature, see: Amirnasr *et al.* (2006); Bowyer *et al.* (1998); Chakraborty *et al.* (1999); Dehghanpour *et al.* (2007); Hannon *et al.* (1999).



Experimental

Crystal data

$[Ag(C_{26}H_{36}N_4)_2](C_{24}H_{20}B)$
M_r = 831.67
Monoclinic, $P2_1/c$
a = 13.2093 (3) Å
b = 15.2132 (2) Å
c = 21.6851 (6) Å
β = 105.462 (2)°
V = 4200.03 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 100 (2) K
0.50 × 0.38 × 0.24 mm

Data collection

Stoe IPDSII diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.781, T_{max} = 0.886
32871 measured reflections
11472 independent reflections
10372 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.079
S = 1.08
11472 reflections
524 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.53 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N2	2.2025 (12)	Ag1*A*—N4	2.045 (4)
Ag1—N3	2.2757 (12)	Ag1*A*—N2	2.310 (3)
Ag1—N4	2.3426 (13)	Ag1*A*—N1	2.444 (3)
Ag1—N1	2.4646 (12)	Ag1*A*—N3	2.449 (4)
N2—Ag1—N3	148.72 (5)	N4—Ag1*A*—N2	152.8 (2)
N2—Ag1—N4	137.23 (5)	N4—Ag1*A*—N1	116.27 (16)
N3—Ag1—N4	73.05 (4)	N2—Ag1*A*—N1	71.57 (9)
N2—Ag1—N1	72.93 (4)	N4—Ag1*A*—N3	74.82 (10)
N3—Ag1—N1	111.61 (4)	N2—Ag1*A*—N3	129.94 (19)
N4—Ag1—N1	105.16 (4)	N1—Ag1*A*—N3	106.54 (14)

Data collection: *X-AREA* (Stoe & Cie, 2006); cell refinement: *X-AREA* data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2033).

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supplementary materials

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Bis[2-(cycloheptyliminomethyl)pyridine-κ^2N,N']silver(I) tetraphenylborate

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Comment

Pyridinecarbaldehyde and its substituted derivatives condense with amines to furnish a range of diimine compounds; such compounds have been used as ligands of transition metals. Among such complexes whose structures have been described are, for example, compounds of copper(I) (Dehghanpour *et al.*, 2007), silver(I) (Bowyer *et al.*, 1998; Hannon *et al.*, 1999) and Ru(II) (Chakraborty *et al.*, 1999). The title complex, (I), was prepared by the reaction of $AgBPh_4$ with the bidentate ligand *N*,*N*'-cycloheptyl-pyridin-2-ylmethylene-amine.

One of the cycloheptyl substituents proved to show disorder with an alternative conformation (shown bright transparent in figure 1a) occupied at 12.7 (2)%, which will be discussed in detail in the next paragraph. The general geometry for the complex is similar with either of the two alternative orientations. While a tetrahedral geometry might be expected for four coordinated silver(I), the coordination sphere around the metal ion in this complex is strongly distorted by the restricting bite angles of the chelating ligand. The intraligand N1–Ag1–N2 and N3–Ag1–N4 angles [72.93 (4), 73.05 (4) °] are much less than 109.5 °. On the contrary the N2–Ag1–N3 and N2–Ag1–N4 angles [148.72 (5), 137.23 (5) °] are much larger than those of a tetrahedral complex. Ag1 is only 0.1135 (5) Å above the plane of N2, N3, and N4, and the bond Ag1—N1 is inclined by 69.72 (3)° with respect to this plane. The Ag–N bond lengths are similar to the corresponding bond distances in related complexes (Amirnasr *et al.*, 2006; Bowyer *et al.*, 1998; Hannon *et al.*, 1999). The dihedral angle between the two chelate rings is 87.06 (4) °. The environments of the imine and pyridine nitrogen atoms are planar with the sums of the three N atom bond angles being 360.0 ° and 359.9 ° for N1 and N2, respectively. Despite the fact that the nitrogen atom (N1) is sp^2 hybridized, some strain in the chelate ring is suggested by the deviation from the 120 ° angle at nitrogen (C25–N1–C29 = 117.6 (1)°).

In the arrangement with the at N4 disordered cycloheptyl rest (bright transparent in figure 1a) the C50 methylene group is more remote of Ag1, the silver atom also moves out by 0.405 (5) Å toward an alternative position. Here the most obtuse angle changes from N2—Ag1—N3 (148.72 (4)°) to N2—Ag1a—N4 (152.8 (2)°), and Ag1 approaches N4. In both alternative conformations, the shortest Ag···H contacts are similar (Ag1···H33*a* 2.85 Å, Ag1···H50*a* 3.14 Å; Ag1a···H33*a* 2.90 Å, Ag1a···H49*c* 3.11 Å) and are close to the sum of the Van der Waals radii (2.92 Å). Apparently the coordinational compromise provoked by the geometrical restrictions of the chelate ligands may find different solutions with similar energy.

Experimental

To a solution of bis(cycloheptyl-pyridin-2-ylmethylene-amine) (37.8 mg, 0.1 mmol) in 20 ml acetonitrile was added silver tetraphenylborate (28.9 mg, 0.1 mmol). The mixture was heated to dissolve the reactants. The solution was filtered and the volume of solvent removed under vacuum to about 5 ml. The diffusion of diethyl ether vapor into the solution gave light-yellow crystals. The crystals were collected and washed with diethylether-dichloromethane (9:1 *v*/*v*); yield 85%. Calc. for $C_{50}H_{56}AgBN_4$: C 72.21, H 6.79, N 6.74%; found: C 72.23, H 6.80, N 6.75%.

Refinement

Hydrogen atoms were generated geometrically (C–H 0.93 to 1.00 Å) and were included in the refinement in the riding model approximation, with U_{iso}(H) set to 1.2 times U_{eq}(C). For Ag1, C48, C49, and C50, alternative positions indicating disorder could be refined in a split atom model with common site occupation factors of 0.127 (2). For the C—C bond lengths in this part restraints of 1.52 (1) Å with a standard deviation of 0.02 Å were used in the refinement. For Ag1 and Ag1a independent anisotropic displacement parameters could be refined, for the splitted C atoms common anisotropic parameters were used for both positions. The H-atom positions were calculated for both alternative conformations. Similar but less resolved disorder phenomena have been observed for a second crystal measured at 193 K.

Figures

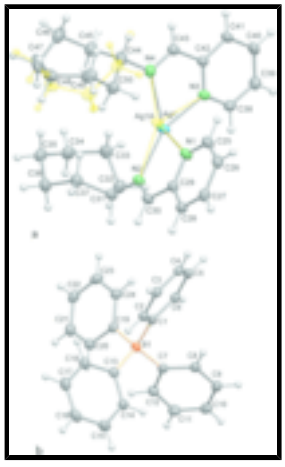


Fig. 1. Structures of a) the cation $[Ag(C_{26}H_{38}N_4)_2]^+$, b) the anion $(C_{24}H_{20}B)^-$ in the crystal. Thermal ellipsoids are drawn at the 50% probability level, and hydrogen atoms are shown as spheres of arbitrary radius. Less occupied alternative positions in the disordered cation are drawn bright transparent.

Bis[2-(cycloheptyliminomethyl)pyridine-k^{2}N,N']silver(I) tetraphenylborate

Crystal data

$[Ag(C_{26}H_{36}N_4)_2]C_{24}H_{20}B$	F_{000} = 1744
M_r = 831.67	D_x = 1.315 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 49514 reflections
a = 13.2093 (3) Å	θ = 1.6–29.8º
b = 15.2132 (2) Å	μ = 0.52 mm^{-1}
c = 21.6851 (6) Å	T = 100 (2) K
β = 105.462 (2)º	Prism, light-yellow
V = 4200.03 (16) Å^3	0.50 × 0.38 × 0.24 mm
Z = 4	

Data collection

Stoe IPDS II	11472 independent reflections

diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 6.7 pixels mm^{-1}

T = 100(2) K

ω scans

Absorption correction: multi-scan (Blessing, 1995)

T_{min} = 0.781, T_{max} = 0.886

32871 measured reflections

10372 reflections with $I > 2\sigma(I)$

R_{int} = 0.017

θ_{max} = 29.4º

θ_{min} = 1.6º

$h = -18 \rightarrow 18$

$k = -21 \rightarrow 20$

$l = -28 \rightarrow 29$

Refinement

Refinement on F^2

Least-squares matrix: full

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

$wR(F^2)$ = 0.079

S = 1.08

11472 reflections

524 parameters

8 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

$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2 + 1.6408P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max}$ = 0.003

$\Delta\rho_{max}$ = 0.53 e $Å^{-3}$

$\Delta\rho_{min}$ = −0.58 e $Å^{-3}$

Extinction correction: none

Special details

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

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

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
B1	0.71523 (11)	0.77457 (9)	0.04699 (7)	0.0190 (2)	
C1	0.65428 (9)	0.77615 (8)	0.10404 (6)	0.0193 (2)	
C2	0.61436 (10)	0.70078 (8)	0.12635 (6)	0.0212 (2)	
H2	0.6256	0.6453	0.1091	0.025*	
C3	0.55857 (10)	0.70357 (9)	0.17289 (6)	0.0226 (2)	
H3	0.5332	0.6506	0.1867	0.027*	
C4	0.54016 (10)	0.78309 (9)	0.19895 (6)	0.0224 (2)	

H4	0.5020	0.7854	0.2304	0.027*	
C5	0.57857 (9)	0.85956 (9)	0.17828 (6)	0.0213 (2)	
H5	0.5667	0.9147	0.1956	0.026*	
C6	0.63446 (9)	0.85551 (8)	0.13219 (6)	0.0205 (2)	
H6	0.6604	0.9087	0.1192	0.025*	
C7	0.82698 (10)	0.83014 (8)	0.06767 (6)	0.0201 (2)	
C8	0.87241 (10)	0.86601 (9)	0.12822 (6)	0.0222 (2)	
H8	0.8364	0.8597	0.1605	0.027*	
C9	0.96835 (10)	0.91059 (9)	0.14326 (7)	0.0259 (3)	
H9	0.9958	0.9342	0.1849	0.031*	
C10	1.02359 (10)	0.92053 (9)	0.09771 (7)	0.0284 (3)	
H10	1.0886	0.9511	0.1076	0.034*	
C11	0.98216 (11)	0.88498 (10)	0.03731 (7)	0.0280 (3)	
H11	1.0193	0.8906	0.0056	0.034*	
C12	0.88647 (10)	0.84116 (9)	0.02314 (7)	0.0241 (2)	
H12	0.8599	0.8175	−0.0186	0.029*	
C13	0.74120 (10)	0.67239 (8)	0.03106 (6)	0.0202 (2)	
C14	0.84116 (10)	0.63461 (9)	0.05230 (6)	0.0224 (2)	
H14	0.8974	0.6698	0.0762	0.027*	
C15	0.86144 (11)	0.54728 (9)	0.03978 (7)	0.0272 (3)	
H15	0.9303	0.5241	0.0556	0.033*	
C16	0.78187 (12)	0.49443 (9)	0.00444 (7)	0.0284 (3)	
H16	0.7955	0.4351	−0.0044	0.034*	
C17	0.68159 (12)	0.52949 (9)	−0.01789 (7)	0.0276 (3)	
H17	0.6260	0.4941	−0.0423	0.033*	
C18	0.66253 (10)	0.61634 (9)	−0.00446 (7)	0.0245 (2)	
H18	0.5933	0.6388	−0.0200	0.029*	
C19	0.63786 (10)	0.81801 (8)	−0.01880 (6)	0.0201 (2)	
C20	0.65518 (11)	0.80003 (9)	−0.07887 (6)	0.0236 (2)	
H20	0.7107	0.7612	−0.0806	0.028*	
C21	0.59516 (11)	0.83618 (9)	−0.13563 (6)	0.0264 (3)	
H21	0.6111	0.8232	−0.1749	0.032*	
C22	0.51163 (11)	0.89140 (9)	−0.13496 (7)	0.0268 (3)	
H22	0.4695	0.9160	−0.1736	0.032*	
C23	0.49090 (10)	0.90999 (9)	−0.07703 (7)	0.0268 (3)	
H23	0.4338	0.9473	−0.0759	0.032*	
C24	0.55340 (10)	0.87427 (9)	−0.02035 (6)	0.0231 (2)	
H24	0.5380	0.8887	0.0188	0.028*	
Ag1	0.85288 (4)	0.19026 (4)	0.14911 (2)	0.02404 (7)	0.873 (2)
Ag1A	0.8437 (2)	0.2153 (3)	0.15095 (15)	0.0248 (5)	0.127 (2)
N1	1.01864 (9)	0.26352 (8)	0.14765 (5)	0.0261 (2)	
N2	0.96308 (9)	0.17026 (8)	0.24404 (5)	0.0224 (2)	
N3	0.76931 (8)	0.13463 (7)	0.05138 (5)	0.0215 (2)	
N4	0.72043 (9)	0.29027 (8)	0.10113 (6)	0.0240 (2)	
C25	1.04846 (11)	0.31078 (10)	0.10380 (7)	0.0276 (3)	
H25	0.9986	0.3211	0.0639	0.033*	
C26	1.14861 (11)	0.34568 (9)	0.11333 (7)	0.0254 (3)	
H26	1.1664	0.3797	0.0810	0.031*	
C27	1.22166 (10)	0.32969 (9)	0.17092 (7)	0.0243 (2)	

H27	1.2911	0.3520	0.1787	0.029*	
C28	1.19238 (10)	0.28065 (9)	0.21724 (6)	0.0225 (2)	
H28	1.2412	0.2686	0.2572	0.027*	
C29	1.08999 (10)	0.24949 (9)	0.20387 (6)	0.0220 (2)	
C30	1.05590 (10)	0.20018 (8)	0.25325 (6)	0.0223 (2)	
H30	1.1050	0.1903	0.2935	0.027*	
C31	0.93615 (10)	0.12872 (9)	0.29904 (6)	0.0224 (2)	
H31	1.0028	0.1082	0.3296	0.027*	
C32	0.86636 (10)	0.04840 (9)	0.27667 (7)	0.0261 (3)	
H32A	0.8799	0.0055	0.3123	0.031*	
H32B	0.8883	0.0206	0.2410	0.031*	
C33	0.74781 (11)	0.06488 (10)	0.25437 (7)	0.0282 (3)	
H33A	0.7351	0.1215	0.2310	0.034*	
H33B	0.7148	0.0179	0.2241	0.034*	
C34	0.69492 (11)	0.06756 (10)	0.30913 (7)	0.0283 (3)	
H34A	0.6180	0.0632	0.2905	0.034*	
H34B	0.7173	0.0149	0.3362	0.034*	
C35	0.71723 (11)	0.14850 (10)	0.35198 (7)	0.0277 (3)	
H35A	0.6832	0.1405	0.3871	0.033*	
H35B	0.6840	0.2000	0.3266	0.033*	
C36	0.83336 (11)	0.16900 (10)	0.38129 (7)	0.0274 (3)	
H36A	0.8690	0.1154	0.4024	0.033*	
H36B	0.8396	0.2148	0.4146	0.033*	
C37	0.88903 (11)	0.20085 (9)	0.33188 (7)	0.0254 (3)	
H37A	0.8381	0.2347	0.2986	0.031*	
H37B	0.9460	0.2416	0.3533	0.031*	
C38	0.78747 (10)	0.05777 (9)	0.02625 (6)	0.0241 (2)	
H38	0.8369	0.0185	0.0522	0.029*	
C39	0.73743 (11)	0.03279 (9)	−0.03600 (7)	0.0258 (3)	
H39	0.7516	−0.0227	−0.0520	0.031*	
C40	0.66676 (11)	0.08999 (9)	−0.07412 (6)	0.0257 (3)	
H40	0.6321	0.0749	−0.1171	0.031*	
C41	0.64692 (10)	0.16987 (9)	−0.04885 (6)	0.0235 (2)	
H41	0.5986	0.2104	−0.0742	0.028*	
C42	0.69887 (10)	0.18943 (8)	0.01403 (6)	0.0206 (2)	
C43	0.67639 (10)	0.27201 (9)	0.04304 (6)	0.0231 (2)	
H43	0.6279	0.3125	0.0178	0.028*	
C44	0.69530 (11)	0.37288 (9)	0.12804 (7)	0.0270 (3)	
H44A	0.6708	0.4165	0.0927	0.032*	0.873 (2)
H44B	0.6503	0.3977	0.0872	0.032*	0.127 (2)
C45	0.60658 (11)	0.35548 (9)	0.15949 (7)	0.0278 (3)	
H54A	0.5455	0.3316	0.1268	0.033*	0.873 (2)
H54B	0.6300	0.3100	0.1929	0.033*	0.873 (2)
H54C	0.5455	0.3316	0.1268	0.033*	0.127 (2)
H54D	0.6300	0.3100	0.1929	0.033*	0.127 (2)
C46	0.57134 (13)	0.43643 (10)	0.18983 (8)	0.0349 (3)	
H46A	0.5014	0.4247	0.1967	0.042*	
H46B	0.5639	0.4864	0.1597	0.042*	
C47	0.64702 (17)	0.46260 (11)	0.25355 (8)	0.0444 (4)	

H47A	0.6729	0.4082	0.2777	0.053*	0.873 (2)
H47B	0.6071	0.4960	0.2785	0.053*	0.873 (2)
H47C	0.6133	0.5117	0.2706	0.053*	0.127 (2)
H47D	0.6499	0.4124	0.2830	0.053*	0.127 (2)
C48	0.74320 (17)	0.51826 (15)	0.24986 (9)	0.0389 (4)	0.873 (2)
H48A	0.7222	0.5809	0.2480	0.047*	0.873 (2)
H48B	0.7985	0.5098	0.2904	0.047*	0.873 (2)
C49	0.79177 (14)	0.50138 (11)	0.19561 (10)	0.0345 (4)	0.873 (2)
H49A	0.8639	0.5258	0.2079	0.041*	0.873 (2)
H49B	0.7514	0.5352	0.1581	0.041*	0.873 (2)
C50	0.79858 (12)	0.40667 (10)	0.17443 (8)	0.0262 (3)	0.873 (2)
H50A	0.8167	0.3684	0.2127	0.031*	0.873 (2)
H50B	0.8560	0.4019	0.1531	0.031*	0.873 (2)
C50A	0.7656 (8)	0.4468 (6)	0.1444 (5)	0.0262 (3)	0.127 (2)
H50C	0.7273	0.5025	0.1308	0.031*	0.127 (2)
H50D	0.8231	0.4419	0.1232	0.031*	0.127 (2)
C49A	0.8086 (9)	0.4445 (8)	0.2158 (5)	0.0345 (4)	0.127 (2)
H49C	0.8170	0.3817	0.2281	0.041*	0.127 (2)
H49D	0.8802	0.4697	0.2254	0.041*	0.127 (2)
C48A	0.7548 (8)	0.4876 (10)	0.2607 (7)	0.0389 (4)	0.127 (2)
H48C	0.7954	0.4743	0.3050	0.047*	0.127 (2)
H48D	0.7573	0.5520	0.2549	0.047*	0.127 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
B1	0.0198 (6)	0.0187 (6)	0.0186 (6)	0.0007 (5)	0.0055 (5)	0.0005 (5)
C1	0.0166 (5)	0.0217 (5)	0.0184 (5)	0.0013 (4)	0.0025 (4)	0.0011 (4)
C2	0.0204 (5)	0.0212 (5)	0.0214 (6)	0.0015 (4)	0.0046 (4)	0.0008 (4)
C3	0.0202 (5)	0.0246 (6)	0.0231 (6)	−0.0009 (4)	0.0058 (5)	0.0034 (5)
C4	0.0176 (5)	0.0297 (6)	0.0195 (5)	0.0015 (4)	0.0046 (4)	0.0013 (5)
C5	0.0183 (5)	0.0242 (6)	0.0202 (5)	0.0020 (4)	0.0032 (4)	−0.0016 (4)
C6	0.0184 (5)	0.0217 (5)	0.0207 (5)	0.0004 (4)	0.0040 (4)	0.0006 (4)
C7	0.0201 (5)	0.0180 (5)	0.0224 (6)	0.0023 (4)	0.0060 (4)	0.0016 (4)
C8	0.0203 (5)	0.0229 (6)	0.0231 (6)	0.0019 (4)	0.0053 (4)	0.0007 (5)
C9	0.0210 (6)	0.0269 (6)	0.0274 (6)	0.0003 (5)	0.0024 (5)	−0.0033 (5)
C10	0.0201 (6)	0.0268 (6)	0.0377 (7)	−0.0023 (5)	0.0068 (5)	−0.0007 (6)
C11	0.0241 (6)	0.0298 (6)	0.0334 (7)	−0.0009 (5)	0.0132 (5)	0.0001 (5)
C12	0.0237 (6)	0.0246 (6)	0.0250 (6)	−0.0003 (5)	0.0085 (5)	−0.0007 (5)
C13	0.0222 (6)	0.0212 (5)	0.0178 (5)	0.0007 (4)	0.0064 (4)	0.0015 (4)
C14	0.0236 (6)	0.0227 (6)	0.0198 (5)	0.0025 (4)	0.0036 (4)	0.0009 (4)
C15	0.0299 (6)	0.0249 (6)	0.0266 (6)	0.0077 (5)	0.0071 (5)	0.0031 (5)
C16	0.0396 (7)	0.0197 (6)	0.0282 (7)	0.0025 (5)	0.0132 (6)	0.0001 (5)
C17	0.0330 (7)	0.0234 (6)	0.0266 (6)	−0.0046 (5)	0.0084 (5)	−0.0026 (5)
C18	0.0243 (6)	0.0236 (6)	0.0253 (6)	−0.0008 (5)	0.0060 (5)	−0.0003 (5)
C19	0.0201 (5)	0.0201 (5)	0.0199 (5)	−0.0012 (4)	0.0049 (4)	0.0016 (4)
C20	0.0247 (6)	0.0248 (6)	0.0211 (6)	0.0022 (5)	0.0056 (5)	0.0000 (5)
C21	0.0303 (6)	0.0277 (6)	0.0199 (6)	−0.0018 (5)	0.0046 (5)	0.0007 (5)

C22	0.0249 (6)	0.0280 (6)	0.0240 (6)	−0.0019 (5)	0.0004 (5)	0.0063 (5)
C23	0.0203 (6)	0.0283 (6)	0.0310 (7)	0.0032 (5)	0.0053 (5)	0.0061 (5)
C24	0.0216 (5)	0.0246 (6)	0.0237 (6)	0.0013 (4)	0.0072 (5)	0.0026 (5)
Ag1	0.02016 (9)	0.02887 (17)	0.01943 (8)	−0.00104 (10)	−0.00109 (6)	0.00182 (11)
Ag1A	0.0202 (6)	0.0317 (12)	0.0183 (5)	−0.0034 (8)	−0.0019 (4)	0.0030 (8)
N1	0.0232 (5)	0.0343 (6)	0.0197 (5)	−0.0017 (4)	0.0038 (4)	0.0028 (4)
N2	0.0209 (5)	0.0265 (5)	0.0192 (5)	−0.0027 (4)	0.0041 (4)	0.0012 (4)
N3	0.0193 (5)	0.0232 (5)	0.0207 (5)	−0.0001 (4)	0.0029 (4)	0.0021 (4)
N4	0.0250 (5)	0.0243 (5)	0.0239 (5)	−0.0027 (4)	0.0085 (4)	−0.0021 (4)
C25	0.0273 (6)	0.0350 (7)	0.0199 (6)	0.0002 (5)	0.0055 (5)	0.0039 (5)
C26	0.0298 (6)	0.0256 (6)	0.0235 (6)	−0.0002 (5)	0.0117 (5)	0.0011 (5)
C27	0.0230 (6)	0.0249 (6)	0.0269 (6)	−0.0019 (5)	0.0100 (5)	−0.0020 (5)
C28	0.0197 (5)	0.0260 (6)	0.0212 (6)	−0.0008 (4)	0.0046 (4)	−0.0009 (5)
C29	0.0213 (5)	0.0253 (6)	0.0194 (5)	−0.0007 (4)	0.0056 (4)	0.0001 (5)
C30	0.0213 (6)	0.0263 (6)	0.0181 (5)	−0.0015 (4)	0.0030 (4)	0.0007 (4)
C31	0.0189 (5)	0.0274 (6)	0.0200 (5)	−0.0028 (4)	0.0035 (4)	0.0025 (5)
C32	0.0248 (6)	0.0246 (6)	0.0306 (7)	−0.0026 (5)	0.0103 (5)	−0.0020 (5)
C33	0.0240 (6)	0.0316 (7)	0.0282 (6)	−0.0085 (5)	0.0056 (5)	−0.0048 (5)
C34	0.0217 (6)	0.0310 (7)	0.0335 (7)	−0.0041 (5)	0.0093 (5)	−0.0002 (6)
C35	0.0245 (6)	0.0292 (7)	0.0314 (7)	0.0013 (5)	0.0110 (5)	0.0022 (5)
C36	0.0272 (6)	0.0324 (7)	0.0239 (6)	−0.0031 (5)	0.0091 (5)	−0.0016 (5)
C37	0.0256 (6)	0.0263 (6)	0.0248 (6)	−0.0056 (5)	0.0074 (5)	−0.0018 (5)
C38	0.0230 (6)	0.0234 (6)	0.0255 (6)	0.0020 (4)	0.0057 (5)	0.0036 (5)
C39	0.0294 (6)	0.0218 (6)	0.0280 (6)	−0.0018 (5)	0.0107 (5)	−0.0019 (5)
C40	0.0257 (6)	0.0304 (6)	0.0201 (6)	−0.0035 (5)	0.0044 (5)	−0.0030 (5)
C41	0.0217 (6)	0.0280 (6)	0.0189 (6)	0.0003 (5)	0.0023 (4)	0.0015 (5)
C42	0.0190 (5)	0.0219 (5)	0.0202 (6)	−0.0006 (4)	0.0043 (4)	0.0013 (4)
C43	0.0230 (6)	0.0232 (6)	0.0227 (6)	0.0012 (4)	0.0055 (5)	0.0018 (5)
C44	0.0334 (7)	0.0237 (6)	0.0270 (6)	−0.0018 (5)	0.0135 (5)	−0.0016 (5)
C45	0.0282 (6)	0.0254 (6)	0.0329 (7)	−0.0010 (5)	0.0134 (5)	−0.0004 (5)
C46	0.0377 (8)	0.0293 (7)	0.0448 (9)	0.0043 (6)	0.0236 (7)	0.0024 (6)
C47	0.0813 (13)	0.0296 (8)	0.0296 (8)	0.0048 (8)	0.0272 (8)	−0.0001 (6)
C48	0.0478 (10)	0.0364 (11)	0.0262 (9)	0.0132 (8)	−0.0009 (7)	−0.0059 (8)
C49	0.0322 (8)	0.0241 (7)	0.0437 (10)	−0.0002 (6)	0.0042 (7)	−0.0069 (7)
C50	0.0251 (7)	0.0228 (7)	0.0297 (8)	0.0001 (5)	0.0056 (6)	−0.0034 (6)
C50A	0.0251 (7)	0.0228 (7)	0.0297 (8)	0.0001 (5)	0.0056 (6)	−0.0034 (6)
C49A	0.0322 (8)	0.0241 (7)	0.0437 (10)	−0.0002 (6)	0.0042 (7)	−0.0069 (7)
C48A	0.0478 (10)	0.0364 (11)	0.0262 (9)	0.0132 (8)	−0.0009 (7)	−0.0059 (8)

Geometric parameters (Å, °)

B1—C1	1.6463 (18)	C28—C29	1.3890 (17)
B1—C13	1.6483 (18)	C28—H28	0.9500
B1—C19	1.6550 (19)	C29—C30	1.4728 (17)
B1—C7	1.6558 (19)	C30—H30	0.9500
C1—C2	1.4009 (17)	C31—C37	1.5281 (19)
C1—C6	1.4086 (17)	C31—C32	1.5296 (18)
C2—C3	1.4002 (18)	C31—H31	1.0000
C2—H2	0.9500	C32—C33	1.5314 (19)

C3—C4	1.3839 (19)	C32—H32A	0.9900
C3—H3	0.9500	C32—H32B	0.9900
C4—C5	1.3902 (18)	C33—C34	1.5305 (19)
C4—H4	0.9500	C33—H33A	0.9900
C5—C6	1.3934 (17)	C33—H33B	0.9900
C5—H5	0.9500	C34—C35	1.523 (2)
C6—H6	0.9500	C34—H34A	0.9900
C7—C8	1.4006 (18)	C34—H34B	0.9900
C7—C12	1.4081 (17)	C35—C36	1.528 (2)
C8—C9	1.3972 (18)	C35—H35A	0.9900
C8—H8	0.9500	C35—H35B	0.9900
C9—C10	1.384 (2)	C36—C37	1.5309 (19)
C9—H9	0.9500	C36—H36A	0.9900
C10—C11	1.388 (2)	C36—H36B	0.9900
C10—H10	0.9500	C37—H37A	0.9900
C11—C12	1.3891 (18)	C37—H37B	0.9900
C11—H11	0.9500	C38—C39	1.3885 (19)
C12—H12	0.9500	C38—H38	0.9500
C13—C14	1.4006 (17)	C39—C40	1.3786 (19)
C13—C18	1.4049 (18)	C39—H39	0.9500
C14—C15	1.3961 (18)	C40—C41	1.3866 (19)
C14—H14	0.9500	C40—H40	0.9500
C15—C16	1.382 (2)	C41—C42	1.3854 (18)
C15—H15	0.9500	C41—H41	0.9500
C16—C17	1.390 (2)	C42—C43	1.4705 (18)
C16—H16	0.9500	C43—H43	0.9500
C17—C18	1.3904 (19)	C44—C50A	1.441 (7)
C17—H17	0.9500	C44—C45	1.5279 (18)
C18—H18	0.9500	C44—C50	1.551 (2)
C19—C24	1.3995 (17)	C44—H44A	1.0000
C19—C20	1.4082 (18)	C44—H44B	1.0000
C20—C21	1.3876 (19)	C45—C46	1.526 (2)
C20—H20	0.9500	C45—H54A	0.9900
C21—C22	1.390 (2)	C45—H54B	0.9900
C21—H21	0.9500	C45—H54C	0.9900
C22—C23	1.384 (2)	C45—H54D	0.9900
C22—H22	0.9500	C46—C47	1.527 (3)
C23—C24	1.3951 (18)	C46—H46A	0.9900
C23—H23	0.9500	C46—H46B	0.9900
C24—H24	0.9500	C47—C48A	1.441 (9)
Ag1—N2	2.2025 (12)	C47—C48	1.547 (3)
Ag1—N3	2.2757 (12)	C47—H47A	0.9900
Ag1—N4	2.3426 (13)	C47—H47B	0.9900
Ag1—N1	2.4646 (12)	C47—H47C	0.9899
Ag1A—N4	2.045 (4)	C47—H47D	0.9899
Ag1A—N2	2.310 (3)	C48—C49	1.505 (3)
Ag1A—N1	2.444 (3)	C48—H48A	0.9900
Ag1A—N3	2.449 (4)	C48—H48B	0.9900
N1—C25	1.3327 (18)	C49—C50	1.522 (2)

N1—C29	1.3444 (17)	C49—H49A	0.9900
N2—C30	1.2728 (17)	C49—H49B	0.9900
N2—C31	1.4746 (16)	C50—H50A	0.9900
N3—C38	1.3386 (17)	C50—H50B	0.9900
N3—C42	1.3472 (16)	C50A—C49A	1.501 (9)
N4—C43	1.2695 (17)	C50A—H50C	0.9900
N4—C44	1.4606 (17)	C50A—H50D	0.9900
C25—C26	1.389 (2)	C49A—C48A	1.500 (9)
C25—H25	0.9500	C49A—H49C	0.9900
C26—C27	1.381 (2)	C49A—H49D	0.9900
C26—H26	0.9500	C48A—H48C	0.9900
C27—C28	1.3866 (18)	C48A—H48D	0.9900
C27—H27	0.9500		
C1—B1—C13	110.00 (10)	H32A—C32—H32B	107.3
C1—B1—C19	109.19 (10)	C34—C33—C32	113.54 (12)
C13—B1—C19	108.13 (10)	C34—C33—H33A	108.9
C1—B1—C7	111.61 (10)	C32—C33—H33A	108.9
C13—B1—C7	108.54 (10)	C34—C33—H33B	108.9
C19—B1—C7	109.31 (10)	C32—C33—H33B	108.9
C2—C1—C6	114.91 (11)	H33A—C33—H33B	107.7
C2—C1—B1	123.51 (11)	C35—C34—C33	116.15 (11)
C6—C1—B1	121.52 (11)	C35—C34—H34A	108.2
C3—C2—C1	122.90 (12)	C33—C34—H34A	108.2
C3—C2—H2	118.6	C35—C34—H34B	108.2
C1—C2—H2	118.6	C33—C34—H34B	108.2
C4—C3—C2	120.28 (12)	H34A—C34—H34B	107.4
C4—C3—H3	119.9	C34—C35—C36	115.36 (12)
C2—C3—H3	119.9	C34—C35—H35A	108.4
C3—C4—C5	118.75 (12)	C36—C35—H35A	108.4
C3—C4—H4	120.6	C34—C35—H35B	108.4
C5—C4—H4	120.6	C36—C35—H35B	108.4
C4—C5—C6	120.20 (12)	H35A—C35—H35B	107.5
C4—C5—H5	119.9	C35—C36—C37	112.94 (12)
C6—C5—H5	119.9	C35—C36—H36A	109.0
C5—C6—C1	122.96 (12)	C37—C36—H36A	109.0
C5—C6—H6	118.5	C35—C36—H36B	109.0
C1—C6—H6	118.5	C37—C36—H36B	109.0
C8—C7—C12	114.75 (11)	H36A—C36—H36B	107.8
C8—C7—B1	125.52 (11)	C31—C37—C36	115.48 (11)
C12—C7—B1	119.69 (11)	C31—C37—H37A	108.4
C9—C8—C7	122.90 (12)	C36—C37—H37A	108.4
C9—C8—H8	118.5	C31—C37—H37B	108.4
C7—C8—H8	118.5	C36—C37—H37B	108.4
C10—C9—C8	120.30 (13)	H37A—C37—H37B	107.5
C10—C9—H9	119.9	N3—C38—C39	122.99 (12)
C8—C9—H9	119.9	N3—C38—H38	118.5
C9—C10—C11	118.74 (12)	C39—C38—H38	118.5
C9—C10—H10	120.6	C40—C39—C38	118.75 (12)
C11—C10—H10	120.6	C40—C39—H39	120.6

C10—C11—C12	120.17 (13)	C38—C39—H39	120.6
C10—C11—H11	119.9	C39—C40—C41	119.04 (12)
C12—C11—H11	119.9	C39—C40—H40	120.5
C11—C12—C7	123.14 (13)	C41—C40—H40	120.5
C11—C12—H12	118.4	C42—C41—C40	118.75 (12)
C7—C12—H12	118.4	C42—C41—H41	120.6
C14—C13—C18	115.21 (12)	C40—C41—H41	120.6
C14—C13—B1	123.28 (11)	N3—C42—C41	122.71 (12)
C18—C13—B1	121.50 (11)	N3—C42—C43	117.21 (11)
C15—C14—C13	122.65 (12)	C41—C42—C43	120.07 (12)
C15—C14—H14	118.7	N4—C43—C42	121.34 (12)
C13—C14—H14	118.7	N4—C43—H43	119.3
C16—C15—C14	120.31 (13)	C42—C43—H43	119.3
C16—C15—H15	119.8	C50A—C44—N4	124.7 (4)
C14—C15—H15	119.8	C50A—C44—C45	123.1 (4)
C15—C16—C17	118.90 (13)	N4—C44—C45	108.20 (11)
C15—C16—H16	120.5	C50A—C44—C50	35.3 (4)
C17—C16—H16	120.5	N4—C44—C50	106.86 (12)
C16—C17—C18	120.05 (13)	C45—C44—C50	114.51 (12)
C16—C17—H17	120.0	C50A—C44—H44A	74.2
C18—C17—H17	120.0	N4—C44—H44A	109.1
C17—C18—C13	122.88 (13)	C45—C44—H44A	109.1
C17—C18—H18	118.6	C50—C44—H44A	109.1
C13—C18—H18	118.6	C50A—C44—H44B	96.6
C24—C19—C20	114.93 (12)	N4—C44—H44B	96.6
C24—C19—B1	124.76 (11)	C45—C44—H44B	96.6
C20—C19—B1	120.31 (11)	C50—C44—H44B	131.4
C21—C20—C19	123.25 (12)	H44A—C44—H44B	22.5
C21—C20—H20	118.4	C46—C45—C44	114.26 (12)
C19—C20—H20	118.4	C46—C45—H54A	108.7
C20—C21—C22	119.85 (13)	C44—C45—H54A	108.7
C20—C21—H21	120.1	C46—C45—H54B	108.7
C22—C21—H21	120.1	C44—C45—H54B	108.7
C23—C22—C21	118.86 (12)	H54A—C45—H54B	107.6
C23—C22—H22	120.6	C46—C45—H54C	108.7
C21—C22—H22	120.6	C44—C45—H54C	108.7
C22—C23—C24	120.40 (12)	H54A—C45—H54C	0.0
C22—C23—H23	119.8	H54B—C45—H54C	107.6
C24—C23—H23	119.8	C46—C45—H54D	108.7
C23—C24—C19	122.70 (12)	C44—C45—H54D	108.7
C23—C24—H24	118.7	H54A—C45—H54D	107.6
C19—C24—H24	118.7	H54B—C45—H54D	0.0
N2—Ag1—N3	148.72 (5)	H54C—C45—H54D	107.6
N2—Ag1—N4	137.23 (5)	C45—C46—C47	113.53 (14)
N3—Ag1—N4	73.05 (4)	C45—C46—H46A	108.9
N2—Ag1—N1	72.93 (4)	C47—C46—H46A	108.9
N3—Ag1—N1	111.61 (4)	C45—C46—H46B	108.9
N4—Ag1—N1	105.16 (4)	C47—C46—H46B	108.9
N4—Ag1A—N2	152.8 (2)	H46A—C46—H46B	107.7

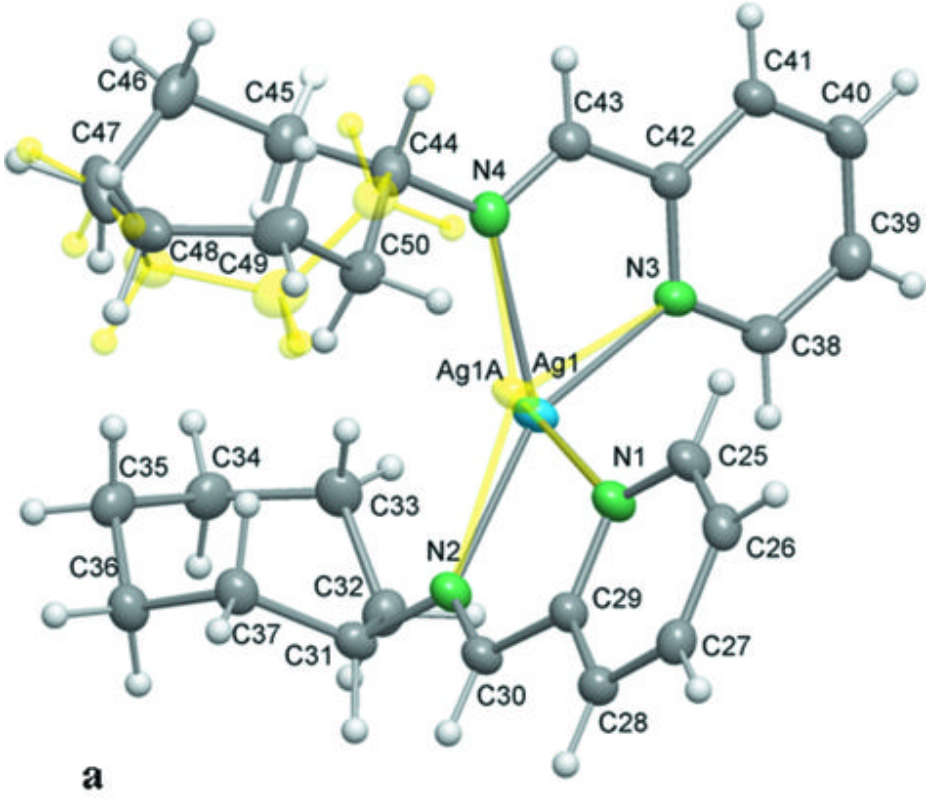
N4—Ag1A—N1	116.27 (16)	C48A—C47—C46	123.7 (6)
N2—Ag1A—N1	71.57 (9)	C48A—C47—C48	19.9 (6)
N4—Ag1A—N3	74.82 (10)	C46—C47—C48	116.40 (14)
N2—Ag1A—N3	129.94 (19)	C48A—C47—H47A	88.4
N1—Ag1A—N3	106.54 (14)	C46—C47—H47A	108.2
C25—N1—C29	117.62 (12)	C48—C47—H47A	108.2
C25—N1—Ag1A	130.14 (12)	C48A—C47—H47B	117.5
C29—N1—Ag1A	111.44 (11)	C46—C47—H47B	108.2
C25—N1—Ag1	133.29 (10)	C48—C47—H47B	108.2
C29—N1—Ag1	109.08 (8)	H47A—C47—H47B	107.3
Ag1A—N1—Ag1	9.44 (9)	C48A—C47—H47C	106.9
C30—N2—C31	117.15 (11)	C46—C47—H47C	106.5
C30—N2—Ag1	117.79 (9)	C48—C47—H47C	93.6
C31—N2—Ag1	124.98 (8)	H47A—C47—H47C	124.0
C30—N2—Ag1A	115.85 (12)	H47B—C47—H47C	18.5
C31—N2—Ag1A	125.32 (11)	C48A—C47—H47D	105.5
Ag1—N2—Ag1A	9.92 (9)	C46—C47—H47D	106.7
C38—N3—C42	117.76 (11)	C48—C47—H47D	124.4
C38—N3—Ag1	127.51 (9)	H47A—C47—H47D	20.8
C42—N3—Ag1	114.56 (9)	H47B—C47—H47D	88.7
C38—N3—Ag1A	136.31 (13)	H47C—C47—H47D	106.5
C42—N3—Ag1A	105.70 (12)	C49—C48—C47	118.32 (16)
Ag1—N3—Ag1A	8.87 (9)	C49—C48—H48A	107.7
C43—N4—C44	119.47 (12)	C47—C48—H48A	107.7
C43—N4—Ag1A	119.45 (14)	C49—C48—H48B	107.7
C44—N4—Ag1A	120.19 (14)	C47—C48—H48B	107.7
C43—N4—Ag1	112.89 (9)	H48A—C48—H48B	107.1
C44—N4—Ag1	127.14 (9)	C48—C49—C50	117.99 (16)
Ag1A—N4—Ag1	7.17 (11)	C48—C49—H49A	107.8
N1—C25—C26	123.44 (13)	C50—C49—H49A	107.8
N1—C25—H25	118.3	C48—C49—H49B	107.8
C26—C25—H25	118.3	C50—C49—H49B	107.8
C27—C26—C25	118.38 (12)	H49A—C49—H49B	107.1
C27—C26—H26	120.8	C49—C50—C44	113.38 (13)
C25—C26—H26	120.8	C49—C50—H50A	108.9
C26—C27—C28	119.16 (12)	C44—C50—H50A	108.9
C26—C27—H27	120.4	C49—C50—H50B	108.9
C28—C27—H27	120.4	C44—C50—H50B	108.9
C27—C28—C29	118.46 (12)	H50A—C50—H50B	107.7
C27—C28—H28	120.8	C44—C50A—C49A	106.1 (7)
C29—C28—H28	120.8	C44—C50A—H50C	110.5
N1—C29—C28	122.91 (12)	C49A—C50A—H50C	110.5
N1—C29—C30	117.64 (11)	C44—C50A—H50D	110.5
C28—C29—C30	119.44 (12)	C49A—C50A—H50D	110.5
N2—C30—C29	122.45 (12)	H50C—C50A—H50D	108.7
N2—C30—H30	118.8	C48A—C49A—C50A	123.0 (10)
C29—C30—H30	118.8	C48A—C49A—H49C	106.6
N2—C31—C37	106.57 (11)	C50A—C49A—H49C	106.6
N2—C31—C32	109.93 (11)	C48A—C49A—H49D	106.6

C37—C31—C32	115.82 (11)	C50A—C49A—H49D	106.6
N2—C31—H31	108.1	H49C—C49A—H49D	106.6
C37—C31—H31	108.1	C47—C48A—C49A	116.1 (9)
C32—C31—H31	108.1	C47—C48A—H48C	108.3
C31—C32—C33	116.64 (11)	C49A—C48A—H48C	108.3
C31—C32—H32A	108.1	C47—C48A—H48D	108.3
C33—C32—H32A	108.1	C49A—C48A—H48D	108.3
C31—C32—H32B	108.1	H48C—C48A—H48D	107.4
C33—C32—H32B	108.1		
C13—B1—C1—C2	−10.75 (16)	N2—Ag1A—N3—C42	176.26 (16)
C19—B1—C1—C2	107.76 (13)	N1—Ag1A—N3—C42	−104.20 (15)
C7—B1—C1—C2	−131.28 (12)	N4—Ag1A—N3—Ag1	−168.6 (6)
C13—B1—C1—C6	172.15 (11)	N2—Ag1A—N3—Ag1	−1.6 (4)
C19—B1—C1—C6	−69.35 (14)	N1—Ag1A—N3—Ag1	77.9 (5)
C7—B1—C1—C6	51.61 (15)	N2—Ag1A—N4—C43	−168.7 (3)
C6—C1—C2—C3	0.23 (18)	N1—Ag1A—N4—C43	90.4 (2)
B1—C1—C2—C3	−177.05 (12)	N3—Ag1A—N4—C43	−10.82 (14)
C1—C2—C3—C4	0.3 (2)	N2—Ag1A—N4—C44	22.2 (4)
C2—C3—C4—C5	−0.37 (19)	N1—Ag1A—N4—C44	−78.70 (19)
C3—C4—C5—C6	0.00 (19)	N3—Ag1A—N4—C44	−179.94 (10)
C4—C5—C6—C1	0.52 (19)	N2—Ag1A—N4—Ag1	−144.2 (11)
C2—C1—C6—C5	−0.61 (18)	N1—Ag1A—N4—Ag1	115.0 (9)
B1—C1—C6—C5	176.73 (11)	N3—Ag1A—N4—Ag1	13.7 (8)
C1—B1—C7—C8	7.04 (17)	N2—Ag1—N4—C43	−178.67 (9)
C13—B1—C7—C8	−114.34 (13)	N3—Ag1—N4—C43	−8.19 (9)
C19—B1—C7—C8	127.93 (13)	N1—Ag1—N4—C43	100.25 (10)
C1—B1—C7—C12	−175.64 (11)	N2—Ag1—N4—C44	9.61 (14)
C13—B1—C7—C12	62.98 (14)	N3—Ag1—N4—C44	−179.92 (11)
C19—B1—C7—C12	−54.75 (14)	N1—Ag1—N4—C44	−71.48 (11)
C12—C7—C8—C9	1.03 (18)	N2—Ag1—N4—Ag1A	24.4 (8)
B1—C7—C8—C9	178.47 (12)	N3—Ag1—N4—Ag1A	−165.1 (8)
C7—C8—C9—C10	−0.5 (2)	N1—Ag1—N4—Ag1A	−56.6 (8)
C8—C9—C10—C11	−0.4 (2)	C29—N1—C25—C26	0.1 (2)
C9—C10—C11—C12	0.6 (2)	Ag1A—N1—C25—C26	168.83 (17)
C10—C11—C12—C7	0.0 (2)	Ag1—N1—C25—C26	−179.24 (10)
C8—C7—C12—C11	−0.77 (19)	N1—C25—C26—C27	0.9 (2)
B1—C7—C12—C11	−178.37 (12)	C25—C26—C27—C28	−0.8 (2)
C1—B1—C13—C14	−103.12 (13)	C26—C27—C28—C29	−0.1 (2)
C19—B1—C13—C14	137.73 (12)	C25—N1—C29—C28	−1.1 (2)
C7—B1—C13—C14	19.25 (16)	Ag1A—N1—C29—C28	−171.90 (15)
C1—B1—C13—C18	75.83 (14)	Ag1—N1—C29—C28	178.35 (11)
C19—B1—C13—C18	−43.33 (15)	C25—N1—C29—C30	177.69 (12)
C7—B1—C13—C18	−161.80 (11)	Ag1A—N1—C29—C30	6.92 (18)
C18—C13—C14—C15	−0.65 (19)	Ag1—N1—C29—C30	−2.82 (14)
B1—C13—C14—C15	178.36 (12)	C27—C28—C29—N1	1.2 (2)
C13—C14—C15—C16	0.9 (2)	C27—C28—C29—C30	−177.64 (12)
C14—C15—C16—C17	−0.5 (2)	C31—N2—C30—C29	−174.87 (12)
C15—C16—C17—C18	−0.1 (2)	Ag1—N2—C30—C29	2.10 (17)
C16—C17—C18—C13	0.4 (2)	Ag1A—N2—C30—C29	−8.8 (2)

C14—C13—C18—C17	0.00 (19)	N1—C29—C30—N2	0.8 (2)
B1—C13—C18—C17	−179.03 (12)	C28—C29—C30—N2	179.70 (13)
C1—B1—C19—C24	20.96 (16)	C30—N2—C31—C37	92.35 (14)
C13—B1—C19—C24	140.62 (12)	Ag1—N2—C31—C37	−84.38 (12)
C7—B1—C19—C24	−101.40 (14)	Ag1A—N2—C31—C37	−72.25 (18)
C1—B1—C19—C20	−159.69 (11)	C30—N2—C31—C32	−141.41 (12)
C13—B1—C19—C20	−40.03 (15)	Ag1—N2—C31—C32	41.87 (14)
C7—B1—C19—C20	77.95 (14)	Ag1A—N2—C31—C32	54.00 (19)
C24—C19—C20—C21	1.25 (19)	N2—C31—C32—C33	−87.85 (14)
B1—C19—C20—C21	−178.16 (12)	C37—C31—C32—C33	32.98 (17)
C19—C20—C21—C22	−1.7 (2)	C31—C32—C33—C34	−84.03 (15)
C20—C21—C22—C23	0.8 (2)	C32—C33—C34—C35	72.20 (16)
C21—C22—C23—C24	0.4 (2)	C33—C34—C35—C36	−54.07 (18)
C22—C23—C24—C19	−0.8 (2)	C34—C35—C36—C37	69.82 (16)
C20—C19—C24—C23	−0.01 (19)	N2—C31—C37—C36	167.12 (11)
B1—C19—C24—C23	179.37 (12)	C32—C31—C37—C36	44.50 (17)
N4—Ag1A—N1—C25	−25.6 (3)	C35—C36—C37—C31	−88.65 (15)
N2—Ag1A—N1—C25	−177.30 (14)	C42—N3—C38—C39	0.16 (19)
N3—Ag1A—N1—C25	55.3 (2)	Ag1—N3—C38—C39	−174.86 (10)
N4—Ag1A—N1—C29	143.70 (16)	Ag1A—N3—C38—C39	−173.28 (14)
N2—Ag1A—N1—C29	−8.02 (15)	N3—C38—C39—C40	0.9 (2)
N3—Ag1A—N1—C29	−135.39 (13)	C38—C39—C40—C41	−0.9 (2)
N4—Ag1A—N1—Ag1	−139.0 (6)	C39—C40—C41—C42	−0.08 (19)
N2—Ag1A—N1—Ag1	69.3 (5)	C38—N3—C42—C41	−1.19 (18)
N3—Ag1A—N1—Ag1	−58.1 (5)	Ag1—N3—C42—C41	174.47 (10)
N2—Ag1—N1—C25	−177.82 (15)	Ag1A—N3—C42—C41	174.10 (13)
N3—Ag1—N1—C25	35.04 (15)	C38—N3—C42—C43	177.52 (11)
N4—Ag1—N1—C25	−42.39 (14)	Ag1—N3—C42—C43	−6.81 (14)
N2—Ag1—N1—C29	2.80 (9)	Ag1A—N3—C42—C43	−7.18 (15)
N3—Ag1—N1—C29	−144.33 (9)	C40—C41—C42—N3	1.2 (2)
N4—Ag1—N1—C29	138.23 (9)	C40—C41—C42—C43	−177.52 (12)
N2—Ag1—N1—Ag1A	−103.3 (5)	C44—N4—C43—C42	−179.68 (11)
N3—Ag1—N1—Ag1A	109.6 (5)	Ag1A—N4—C43—C42	11.1 (2)
N4—Ag1—N1—Ag1A	32.1 (5)	Ag1—N4—C43—C42	7.90 (16)
N3—Ag1—N2—C30	101.11 (13)	N3—C42—C43—N4	−0.98 (18)
N4—Ag1—N2—C30	−96.63 (11)	C41—C42—C43—N4	177.77 (12)
N1—Ag1—N2—C30	−2.57 (10)	C43—N4—C44—C50A	−108.7 (5)
N3—Ag1—N2—C31	−82.18 (13)	Ag1A—N4—C44—C50A	60.4 (5)
N4—Ag1—N2—C31	80.08 (12)	Ag1—N4—C44—C50A	62.5 (5)
N1—Ag1—N2—C31	174.14 (11)	C43—N4—C44—C45	93.33 (15)
N3—Ag1—N2—Ag1A	−177.6 (6)	Ag1A—N4—C44—C45	−97.55 (16)
N4—Ag1—N2—Ag1A	−15.4 (5)	Ag1—N4—C44—C45	−95.43 (13)
N1—Ag1—N2—Ag1A	78.7 (5)	C43—N4—C44—C50	−142.90 (13)
N4—Ag1A—N2—C30	−103.1 (4)	Ag1A—N4—C44—C50	26.22 (17)
N1—Ag1A—N2—C30	8.72 (15)	Ag1—N4—C44—C50	28.34 (15)
N3—Ag1A—N2—C30	105.17 (19)	C50A—C44—C45—C46	21.7 (5)
N4—Ag1A—N2—C31	61.6 (4)	N4—C44—C45—C46	−179.86 (13)
N1—Ag1A—N2—C31	173.49 (11)	C50—C44—C45—C46	61.11 (17)
N3—Ag1A—N2—C31	−90.1 (2)	C44—C45—C46—C47	−76.13 (17)

N4—Ag1A—N2—Ag1	153.2 (8)	C45—C46—C47—C48A	61.1 (8)
N1—Ag1A—N2—Ag1	−95.0 (5)	C45—C46—C47—C48	82.50 (18)
N3—Ag1A—N2—Ag1	1.5 (4)	C48A—C47—C48—C49	82.3 (16)
N2—Ag1—N3—C38	−9.59 (16)	C46—C47—C48—C49	−34.4 (2)
N4—Ag1—N3—C38	−177.09 (11)	C47—C48—C49—C50	−38.3 (3)
N1—Ag1—N3—C38	82.93 (11)	C48—C49—C50—C44	82.40 (19)
N2—Ag1—N3—C42	175.25 (9)	C50A—C44—C50—C49	40.5 (7)
N4—Ag1—N3—C42	7.75 (9)	N4—C44—C50—C49	167.58 (13)
N1—Ag1—N3—C42	−92.23 (9)	C45—C44—C50—C49	−72.63 (17)
N2—Ag1—N3—Ag1A	177.5 (6)	N4—C44—C50A—C49A	−102.4 (7)
N4—Ag1—N3—Ag1A	10.0 (5)	C45—C44—C50A—C49A	52.4 (9)
N1—Ag1—N3—Ag1A	−90.0 (6)	C50—C44—C50A—C49A	−34.0 (5)
N4—Ag1A—N3—C38	−176.78 (13)	C44—C50A—C49A—C48A	−87.5 (12)
N2—Ag1A—N3—C38	−9.8 (3)	C46—C47—C48A—C49A	−31.6 (15)
N1—Ag1A—N3—C38	69.8 (2)	C48—C47—C48A—C49A	−106 (2)
N4—Ag1A—N3—C42	9.25 (12)	C50A—C49A—C48A—C47	54.7 (17)

Fig. 1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