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# Bis[*N*′-(3-cyanobenzylidene)isonicotinohydrazide]silver(I) trifluoroacetate

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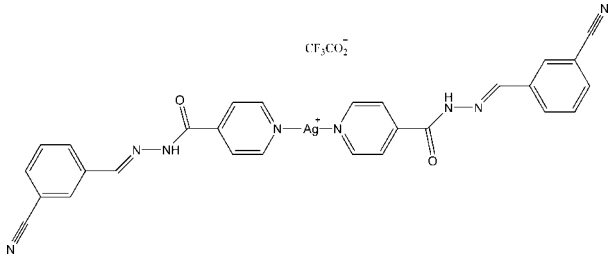
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.005 Å; disorder in solvent or counterion; $R$ factor = 0.046; $wR$ factor = 0.137; data-to-parameter ratio = 12.0.

In the title compound, $[Ag(C_{14}H_{10}N_4O)_2]CF_3CO_2$, the $Ag^I$ ion is coordinated by two N atoms of the pyridine rings of two *N*′-(3-cyanobenzylidene)isonicotinohydrazide ligands in a nearly linear geometry. In the crystal structure, a combination of close contacts formed *via* Ag···N interactions [Ag···N = 3.098 (2) and 3.261 (2) Å] from symmetry-related molecules and intermolecular N—H···O hydrogen bonds between $CF_3CO_2^-$ anions and the hydrazone groups of two ligands give rise to chains. Furthermore, there are Ag···O interactions with a separation of 2.765 (2) Å between chains. The F atoms of the $CF_3CO_2^-$ anion are disordered over two sites with refined occupancies of 0.593 (5) and 0.407 (5).

## Related literature

For related silver complexes, see: Dong *et al.* (2004); Niu *et al.* (2008, 2009); Sumby & Hardie (2005); Abu-Youssef *et al.* (2007); Zheng *et al.* (2003).




## Experimental

### Crystal data

$[Ag(C_{14}H_{10}N_4O)_2]C_2F_3O_2$
$M_r$ = 721.41
Triclinic, $P\overline{1}$
$a$ = 7.5345 (14) Å
$b$ = 13.744 (3) Å
$c$ = 14.098 (3) Å
$\alpha$ = 86.562 (3)°
$\beta$ = 88.126 (3)°
$\gamma$ = 83.792 (3)°
$V$ = 1448.2 (5) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.77 mm$^{-1}$
$T$ = 173 K
0.32 × 0.22 × 0.17 mm

### Data collection

Bruker APEXII CCD detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.791, $T_{max}$ = 0.881
8015 measured reflections
5306 independent reflections
4046 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.137
$S$ = 1.03
5306 reflections
443 parameters
48 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.95 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.83 e Å$^{-3}$

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

| | | | |
|---|---|---|---|
| Ag1—N5 | 2.143 (3) | Ag1—N1 | 2.147 (3) |
| N5—Ag1—N1 | 174.20 (11) | | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H40···O4$^{i}$ | 0.88 | 1.93 | 2.805 (4) | 172 |
| N6—H39···O3$^{ii}$ | 0.90 | 2.13 | 2.936 (4) | 149 |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXL97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 2005); software used to prepare material for publication: *SHELXL97*.

We are grateful to Mrs Li (Wuhan University) for her assistance with the X-ray crystallographic analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2867).

## References

Abu-Youssef, M. A. M., Dey, R., Gohar, Y., Massoud, A. A., Ohrstrom, L. & Langer, V. (2007). *Inorg. Chem.*. **46**, 5893–5903.
Brandenburg, K. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2002). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Dong, Y.-B., Zhao, X. & Huang, R.-Q. (2004). *Inorg. Chem.* **43**, 5603–5612.
Niu, C.-Y., Wu, B.-L., Zheng, X.-F., Wan, X.-S., Zhang, H.-Y., Niu, Y.-Y. & Meng, L.-Y. (2009). *CrystEngComm*, **11**, 1373–1382.
Niu, C.-Y., Zheng, X.-F., Bai, L.-L., Wu, X.-L. & Kou, C.-H. (2008). *Acta Cryst.* C**64**, m305–m307.
Sheldrick, G. M. (1996). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1994). *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Sumby, C. J. & Hardie, M. J. (2005). *Angew. Chem. Int. Ed.* **44**, 6395–6399.
Zheng, Y., Du, M., Li, J.-R., Zhang, R.-H. & Bu, X.-H. (2003). *Dalton Trans.* pp. 1509–1514.

# supporting information

*Acta Cryst.* (2009). E**65**, m1029 [doi:10.1107/S1600536809029183]

## Bis[*N*′-(3-cyanobenzylidene)isonicotinohydrazide]silver(I) trifluoroacetate

**Cao-Yuan Niu, Hai-Yan Zhang, Yu-Li Dang and Chun-Hong Kou**

### S1. Comment

Silver coordination complexes with pyridyl organic ligands are of great interests for their utilities in fluorescent materials and antibiotic aspects (Dong *et al.*, 2004; Abu-Youssef, *et al.*, 2007). In the title compound, (I), the central $Ag^{I}$ ion is coordinated by two nitrogen atoms from two pyridine rings of two different ligands, defining a slightly distorted linear coordination geometry (Fig. 1). Coordinating bond distances and angle around metal center are shown in Table 1. In the crystal structure, there are N—H···O hydrogen bonds between the hydrazone groups of 3-cyanobenzylidene isonicotinohydrazide ligands and $CF_3CO_2^-$ anions (Table 2). In addition, there are weak Ag···N interactions between two neighbouring silver monomers with separations of 3.098 (2) and 3.261 (2) Å and Ag···O interactions between two neighbouring silver monomers with separations of 2.765 (2) Å. Hydrogen bonds and Ag···N interactions link parallel silver monomers together to construct one-dimensional chains (Fig. 2) and Ag···O interactions contribute to the three-dimensional structure.

### S2. Experimental

A solution of $AgCF_3CO_2$ (0.022 g, 0.1 mmol) in $CH_3OH$ (10 ml) was carefully layered on a $CH_3OH/CHCl_3$ solution (5 ml/10 ml) of 3-Cyanobenzylidene isonicotinohydrazide (0.025 g, 0.1 mmol) in a straight glass tube. About ten days later, colourless single crystals suitable for X-ray analysis were obtained (yield about 43%).

### S3. Refinement

C-bound H atoms were placed in calculated positions and refined using a riding model [C—H = 0.95 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C)]. The N-bound H atoms were first introduced in calculated positions and refined freely with $U_{iso}$(H) = 1.2$U_{eq}$(carrier N). Three F atoms (F1—F3) of the trifluoroacetate anion are disordered over two positions, with maximum and minimum occupancies of 0.593 (5) and 0.407 (5), respectively. All C—F bond lengths were restrained to 1.26 (2) Å. Restraints of displacement parameters for three F or disordered F atoms were also performed. The final difference Fourier map had a highest peak at 0.96 Å from atom Ag1 and a deepest hole at 0.96 Å from atom Ag1, but were otherwise featureless.

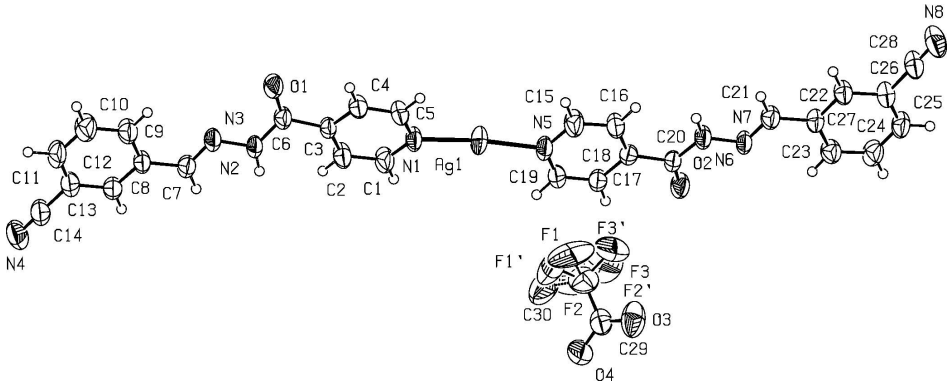



**Figure 1**

The asymmetric unit of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. In the anion, the dashed lines indicate the minor component of disorder.

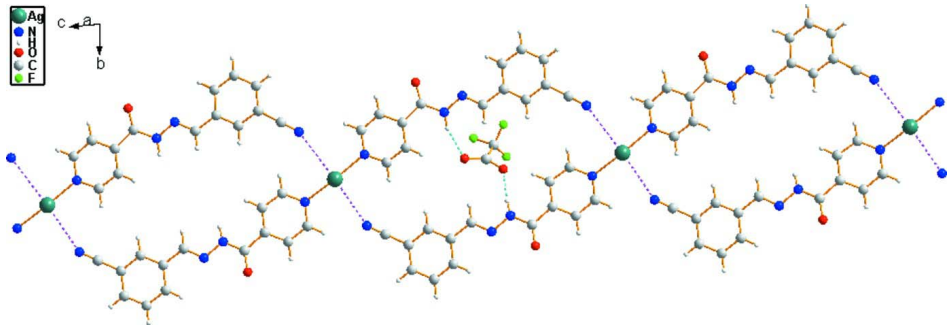



**Figure 2**

Part of the the one-dimensional chain formed *via* intermolecular hydrogen bonds indicated by green dashed lines and Ag···N interactions indicated by pink dashed lines.

**Bis[*N*′-(3-cyanobenzylidene)isonicotinohydrazide]silver(I) trifluoroacetate**

*Crystal data*

$[Ag(C_{14}H_{10}N_4O)_2]C_2F_3O_2$
$M_r = 721.41$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5345\ (14)$ Å
$b = 13.744\ (3)$ Å
$c = 14.098\ (3)$ Å
$\alpha = 86.562\ (3)°$
$\beta = 88.126\ (3)°$
$\gamma = 83.792\ (3)°$
$V = 1448.2\ (5)$ Å$^3$
$Z = 2$
$F(000) = 724$
$D_x = 1.654$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2885 reflections
$\theta = 2.1–25.5°$
$\mu = 0.77$ mm$^{-1}$
$T = 173$ K
Needle, yellow
0.32 × 0.22 × 0.17 mm

*Data collection*

Bruker APEXII CCD detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.791$, $T_{max} = 0.881$
8015 measured reflections
5306 independent reflections
4046 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.025
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.1°
$h$ = −9→9
$k$ = −16→16
$l$ = −8→17

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.137
$S$ = 1.03
5306 reflections
443 parameters
48 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
$w = 1/[\sigma^2(F_o^2) + (0.0871P)^2 + 0.05P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.95 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.83 e Å$^{-3}$

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Ag1 | 0.07174 (4) | 0.80139 (2) | 0.31966 (2) | 0.07153 (17) | |
| N1 | 0.1905 (4) | 0.8820 (2) | 0.4222 (2) | 0.0511 (7) | |
| N2 | 0.4458 (4) | 1.0110 (2) | 0.71224 (19) | 0.0467 (6) | |
| H40 | 0.4975 | 0.9505 | 0.7165 | 0.056* | |
| N3 | 0.4965 (4) | 1.0684 (2) | 0.78081 (19) | 0.0499 (7) | |
| N4 | 0.9740 (5) | 0.9994 (3) | 1.2069 (2) | 0.0771 (10) | |
| N5 | −0.0205 (4) | 0.7130 (2) | 0.2151 (2) | 0.0542 (7) | |
| N6 | −0.3086 (4) | 0.5740 (2) | −0.06091 (19) | 0.0499 (7) | |
| H39 | −0.3230 | 0.6397 | −0.0717 | 0.060* | |
| N7 | −0.3701 (4) | 0.5149 (2) | −0.12433 (19) | 0.0473 (6) | |
| N8 | −0.8578 (6) | 0.5997 (3) | −0.5468 (3) | 0.0829 (11) | |
| O1 | 0.2840 (4) | 1.14121 (17) | 0.63867 (18) | 0.0630 (7) | |
| O2 | −0.2138 (4) | 0.44400 (17) | 0.03838 (17) | 0.0601 (6) | |
| O3 | 0.2518 (5) | 0.2337 (2) | 0.1519 (2) | 0.0957 (11) | |
| O4 | 0.3698 (5) | 0.1775 (2) | 0.2890 (2) | 0.0950 (11) | |
| C1 | 0.2540 (6) | 0.8390 (3) | 0.5037 (3) | 0.0623 (10) | |
| H28 | 0.2629 | 0.7695 | 0.5111 | 0.075* | |
| C2 | 0.3069 (5) | 0.8889 (3) | 0.5766 (3) | 0.0577 (9) | |
| H29 | 0.3509 | 0.8547 | 0.6331 | 0.069* | |
| C3 | 0.2955 (4) | 0.9898 (2) | 0.5673 (2) | 0.0413 (7) | |
| C4 | 0.2324 (4) | 1.0347 (2) | 0.4829 (2) | 0.0480 (8) | |
| H30 | 0.2240 | 1.1040 | 0.4733 | 0.058* | |

| | | | | | |
|---|---|---|---|---|---|
| C5 | 0.1822 (4) | 0.9791 (3) | 0.4135 (2) | 0.0492 (8) | |
| H31 | 0.1392 | 1.0115 | 0.3560 | 0.059* | |
| C6 | 0.3404 (4) | 1.0549 (2) | 0.6427 (2) | 0.0470 (8) | |
| C7 | 0.5898 (4) | 1.0245 (3) | 0.8475 (2) | 0.0488 (8) | |
| H32 | 0.6173 | 0.9553 | 0.8495 | 0.059* | |
| C8 | 0.6539 (4) | 1.0815 (2) | 0.9204 (2) | 0.0461 (7) | |
| C9 | 0.6270 (5) | 1.1842 (3) | 0.9143 (3) | 0.0606 (10) | |
| H33 | 0.5639 | 1.2171 | 0.8623 | 0.073* | |
| C10 | 0.6902 (6) | 1.2380 (3) | 0.9820 (3) | 0.0748 (12) | |
| H34 | 0.6709 | 1.3075 | 0.9768 | 0.090* | |
| C11 | 0.7812 (6) | 1.1916 (3) | 1.0576 (3) | 0.0672 (11) | |
| H35 | 0.8269 | 1.2289 | 1.1040 | 0.081* | |
| C12 | 0.8062 (5) | 1.0904 (3) | 1.0659 (3) | 0.0545 (9) | |
| C13 | 0.7428 (5) | 1.0354 (3) | 0.9974 (2) | 0.0481 (8) | |
| H36 | 0.7606 | 0.9658 | 1.0037 | 0.058* | |
| C14 | 0.9005 (5) | 1.0402 (3) | 1.1449 (3) | 0.0603 (9) | |
| C15 | −0.1106 (6) | 0.7536 (3) | 0.1400 (3) | 0.0700 (11) | |
| H22 | −0.1284 | 0.8231 | 0.1327 | 0.084* | |
| C16 | −0.1786 (5) | 0.7013 (3) | 0.0732 (3) | 0.0590 (9) | |
| H21 | −0.2389 | 0.7340 | 0.0203 | 0.071* | |
| C17 | −0.1585 (4) | 0.6002 (2) | 0.0834 (2) | 0.0417 (7) | |
| C18 | −0.0668 (5) | 0.5584 (2) | 0.1616 (2) | 0.0499 (8) | |
| H20 | −0.0499 | 0.4890 | 0.1715 | 0.060* | |
| C19 | −0.0005 (5) | 0.6156 (3) | 0.2244 (2) | 0.0530 (8) | |
| H19 | 0.0627 | 0.5847 | 0.2772 | 0.064* | |
| C20 | −0.2274 (4) | 0.5316 (2) | 0.0187 (2) | 0.0442 (7) | |
| C21 | −0.4550 (5) | 0.5585 (3) | −0.1937 (2) | 0.0508 (8) | |
| H23 | −0.4746 | 0.6280 | −0.1976 | 0.061* | |
| C22 | −0.5228 (4) | 0.5035 (2) | −0.2675 (2) | 0.0461 (7) | |
| C23 | −0.4960 (5) | 0.4015 (3) | −0.2652 (3) | 0.0542 (9) | |
| H24 | −0.4279 | 0.3667 | −0.2161 | 0.065* | |
| C24 | −0.5667 (6) | 0.3510 (3) | −0.3331 (3) | 0.0628 (10) | |
| H25 | −0.5495 | 0.2813 | −0.3297 | 0.075* | |
| C25 | −0.6625 (5) | 0.3998 (3) | −0.4062 (3) | 0.0591 (9) | |
| H26 | −0.7109 | 0.3643 | −0.4532 | 0.071* | |
| C26 | −0.6874 (5) | 0.5011 (3) | −0.4105 (2) | 0.0533 (8) | |
| C27 | −0.6184 (5) | 0.5528 (3) | −0.3409 (2) | 0.0510 (8) | |
| H27 | −0.6372 | 0.6224 | −0.3438 | 0.061* | |
| C28 | −0.7845 (5) | 0.5554 (3) | −0.4867 (3) | 0.0626 (10) | |
| C29 | 0.2595 (5) | 0.2239 (3) | 0.2380 (3) | 0.0611 (10) | |
| C30 | 0.1058 (7) | 0.2780 (3) | 0.2934 (4) | 0.0814 (13) | |
| F1 | 0.1449 (15) | 0.3562 (8) | 0.3268 (9) | 0.132 (5) | 0.593 (15) |
| F2 | 0.0334 (14) | 0.2268 (7) | 0.3564 (11) | 0.156 (6) | 0.593 (15) |
| F3 | −0.0247 (13) | 0.3127 (8) | 0.2334 (8) | 0.144 (5) | 0.593 (15) |
| F1′ | 0.141 (3) | 0.2689 (11) | 0.3907 (7) | 0.145 (6) | 0.407 (15) |
| F2′ | −0.0425 (19) | 0.2452 (15) | 0.2912 (13) | 0.153 (7) | 0.407 (15) |
| F3′ | 0.093 (2) | 0.3702 (7) | 0.2843 (13) | 0.132 (7) | 0.407 (15) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ag1 | 0.0812 (3) | 0.0767 (3) | 0.0630 (2) | −0.01527 (17) | −0.01994 (17) | −0.03412 (17) |
| N1 | 0.0622 (17) | 0.0518 (17) | 0.0435 (16) | −0.0139 (13) | −0.0157 (13) | −0.0136 (12) |
| N2 | 0.0567 (15) | 0.0441 (15) | 0.0412 (15) | −0.0050 (12) | −0.0149 (12) | −0.0128 (11) |
| N3 | 0.0594 (16) | 0.0477 (16) | 0.0452 (16) | −0.0078 (13) | −0.0152 (13) | −0.0137 (12) |
| N4 | 0.079 (2) | 0.103 (3) | 0.050 (2) | −0.011 (2) | −0.0193 (18) | −0.0021 (19) |
| N5 | 0.0699 (18) | 0.0492 (18) | 0.0460 (16) | −0.0064 (14) | −0.0174 (14) | −0.0158 (13) |
| N6 | 0.0672 (17) | 0.0418 (15) | 0.0435 (15) | −0.0091 (13) | −0.0175 (13) | −0.0097 (12) |
| N7 | 0.0606 (16) | 0.0450 (15) | 0.0390 (15) | −0.0093 (12) | −0.0137 (13) | −0.0115 (12) |
| N8 | 0.103 (3) | 0.089 (3) | 0.061 (2) | −0.019 (2) | −0.037 (2) | 0.003 (2) |
| O1 | 0.0821 (17) | 0.0408 (14) | 0.0686 (17) | −0.0027 (12) | −0.0307 (13) | −0.0155 (11) |
| O2 | 0.0886 (18) | 0.0389 (14) | 0.0550 (15) | −0.0067 (12) | −0.0241 (13) | −0.0092 (10) |
| O3 | 0.162 (3) | 0.074 (2) | 0.0531 (18) | −0.024 (2) | −0.0202 (19) | 0.0046 (15) |
| O4 | 0.110 (2) | 0.078 (2) | 0.093 (2) | 0.0287 (18) | −0.046 (2) | −0.0184 (17) |
| C1 | 0.085 (3) | 0.042 (2) | 0.064 (2) | −0.0097 (18) | −0.029 (2) | −0.0104 (17) |
| C2 | 0.084 (2) | 0.0413 (19) | 0.051 (2) | −0.0106 (17) | −0.0296 (18) | −0.0026 (15) |
| C3 | 0.0457 (16) | 0.0413 (17) | 0.0390 (16) | −0.0081 (13) | −0.0106 (13) | −0.0088 (13) |
| C4 | 0.0597 (19) | 0.0429 (18) | 0.0431 (18) | −0.0100 (15) | −0.0137 (15) | −0.0017 (14) |
| C5 | 0.0581 (19) | 0.054 (2) | 0.0377 (17) | −0.0124 (16) | −0.0144 (15) | −0.0001 (14) |
| C6 | 0.0553 (18) | 0.0424 (19) | 0.0459 (19) | −0.0102 (15) | −0.0130 (15) | −0.0101 (14) |
| C7 | 0.0591 (19) | 0.0445 (19) | 0.0445 (18) | −0.0062 (15) | −0.0095 (15) | −0.0106 (14) |
| C8 | 0.0538 (18) | 0.0478 (19) | 0.0389 (17) | −0.0095 (14) | −0.0117 (14) | −0.0084 (14) |
| C9 | 0.081 (3) | 0.045 (2) | 0.057 (2) | −0.0056 (17) | −0.0252 (19) | −0.0060 (16) |
| C10 | 0.099 (3) | 0.047 (2) | 0.082 (3) | −0.012 (2) | −0.032 (2) | −0.0144 (19) |
| C11 | 0.081 (3) | 0.061 (3) | 0.065 (3) | −0.016 (2) | −0.023 (2) | −0.0222 (19) |
| C12 | 0.058 (2) | 0.066 (2) | 0.0423 (19) | −0.0110 (17) | −0.0096 (16) | −0.0090 (16) |
| C13 | 0.0570 (19) | 0.0456 (19) | 0.0430 (18) | −0.0064 (15) | −0.0093 (15) | −0.0058 (14) |
| C14 | 0.062 (2) | 0.076 (3) | 0.046 (2) | −0.0118 (19) | −0.0089 (18) | −0.0125 (18) |
| C15 | 0.106 (3) | 0.041 (2) | 0.066 (2) | −0.008 (2) | −0.035 (2) | −0.0093 (17) |
| C16 | 0.087 (3) | 0.0405 (19) | 0.051 (2) | −0.0024 (17) | −0.0313 (19) | −0.0053 (15) |
| C17 | 0.0482 (17) | 0.0408 (17) | 0.0362 (16) | −0.0028 (13) | −0.0035 (13) | −0.0059 (13) |
| C18 | 0.068 (2) | 0.0406 (18) | 0.0413 (18) | 0.0011 (15) | −0.0147 (15) | −0.0067 (14) |
| C19 | 0.062 (2) | 0.056 (2) | 0.0422 (18) | −0.0019 (16) | −0.0168 (15) | −0.0095 (15) |
| C20 | 0.0528 (18) | 0.0416 (19) | 0.0394 (17) | −0.0034 (14) | −0.0096 (14) | −0.0105 (13) |
| C21 | 0.064 (2) | 0.0436 (19) | 0.047 (2) | −0.0095 (15) | −0.0115 (16) | −0.0071 (15) |
| C22 | 0.0551 (18) | 0.0457 (19) | 0.0403 (17) | −0.0137 (15) | −0.0080 (14) | −0.0072 (14) |
| C23 | 0.065 (2) | 0.046 (2) | 0.054 (2) | −0.0105 (16) | −0.0137 (17) | −0.0035 (15) |
| C24 | 0.077 (2) | 0.047 (2) | 0.068 (3) | −0.0150 (18) | −0.013 (2) | −0.0151 (17) |
| C25 | 0.071 (2) | 0.057 (2) | 0.054 (2) | −0.0169 (18) | −0.0123 (18) | −0.0179 (17) |
| C26 | 0.059 (2) | 0.061 (2) | 0.0434 (19) | −0.0170 (17) | −0.0117 (15) | −0.0073 (16) |
| C27 | 0.064 (2) | 0.0462 (19) | 0.0454 (19) | −0.0128 (16) | −0.0148 (16) | −0.0039 (14) |
| C28 | 0.077 (2) | 0.064 (2) | 0.052 (2) | −0.019 (2) | −0.0222 (19) | −0.0061 (18) |
| C29 | 0.086 (3) | 0.0379 (19) | 0.061 (2) | −0.0105 (18) | −0.021 (2) | 0.0021 (16) |
| C30 | 0.094 (3) | 0.052 (3) | 0.095 (4) | −0.002 (2) | −0.009 (3) | 0.010 (3) |
| F1 | 0.149 (7) | 0.122 (9) | 0.135 (8) | −0.021 (6) | 0.023 (6) | −0.076 (7) |
| F2 | 0.131 (7) | 0.126 (7) | 0.189 (11) | 0.019 (5) | 0.075 (7) | 0.075 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| F3 | 0.124 (6) | 0.121 (7) | 0.180 (8) | 0.056 (5) | −0.066 (6) | −0.036 (6) |
| F1′ | 0.234 (14) | 0.121 (10) | 0.067 (5) | 0.047 (9) | −0.009 (7) | −0.023 (6) |
| F2′ | 0.114 (8) | 0.184 (15) | 0.171 (13) | −0.061 (9) | 0.031 (8) | −0.029 (11) |
| F3′ | 0.171 (12) | 0.037 (5) | 0.168 (13) | 0.038 (6) | 0.048 (9) | 0.032 (7) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ag1—N5 | 2.143 (3) | C9—C10 | 1.369 (5) |
| Ag1—N1 | 2.147 (3) | C9—H33 | 0.9500 |
| N1—C5 | 1.327 (4) | C10—C11 | 1.372 (6) |
| N1—C1 | 1.338 (5) | C10—H34 | 0.9500 |
| N2—C6 | 1.353 (4) | C11—C12 | 1.381 (6) |
| N2—N3 | 1.372 (4) | C11—H35 | 0.9500 |
| N2—H40 | 0.8793 | C12—C13 | 1.388 (5) |
| N3—C7 | 1.275 (4) | C12—C14 | 1.440 (6) |
| N4—C14 | 1.136 (5) | C13—H36 | 0.9500 |
| N5—C19 | 1.330 (5) | C15—C16 | 1.363 (5) |
| N5—C15 | 1.338 (5) | C15—H22 | 0.9500 |
| N6—C20 | 1.364 (4) | C16—C17 | 1.381 (5) |
| N6—N7 | 1.367 (4) | C16—H21 | 0.9500 |
| N6—H39 | 0.9025 | C17—C18 | 1.383 (4) |
| N7—C21 | 1.270 (4) | C17—C20 | 1.493 (4) |
| N8—C28 | 1.135 (5) | C18—C19 | 1.360 (5) |
| O1—C6 | 1.215 (4) | C18—H20 | 0.9500 |
| O2—C20 | 1.214 (4) | C19—H19 | 0.9500 |
| O3—C29 | 1.216 (4) | C21—C22 | 1.458 (5) |
| O4—C29 | 1.218 (4) | C21—H23 | 0.9500 |
| C1—C2 | 1.363 (5) | C22—C27 | 1.381 (5) |
| C1—H28 | 0.9500 | C22—C23 | 1.393 (5) |
| C2—C3 | 1.378 (5) | C23—C24 | 1.369 (5) |
| C2—H29 | 0.9500 | C23—H24 | 0.9500 |
| C3—C4 | 1.381 (4) | C24—C25 | 1.376 (5) |
| C3—C6 | 1.500 (4) | C24—H25 | 0.9500 |
| C4—C5 | 1.365 (5) | C25—C26 | 1.382 (5) |
| C4—H30 | 0.9500 | C25—H26 | 0.9500 |
| C5—H31 | 0.9500 | C26—C27 | 1.391 (5) |
| C7—C8 | 1.454 (4) | C26—C28 | 1.443 (5) |
| C7—H32 | 0.9500 | C27—H27 | 0.9500 |
| C8—C13 | 1.380 (5) | C29—C30 | 1.526 (7) |
| C8—C9 | 1.402 (5) | | |
| | | | |
| N5—Ag1—N1 | 174.20 (11) | C11—C12—C14 | 120.6 (3) |
| C5—N1—C1 | 116.6 (3) | C13—C12—C14 | 118.9 (3) |
| C5—N1—Ag1 | 121.0 (2) | C8—C13—C12 | 120.1 (3) |
| C1—N1—Ag1 | 121.8 (2) | C8—C13—H36 | 119.9 |
| C6—N2—N3 | 117.8 (3) | C12—C13—H36 | 119.9 |
| C6—N2—H40 | 128.2 | N4—C14—C12 | 179.0 (5) |
| N3—N2—H40 | 113.6 | N5—C15—C16 | 123.9 (3) |

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| C7—N3—N2 | 116.5 (3) | N5—C15—H22 | 118.0 |
| C19—N5—C15 | 116.7 (3) | C16—C15—H22 | 118.0 |
| C19—N5—Ag1 | 121.9 (2) | C15—C16—C17 | 119.2 (3) |
| C15—N5—Ag1 | 121.2 (2) | C15—C16—H21 | 120.4 |
| C20—N6—N7 | 118.7 (3) | C17—C16—H21 | 120.4 |
| C20—N6—H39 | 121.2 | C16—C17—C18 | 116.8 (3) |
| N7—N6—H39 | 120.1 | C16—C17—C20 | 126.4 (3) |
| C21—N7—N6 | 115.9 (3) | C18—C17—C20 | 116.8 (3) |
| N1—C1—C2 | 123.9 (3) | C19—C18—C17 | 120.6 (3) |
| N1—C1—H28 | 118.0 | C19—C18—H20 | 119.7 |
| C2—C1—H28 | 118.0 | C17—C18—H20 | 119.7 |
| C1—C2—C3 | 119.0 (3) | N5—C19—C18 | 122.8 (3) |
| C1—C2—H29 | 120.5 | N5—C19—H19 | 118.6 |
| C3—C2—H29 | 120.5 | C18—C19—H19 | 118.6 |
| C2—C3—C4 | 117.5 (3) | O2—C20—N6 | 123.2 (3) |
| C2—C3—C6 | 125.2 (3) | O2—C20—C17 | 120.8 (3) |
| C4—C3—C6 | 117.3 (3) | N6—C20—C17 | 115.9 (3) |
| C5—C4—C3 | 119.7 (3) | N7—C21—C22 | 121.1 (3) |
| C5—C4—H30 | 120.1 | N7—C21—H23 | 119.5 |
| C3—C4—H30 | 120.1 | C22—C21—H23 | 119.5 |
| N1—C5—C4 | 123.3 (3) | C27—C22—C23 | 118.7 (3) |
| N1—C5—H31 | 118.4 | C27—C22—C21 | 119.8 (3) |
| C4—C5—H31 | 118.4 | C23—C22—C21 | 121.5 (3) |
| O1—C6—N2 | 124.1 (3) | C24—C23—C22 | 120.7 (3) |
| O1—C6—C3 | 120.2 (3) | C24—C23—H24 | 119.6 |
| N2—C6—C3 | 115.6 (3) | C22—C23—H24 | 119.6 |
| N3—C7—C8 | 119.3 (3) | C23—C24—C25 | 120.8 (3) |
| N3—C7—H32 | 120.4 | C23—C24—H25 | 119.6 |
| C8—C7—H32 | 120.4 | C25—C24—H25 | 119.6 |
| C13—C8—C9 | 118.5 (3) | C24—C25—C26 | 119.3 (3) |
| C13—C8—C7 | 120.5 (3) | C24—C25—H26 | 120.4 |
| C9—C8—C7 | 121.0 (3) | C26—C25—H26 | 120.4 |
| C10—C9—C8 | 121.0 (3) | C25—C26—C27 | 120.2 (3) |
| C10—C9—H33 | 119.5 | C25—C26—C28 | 121.2 (3) |
| C8—C9—H33 | 119.5 | C27—C26—C28 | 118.6 (3) |
| C9—C10—C11 | 120.1 (4) | C22—C27—C26 | 120.3 (3) |
| C9—C10—H34 | 119.9 | C22—C27—H27 | 119.8 |
| C11—C10—H34 | 119.9 | C26—C27—H27 | 119.8 |
| C10—C11—C12 | 119.8 (3) | N8—C28—C26 | 178.3 (4) |
| C10—C11—H35 | 120.1 | O3—C29—O4 | 131.0 (4) |
| C12—C11—H35 | 120.1 | O3—C29—C30 | 115.8 (4) |
| C11—C12—C13 | 120.5 (3) | O4—C29—C30 | 113.3 (4) |

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|---|---|---|---|
| N5—Ag1—N1—C5 | 122.8 (10) | C14—C12—C13—C8 | −179.2 (3) |
| N5—Ag1—N1—C1 | −66.4 (11) | C11—C12—C14—N4 | 166 (27) |
| C6—N2—N3—C7 | 177.3 (3) | C13—C12—C14—N4 | −15 (28) |
| N1—Ag1—N5—C19 | 56.5 (11) | C19—N5—C15—C16 | −1.2 (7) |
| N1—Ag1—N5—C15 | −127.5 (10) | Ag1—N5—C15—C16 | −177.4 (4) |

| | | | |
|---|---|---|---|
| C20—N6—N7—C21 | 175.5 (3) | N5—C15—C16—C17 | 1.6 (7) |
| C5—N1—C1—C2 | 1.0 (6) | C15—C16—C17—C18 | −0.9 (6) |
| Ag1—N1—C1—C2 | −170.2 (3) | C15—C16—C17—C20 | 178.6 (4) |
| N1—C1—C2—C3 | −0.1 (7) | C16—C17—C18—C19 | −0.1 (5) |
| C1—C2—C3—C4 | −0.8 (6) | C20—C17—C18—C19 | −179.6 (3) |
| C1—C2—C3—C6 | 177.1 (4) | C15—N5—C19—C18 | 0.1 (5) |
| C2—C3—C4—C5 | 0.9 (5) | Ag1—N5—C19—C18 | 176.3 (3) |
| C6—C3—C4—C5 | −177.2 (3) | C17—C18—C19—N5 | 0.5 (6) |
| C1—N1—C5—C4 | −0.9 (5) | N7—N6—C20—O2 | −3.4 (5) |
| Ag1—N1—C5—C4 | 170.4 (3) | N7—N6—C20—C17 | 178.2 (3) |
| C3—C4—C5—N1 | 0.0 (5) | C16—C17—C20—O2 | −174.3 (4) |
| N3—N2—C6—O1 | −2.0 (5) | C18—C17—C20—O2 | 5.1 (5) |
| N3—N2—C6—C3 | 177.5 (3) | C16—C17—C20—N6 | 4.1 (5) |
| C2—C3—C6—O1 | −160.7 (4) | C18—C17—C20—N6 | −176.4 (3) |
| C4—C3—C6—O1 | 17.1 (5) | N6—N7—C21—C22 | 178.3 (3) |
| C2—C3—C6—N2 | 19.7 (5) | N7—C21—C22—C27 | 178.4 (3) |
| C4—C3—C6—N2 | −162.4 (3) | N7—C21—C22—C23 | −0.6 (5) |
| N2—N3—C7—C8 | 177.6 (3) | C27—C22—C23—C24 | −1.6 (5) |
| N3—C7—C8—C13 | 174.7 (3) | C21—C22—C23—C24 | 177.4 (3) |
| N3—C7—C8—C9 | −5.2 (5) | C22—C23—C24—C25 | 1.5 (6) |
| C13—C8—C9—C10 | 1.2 (6) | C23—C24—C25—C26 | −0.2 (6) |
| C7—C8—C9—C10 | −178.8 (4) | C24—C25—C26—C27 | −0.9 (6) |
| C8—C9—C10—C11 | −0.1 (7) | C24—C25—C26—C28 | 179.1 (4) |
| C9—C10—C11—C12 | −1.1 (7) | C23—C22—C27—C26 | 0.5 (5) |
| C10—C11—C12—C13 | 1.2 (6) | C21—C22—C27—C26 | −178.6 (3) |
| C10—C11—C12—C14 | −179.6 (4) | C25—C26—C27—C22 | 0.8 (5) |
| C9—C8—C13—C12 | −1.1 (5) | C28—C26—C27—C22 | −179.2 (3) |
| C7—C8—C13—C12 | 178.9 (3) | C25—C26—C28—N8 | −134 (17) |
| C11—C12—C13—C8 | −0.1 (6) | C27—C26—C28—N8 | 46 (17) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H40···O4$^{i}$ | 0.88 | 1.93 | 2.805 (4) | 172 |
| N6—H39···O3$^{ii}$ | 0.90 | 2.13 | 2.936 (4) | 149 |

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