

## Bis(6,6'-dimethyl-2,2'-dipyridyl- $\kappa^2 N,N'$ )-silver(I) tetrafluoridoborate

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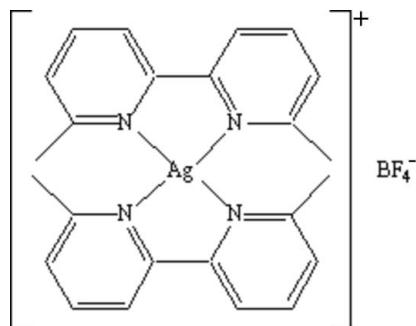
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Key indicators: single-crystal X-ray study;  $T = 110$  K; mean  $\sigma(C-C) = 0.003$  Å;  $R$  factor = 0.025;  $wR$  factor = 0.062; data-to-parameter ratio = 15.4.

In the title compound,  $[Ag(C_{12}H_{12}N_2)_2]BF_4$ , the  $Ag^I$  atom is four-coordinated by two chelating bipyridine groups; thus the crystal structure presents a 2:1 ligand-to-metal ratio. The angles around the metal center describe a distorted tetrahedral geometry, with the  $Ag-N$  distances falling in the range of reported values. The pyridyl rings of the bipyridine ligands are essentially coplanar with small twisting angles between the corresponding mean planes.

### Related literature

For background information, see: Newkome *et al.* (1981); Kaes *et al.* (2000). For related structures, see: Effendy *et al.* (2007); Di Nicola *et al.* (2007).



### Experimental

#### Crystal data

$[Ag(C_{12}H_{12}N_2)_2]BF_4$   
 $M_r = 563.15$

Monoclinic,  $P2_1/c$   
 $a = 12.3994$  (3) Å

$b = 21.8446$  (7) Å  
 $c = 8.8062$  (3) Å  
 $\beta = 98.260$  (1)°  
 $V = 2360.50$  (12) Å<sup>3</sup>  
 $Z = 4$

Mo  $K\alpha$  radiation  
 $\mu = 0.91$  mm<sup>-1</sup>  
 $T = 110$  (2) K  
 $0.30 \times 0.19 \times 0.18$  mm

#### Data collection

Bruker X8 APEX diffractometer  
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)  
 $T_{min} = 0.82$ ,  $T_{max} = 0.84$

26276 measured reflections  
4792 independent reflections  
4152 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.036$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.025$   
 $wR(F^2) = 0.062$   
 $S = 1.06$   
4792 reflections

311 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.39$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.27$  e Å<sup>-3</sup>

**Table 1**  
Selected geometric parameters (Å, °).

Ag1—N1	2.2779 (16)	Ag1—N3	2.3182 (17)
Ag1—N4	2.2939 (16)	Ag1—N2	2.3265 (16)
N1—Ag1—N4	131.17 (6)	N1—Ag1—N2	72.30 (6)
N1—Ag1—N3	136.17 (6)	N4—Ag1—N2	137.80 (6)
N4—Ag1—N3	72.67 (6)	N3—Ag1—N2	117.26 (6)

Data collection: *APEX2* (Bruker, 2003); cell refinement: *SAINT-Plus* (Bruker, 2003); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2000); software used to prepare material for publication: *SHELXTL*.

The Bruker X8 APEX diffractometer was purchased with funds received from the National Science Foundation Major Research Instrumentation Program Grant CHE-0321214. KK thanks the Robert A. Welch Foundation for support (AA-1508).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2455).

### References

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## **supplementary materials**

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## **Bis(6,6'-dimethyl-2,2'-dipyridyl- $\kappa^2N,N'$ )silver(I) tetrafluoridoborate**

**K. K. Klausmeyer, F. Hung-Low and A. Renz**

### **Comment**

Early reports of 2,2'-dipyridyl complexes with a variety of metals, such as Pd, Cu, Co, and Zn (Newkome *et al.*, 1981), have been accompanied by a considerable amount of work on the study the coordination chemistry of these and the related methyl-substituted dipyridyls (Kaes *et al.*, 2000). More recently, the study of these bipyridine ligands with silver salts has shown a predominant coordination form of the type  $[AgL_2]^+X^-$ , which form a five-membered ring that can stabilize different oxidation states of the silver center (I or II) (Effendy *et al.*, 2007; Di Nicola *et al.*, 2007). This is a common mode of binding for these bipyridine fragments, since they are almost universally chelating bidentate ligands by virtue of the close proximity of the aromatic rings. Additionally, it has been seen that the silver coordination environment parameters vary widely with respect to steric changes within the ligand, and external forces associated with the counterion, can affect the formation of close metal—metal interactions. Herein, we continue to enhance the library of silver coordination structures containing substituted bipyridine ligands, by reporting the formation of the title compound, formed by the reaction between the 6,6'-dimethyl-2,2'-dipyridyl ligand and the silver tetrafluoroborate salt, which presents a 2:1 ligand to metal ratio.

The title compound consists of two 6,6'-dimethyl-2,2'-dipyridyl ligands bound to the silver center in a chelating fashion, and the tetrafluoroborate is a non coordinating counteranion. According to the angles around the metal atom, a highly distorted tetrahedral geometry is described with values ranging between 72.30 (6) and 137.80 (6) $^\circ$ . The two pyridyl rings corresponding to the N1 and N2 atoms are nearly coplanar with a twist angle of 6.59 (12) $^\circ$  between the two mean planes. In contrast, the pyridyl rings of the second bipyridine ligand corresponding to N3 and N4, describe a larger angle with a value of 12.19 (10) $^\circ$ .

### **Experimental**

The title compound was obtained by mixing AgBF<sub>4</sub> (0.057 g, 0.3 mmol) and 6,6'-dimethyl-2,2'-dipyridyl (0.110 g, 0.6 mmol) in 10 ml of acetonitrile. The mixture was stirred for 10 min and the solvent removed in vacuo. Diffraction-quality crystals were obtained by slow diffusion of hexanes into a concentrated THF solution of the title compound in the presence of air.

### **Refinement**

All hydrogen atoms were included in calculated positions (C—H = 0.95–0.98 Å); isotropic displacement parameters were fixed [ $U_{iso}(H) = 1.2U_{eq}(C)$  or  $1.5U_{eq}(C)$  for methyl H atoms].

# supplementary materials

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## Figures

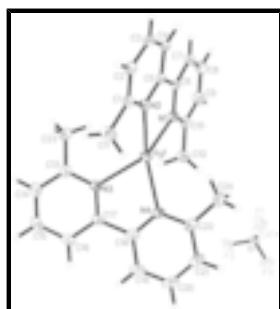


Fig. 1. The molecular structure with displacement ellipsoids drawn at the 50% probability level

### Bis(6,6'-dimethyl-2,2'-dipyridyl-κ<sup>2</sup>N,N')silver(I) tetrafluoridoborate

#### Crystal data

[Ag(C <sub>12</sub> H <sub>12</sub> N <sub>2</sub> ) <sub>2</sub> ]BF <sub>4</sub>	$F_{000} = 1136$
$M_r = 563.15$	$D_x = 1.585 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 12.3994 (3) \text{ \AA}$	Cell parameters from 9987 reflections
$b = 21.8446 (7) \text{ \AA}$	$\theta = 2.5\text{--}26.4^\circ$
$c = 8.8062 (3) \text{ \AA}$	$\mu = 0.91 \text{ mm}^{-1}$
$\beta = 98.260 (1)^\circ$	$T = 110 (2) \text{ K}$
$V = 2360.50 (12) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.30 \times 0.19 \times 0.18 \text{ mm}$

#### Data collection

Bruker X8 APEX diffractometer	4792 independent reflections
Radiation source: fine-focus sealed tube	4152 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.036$
$T = 110(2) \text{ K}$	$\theta_{\max} = 26.4^\circ$
$\varphi$ and $\omega$ scans	$\theta_{\min} = 2.5^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -15 \rightarrow 15$
$T_{\min} = 0.82$ , $T_{\max} = 0.84$	$k = -27 \rightarrow 27$
26276 measured reflections	$l = -10 \rightarrow 11$

#### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.025$	H-atom parameters constrained

$$wR(F^2) = 0.062 \quad w = 1/[\sigma^2(F_o^2) + (0.0265P)^2 + 1.4749P]$$

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

$S = 1.06$   $(\Delta/\sigma)_{\max} = 0.001$

4792 reflections  $\Delta\rho_{\max} = 0.39 \text{ e } \text{\AA}^{-3}$

311 parameters  $\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$

Primary atom site location: structure-invariant direct methods 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 ( $\text{\AA}^2$ )

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.295854 (12)	0.125477 (7)	0.418493 (18)	0.02106 (6)
F1	0.09472 (11)	0.90487 (6)	0.06840 (17)	0.0342 (3)
F2	0.17714 (13)	0.84781 (7)	-0.09586 (17)	0.0428 (4)
F3	0.27821 (12)	0.90684 (8)	0.0810 (2)	0.0592 (5)
F4	0.19308 (13)	0.82196 (7)	0.15473 (18)	0.0452 (4)
N1	0.15613 (13)	0.17466 (7)	0.50906 (19)	0.0175 (4)
N2	0.19705 (13)	0.05261 (7)	0.53331 (19)	0.0171 (3)
N3	0.34190 (13)	0.10206 (7)	0.1792 (2)	0.0177 (4)
N4	0.47489 (13)	0.15253 (7)	0.4213 (2)	0.0186 (4)
C1	0.22313 (16)	-0.00719 (9)	0.5434 (2)	0.0194 (4)
C2	0.16593 (17)	-0.04763 (9)	0.6240 (2)	0.0214 (4)
H2	0.1849	-0.0898	0.6300	0.026*
C3	0.08159 (16)	-0.02604 (9)	0.6950 (2)	0.0214 (4)
H3	0.0428	-0.0531	0.7520	0.026*
C4	0.05368 (16)	0.03523 (9)	0.6828 (2)	0.0185 (4)
H4	-0.0046	0.0509	0.7305	0.022*
C5	0.11300 (15)	0.07351 (9)	0.5988 (2)	0.0165 (4)
C6	0.08694 (16)	0.14045 (9)	0.5790 (2)	0.0168 (4)
C7	-0.00391 (17)	0.16596 (9)	0.6300 (3)	0.0228 (4)
H7	-0.0517	0.1412	0.6789	0.027*
C8	-0.02380 (18)	0.22776 (10)	0.6085 (3)	0.0280 (5)
H8	-0.0856	0.2460	0.6425	0.034*
C9	0.04698 (18)	0.26278 (9)	0.5372 (3)	0.0255 (5)
H9	0.0342	0.3053	0.5214	0.031*
C10	0.13704 (17)	0.23510 (9)	0.4890 (2)	0.0204 (4)

## supplementary materials

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C11	0.31664 (19)	-0.02794 (10)	0.4649 (3)	0.0293 (5)
H11A	0.2926	-0.0309	0.3542	0.044*
H11B	0.3419	-0.0681	0.5049	0.044*
H11C	0.3764	0.0017	0.4846	0.044*
C12	0.21919 (18)	0.27082 (10)	0.4151 (3)	0.0266 (5)
H12A	0.2877	0.2732	0.4858	0.040*
H12B	0.1914	0.3122	0.3911	0.040*
H12C	0.2320	0.2503	0.3204	0.040*
C13	0.27657 (17)	0.07079 (9)	0.0721 (2)	0.0205 (4)
C14	0.31471 (19)	0.04876 (10)	-0.0584 (3)	0.0273 (5)
H14	0.2676	0.0265	-0.1333	0.033*
C15	0.4210 (2)	0.05943 (11)	-0.0781 (3)	0.0310 (5)
H15	0.4477	0.0452	-0.1676	0.037*
C16	0.48874 (18)	0.09098 (10)	0.0333 (3)	0.0279 (5)
H16	0.5628	0.0982	0.0222	0.034*
C17	0.44696 (16)	0.11204 (9)	0.1617 (2)	0.0186 (4)
C18	0.51610 (16)	0.14505 (9)	0.2887 (3)	0.0197 (4)
C19	0.61894 (17)	0.16631 (9)	0.2710 (3)	0.0249 (5)
H19	0.6464	0.1609	0.1766	0.030*
C20	0.68081 (17)	0.19542 (9)	0.3929 (3)	0.0284 (5)
H20	0.7513	0.2105	0.3831	0.034*
C21	0.63940 (18)	0.20234 (9)	0.5283 (3)	0.0266 (5)
H21	0.6815	0.2217	0.6135	0.032*
C22	0.53476 (17)	0.18063 (9)	0.5400 (3)	0.0225 (4)
C23	0.16164 (18)	0.06009 (11)	0.0986 (3)	0.0279 (5)
H23A	0.1482	0.0819	0.1913	0.042*
H23B	0.1498	0.0162	0.1116	0.042*
H23C	0.1116	0.0752	0.0102	0.042*
C24	0.4858 (2)	0.18751 (11)	0.6843 (3)	0.0341 (6)
H24A	0.4538	0.2284	0.6876	0.051*
H24B	0.5425	0.1821	0.7730	0.051*
H24C	0.4289	0.1565	0.6870	0.051*
B1	0.1867 (2)	0.87055 (11)	0.0528 (3)	0.0250 (5)

### *Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.01884 (9)	0.02289 (9)	0.02368 (10)	-0.00269 (6)	0.01069 (7)	-0.00145 (6)
F1	0.0312 (7)	0.0307 (7)	0.0446 (9)	0.0100 (6)	0.0186 (6)	0.0062 (6)
F2	0.0560 (10)	0.0408 (8)	0.0372 (9)	-0.0060 (7)	0.0257 (8)	-0.0059 (7)
F3	0.0309 (8)	0.0673 (11)	0.0842 (14)	-0.0220 (8)	0.0245 (9)	-0.0222 (10)
F4	0.0465 (9)	0.0450 (9)	0.0466 (10)	0.0205 (7)	0.0147 (7)	0.0184 (7)
N1	0.0192 (8)	0.0179 (8)	0.0156 (9)	-0.0008 (7)	0.0032 (7)	-0.0009 (7)
N2	0.0175 (8)	0.0186 (8)	0.0158 (9)	0.0002 (6)	0.0048 (7)	-0.0008 (7)
N3	0.0184 (9)	0.0170 (8)	0.0184 (9)	0.0012 (7)	0.0050 (7)	0.0028 (7)
N4	0.0169 (8)	0.0165 (8)	0.0225 (10)	-0.0011 (6)	0.0035 (7)	0.0030 (7)
C1	0.0201 (10)	0.0198 (10)	0.0183 (11)	0.0011 (8)	0.0028 (8)	-0.0012 (8)
C2	0.0230 (11)	0.0176 (10)	0.0231 (12)	-0.0009 (8)	0.0020 (9)	0.0001 (8)

C3	0.0203 (10)	0.0226 (10)	0.0218 (11)	-0.0057 (8)	0.0043 (9)	0.0033 (8)
C4	0.0157 (10)	0.0237 (10)	0.0163 (10)	-0.0015 (8)	0.0033 (8)	-0.0005 (8)
C5	0.0160 (9)	0.0192 (10)	0.0141 (10)	-0.0010 (7)	0.0013 (8)	-0.0011 (8)
C6	0.0165 (9)	0.0189 (10)	0.0149 (10)	-0.0006 (7)	0.0019 (8)	-0.0027 (8)
C7	0.0219 (11)	0.0241 (11)	0.0239 (12)	0.0018 (8)	0.0083 (9)	-0.0005 (9)
C8	0.0253 (12)	0.0279 (12)	0.0317 (13)	0.0066 (9)	0.0077 (10)	-0.0017 (10)
C9	0.0295 (12)	0.0187 (10)	0.0285 (12)	0.0051 (9)	0.0049 (10)	0.0003 (9)
C10	0.0242 (11)	0.0179 (10)	0.0186 (11)	0.0001 (8)	0.0014 (9)	-0.0010 (8)
C11	0.0340 (13)	0.0225 (11)	0.0346 (13)	0.0065 (9)	0.0157 (11)	0.0046 (10)
C12	0.0290 (12)	0.0208 (10)	0.0313 (13)	-0.0005 (9)	0.0091 (10)	0.0030 (9)
C13	0.0229 (10)	0.0181 (10)	0.0201 (11)	0.0006 (8)	0.0016 (9)	0.0032 (8)
C14	0.0344 (13)	0.0262 (11)	0.0210 (12)	0.0018 (9)	0.0032 (10)	-0.0039 (9)
C15	0.0408 (14)	0.0336 (12)	0.0213 (12)	0.0066 (10)	0.0133 (11)	-0.0015 (10)
C16	0.0237 (11)	0.0327 (12)	0.0302 (13)	0.0025 (9)	0.0133 (10)	0.0022 (10)
C17	0.0192 (10)	0.0183 (10)	0.0195 (11)	0.0018 (8)	0.0074 (8)	0.0054 (8)
C18	0.0174 (10)	0.0145 (9)	0.0278 (12)	0.0023 (8)	0.0053 (9)	0.0051 (8)
C19	0.0186 (10)	0.0222 (11)	0.0355 (14)	0.0021 (8)	0.0099 (10)	0.0080 (9)
C20	0.0152 (10)	0.0199 (10)	0.0499 (16)	-0.0022 (8)	0.0041 (10)	0.0066 (10)
C21	0.0214 (11)	0.0176 (10)	0.0385 (14)	-0.0021 (8)	-0.0043 (10)	0.0005 (9)
C22	0.0246 (11)	0.0165 (10)	0.0253 (12)	-0.0022 (8)	0.0004 (9)	0.0017 (8)
C23	0.0217 (11)	0.0331 (12)	0.0282 (13)	-0.0039 (9)	0.0011 (10)	-0.0043 (10)
C24	0.0379 (14)	0.0364 (13)	0.0269 (13)	-0.0127 (11)	0.0014 (11)	-0.0061 (10)
B1	0.0215 (12)	0.0248 (13)	0.0318 (15)	0.0006 (9)	0.0143 (11)	-0.0005 (10)

*Geometric parameters (Å, °)*

Ag1—N1	2.2779 (16)	C9—H9	0.9500
Ag1—N4	2.2939 (16)	C10—C12	1.503 (3)
Ag1—N3	2.3182 (17)	C11—H11A	0.9800
Ag1—N2	2.3265 (16)	C11—H11B	0.9800
F1—B1	1.388 (3)	C11—H11C	0.9800
F2—B1	1.389 (3)	C12—H12A	0.9800
F3—B1	1.377 (3)	C12—H12B	0.9800
F4—B1	1.385 (3)	C12—H12C	0.9800
N1—C10	1.349 (3)	C13—C14	1.390 (3)
N1—C6	1.351 (3)	C13—C23	1.495 (3)
N2—C5	1.341 (2)	C14—C15	1.374 (3)
N2—C1	1.346 (3)	C14—H14	0.9500
N3—C13	1.339 (3)	C15—C16	1.380 (3)
N3—C17	1.351 (3)	C15—H15	0.9500
N4—C22	1.341 (3)	C16—C17	1.388 (3)
N4—C18	1.350 (3)	C16—H16	0.9500
C1—C2	1.390 (3)	C17—C18	1.493 (3)
C1—C11	1.502 (3)	C18—C19	1.387 (3)
C2—C3	1.376 (3)	C19—C20	1.381 (3)
C2—H2	0.9500	C19—H19	0.9500
C3—C4	1.383 (3)	C20—C21	1.372 (3)
C3—H3	0.9500	C20—H20	0.9500
C4—C5	1.394 (3)	C21—C22	1.399 (3)

## supplementary materials

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C4—H4	0.9500	C21—H21	0.9500
C5—C6	1.502 (3)	C22—C24	1.493 (3)
C6—C7	1.388 (3)	C23—H23A	0.9800
C7—C8	1.380 (3)	C23—H23B	0.9800
C7—H7	0.9500	C23—H23C	0.9800
C8—C9	1.381 (3)	C24—H24A	0.9800
C8—H8	0.9500	C24—H24B	0.9800
C9—C10	1.389 (3)	C24—H24C	0.9800
N1—Ag1—N4	131.17 (6)	C10—C12—H12A	109.5
N1—Ag1—N3	136.17 (6)	C10—C12—H12B	109.5
N4—Ag1—N3	72.67 (6)	H12A—C12—H12B	109.5
N1—Ag1—N2	72.30 (6)	C10—C12—H12C	109.5
N4—Ag1—N2	137.80 (6)	H12A—C12—H12C	109.5
N3—Ag1—N2	117.26 (6)	H12B—C12—H12C	109.5
C10—N1—C6	119.36 (17)	N3—C13—C14	121.04 (19)
C10—N1—Ag1	122.94 (13)	N3—C13—C23	117.64 (19)
C6—N1—Ag1	117.61 (12)	C14—C13—C23	121.3 (2)
C5—N2—C1	119.75 (17)	C15—C14—C13	119.5 (2)
C5—N2—Ag1	116.36 (12)	C15—C14—H14	120.3
C1—N2—Ag1	123.80 (13)	C13—C14—H14	120.3
C13—N3—C17	119.85 (18)	C14—C15—C16	119.5 (2)
C13—N3—Ag1	123.34 (13)	C14—C15—H15	120.3
C17—N3—Ag1	115.81 (13)	C16—C15—H15	120.3
C22—N4—C18	119.60 (17)	C15—C16—C17	118.9 (2)
C22—N4—Ag1	123.55 (14)	C15—C16—H16	120.5
C18—N4—Ag1	116.46 (13)	C17—C16—H16	120.5
N2—C1—C2	121.02 (19)	N3—C17—C16	121.2 (2)
N2—C1—C11	117.16 (18)	N3—C17—C18	116.86 (18)
C2—C1—C11	121.82 (18)	C16—C17—C18	121.92 (19)
C3—C2—C1	119.40 (19)	N4—C18—C19	121.7 (2)
C3—C2—H2	120.3	N4—C18—C17	117.26 (17)
C1—C2—H2	120.3	C19—C18—C17	121.1 (2)
C2—C3—C4	119.62 (19)	C20—C19—C18	119.0 (2)
C2—C3—H3	120.2	C20—C19—H19	120.5
C4—C3—H3	120.2	C18—C19—H19	120.5
C3—C4—C5	118.46 (18)	C21—C20—C19	119.4 (2)
C3—C4—H4	120.8	C21—C20—H20	120.3
C5—C4—H4	120.8	C19—C20—H20	120.3
N2—C5—C4	121.71 (18)	C20—C21—C22	119.6 (2)
N2—C5—C6	116.67 (17)	C20—C21—H21	120.2
C4—C5—C6	121.62 (17)	C22—C21—H21	120.2
N1—C6—C7	121.57 (18)	N4—C22—C21	120.9 (2)
N1—C6—C5	116.81 (17)	N4—C22—C24	117.56 (19)
C7—C6—C5	121.62 (18)	C21—C22—C24	121.6 (2)
C8—C7—C6	119.1 (2)	C13—C23—H23A	109.5
C8—C7—H7	120.5	C13—C23—H23B	109.5
C6—C7—H7	120.5	H23A—C23—H23B	109.5
C7—C8—C9	119.4 (2)	C13—C23—H23C	109.5
C7—C8—H8	120.3	H23A—C23—H23C	109.5

## supplementary materials

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C9—C8—H8	120.3	H23B—C23—H23C	109.5
C8—C9—C10	119.29 (19)	C22—C24—H24A	109.5
C8—C9—H9	120.4	C22—C24—H24B	109.5
C10—C9—H9	120.4	H24A—C24—H24B	109.5
N1—C10—C9	121.30 (19)	C22—C24—H24C	109.5
N1—C10—C12	116.61 (18)	H24A—C24—H24C	109.5
C9—C10—C12	122.07 (18)	H24B—C24—H24C	109.5
C1—C11—H11A	109.5	F3—B1—F4	110.8 (2)
C1—C11—H11B	109.5	F3—B1—F1	109.79 (19)
H11A—C11—H11B	109.5	F4—B1—F1	108.70 (18)
C1—C11—H11C	109.5	F3—B1—F2	109.43 (19)
H11A—C11—H11C	109.5	F4—B1—F2	109.03 (19)
H11B—C11—H11C	109.5	F1—B1—F2	109.0 (2)

## supplementary materials

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Fig. 1

