# metal-organic compounds

# *catena*-Poly[[silver(I)-*μ*-bis{2-[(*E*)-phenyl-diazenyl]-1*H*-imidazol-1-yl}methane] trifluoromethanesulfonate]

## Tao Wang, Ji-Jun Xu and Chuan-Ming Jin*

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The title compound, $\{[Ag(C_{19}H_{16}N_8)](CF_3SO_3)\}_n$, is a coordination polymer with cationic chain motif. The Ag$^+$ cation is coordinated by two unsubstituted imidazolyl N atoms of two independent 2-paBIM ligands [2-paBIM is bis{2-[(*E*)-phenyldiazenyl]-1*H*-imidazol-1-yl}methane]. The shortest Ag⋯Ag separation in a cationic chain is 8.841 (2) Å and the dihedral angle between two 2-phenyldiazenyl-imidazole planes in the same ligand is 74.7 (3)°. Weak C—H⋯O interactions are seen in the crystal.

## Related literature

For background to metal-organic frameworks, see: Batten & Robson (1998); Burrows (2011); Leininger *et al.* (2000); Tanabe & Cohen (2011). For examples of supramolecular arrangements using multidentate *N*-donor spacer ligands, see: Custelcean (2010); Pschirer *et al.* (2002). For structures of related ligands, see: Hamilton & Ziegler (2004); Jin *et al.* (2009).
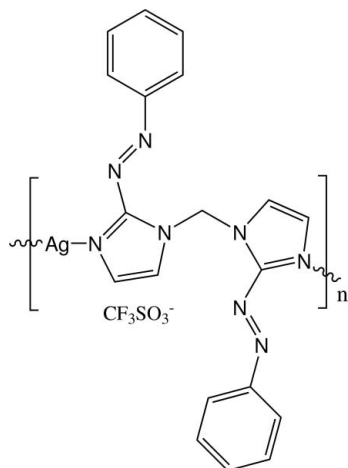


# Experimental

## Crystal data

| | |
|---|---|
| [Ag(C$_{19}$H$_{16}$N$_8$)](CF$_3$SO$_3$) | $V$ = 2343.0 (5) Å$^3$ |
| $M_r$ = 613.34 | $Z$ = 4 |
| Orthorhombic, $Pna2_1$ | Mo $K\alpha$ radiation |
| $a$ = 16.0251 (19) Å | $\mu$ = 1.01 mm$^{-1}$ |
| $b$ = 8.455 (1) Å | $T$ = 298 K |
| $c$ = 17.293 (2) Å | 0.13 × 0.10 × 0.10 mm |

## Data collection

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 11674 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 4823 independent reflections |
| | 4073 reflections with $I > 2\sigma(I)$ |
| $T_{min}$ = 0.879, $T_{max}$ = 0.905 | $R_{int}$ = 0.057 |

## Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.065 | H-atom parameters constrained |
| $wR(F^2)$ = 0.167 | $\Delta\rho_{max}$ = 1.08 e Å$^{-3}$ |
| $S$ = 1.13 | $\Delta\rho_{min}$ = −0.54 e Å$^{-3}$ |
| 4823 reflections | Absolute structure: Flack (1983), 1807 Friedel pairs |
| 326 parameters | Flack parameter: 0.54 (5) |
| 1 restraint | |

**Table 1**
Selected bond lengths (Å).

| Ag1—N3 | 2.152 (5) | Ag1—N6$^i$ | 2.174 (6) |
|---|---|---|---|

Symmetry code: (i) $-x + 1, -y + 2, z + \frac{1}{2}$.

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

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C10—H10$B$⋯O1$^i$ | 0.97 | 2.50 | 3.285 (10) | 138 |
| C8—H8⋯O2$^{ii}$ | 0.93 | 2.31 | 3.021 (10) | 133 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

# References

Batten, S. R. & Robson, R. (1998). *Angew. Chem. Int. Ed. Engl.* **37**, 1460–1494.
Bruker (2001). *SAINT-Plus* and *SMART*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Burrows, A. D. (2011). *CrystEngComm*, **13**, 3623–3642.
Custelcean, R. (2010). *Chem. Soc. Rev.* **39**, 3675–3685.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.

Hamilton, B. H. & Ziegler, C. J. (2004). *Inorg. Chem.* **43**, 4272–4277.

Jin, C. M., Chen, Z. F., Mei, H. F. & Shi, X. K. (2009). *J. Mol. Struct.* **921**, 58–62.

Leininger, S., Olenyuk, B. & Stang, P. J. (2000). *Chem. Rev.* **100**, 853–908.

Pschirer, N. G., Curtin, D. M., Smith, M. D., Bunz, W. H. F. & Zur Loye, H.-C. (2002). *Angew. Chem. Int. Ed. Engl.* **41**, 583–585.

Sheldrick, G. M. (1996). *SADABS.* Bruker AXS Inc., Madison, Wisconsin, USA.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Tanabe, K. K. & Cohen, S. M. (2011). *Chem. Soc. Rev.* **40**, 498–519.

# *catena*-Poly[[silver(I)-*μ*-bis{2-[(*E*)-phenyldiazenyl]-1*H*-imidazol-1-yl}methane] trifluoromethanesulfonate]

## Tao Wang, Ji-Jun Xu and Chuan-Ming Jin

### S1. Comment

The construction of functional metal-organic frameworks is of great interest due to their intriguing network topologies and their potential applications as microporous, magnetic or catalytically active species or in the fields of nonlinear optics, molecular separation, toxic materials adsorption and molecular sensors *etc.* (Batten & Robson, 1998; Burrows, 2011; Leininger *et al.*, 2000; Tanabe & Cohen, 2011). Such molecular architectures have been successfully designed and synthesized by judicious combination of a metal 'node′ and an organic ligands as 'spacer′. The roles of counter anions and different solvent molecules are also of significant effect on supramolecular self-assembly. More recently, the molecular geometry and flexibility of multidentate N-donor spacer ligands play key roles in the field of molecular materials and supramolecular self-assemble crystal engineering. For example, 4, 4′-bipyridine, 1, 2-bis(4-pyridyl)ethane and *trans*-bis-(4-pyridyl)ethene as ligands can form a lot of coordination polymers with different structural features (Custelcean, 2010; Pschirer *et al.*, 2002). The coordination polymer frameworks which were built by methylene C-bridged bipyridine, bitriazole and bisimidazole ligands have also been described widely (Hamilton & Ziegler, 2004; Jin *et al.*, 2009). Bis[2-((*E*)-phenyldiazenyl)-1*H*-imidazol-1-yl- methane (2-paBIM) is a flexibie V-shaped N-donor ligand containing azo groups which is built up by two methylene C-bridged substituted imidazole rings. The title compound, [Ag(2-paBIM)SO$_3$CF$_3$]$_n$, (I), with a one-dimensional zigzag cationic chain structural motif was formed by the addition of a solution of 2-paBIM to AgSO$_3$CF$_3$.

Single crystal X-ray diffraction analysis reveals that complex (I) consists of one-dimensional cationic polymeric chains and uncoordinated CF$_3$SO$_3^-$. The Ag$^+$ ions are coordinated by two imidazolyl unsubstituted nitrogen atoms of independent 2-paBIM ligands, which act as bridges between silver(I) centers (Fig.1). The Ag$^+$ ions show a coordination mode that is bent out of linearity with the bond angles of N—Ag—N being 153.9 (2)°. Ag—N bond lengths are 2.157 (5) Å and 2.170 (6) Å, respectively. Adjacent Ag······Ag distances in the same cationic chain are 8.841 (2) Å and the dihedral angle of the two 2-phenyldiazenyl-imidazole planes in the same ligand is 74.7 (3)°. Non-coordinated CF$_3$SO$_3^-$ anions are filled in the voids of each zigzag cationic chain and show through the weak C—H······O hydrogen-bond interactions (Table 1).

### S2. Experimental

An CH$_3$CN solution (5 ml) of 2-paBIM (178 mg, 0.5 mmol) was slowly diffused into an aqueous solution (5 ml) of AgSO$_3$CF$_3$(128 mg, 0.5 mmol) in a test tube. Red crystals of [Ag(2-paBIM)SO$_3$CF$_3$]$_n$ were formed at the interface of solvent in two weeks and were obtained in 62% yield.

### S3. Refinement

The structure was refined as a racemic twin using TWIN and BASF keywords. H atoms were positioned geometrically at distances of 0.93 (CH), and 0.97 (CH$_2$) from the parent C atoms. A riding model was used during the refinement process.

The $U_{iso}$ values were constrained to be $1.2U_{eq}$ of the corresponding carrier atom.
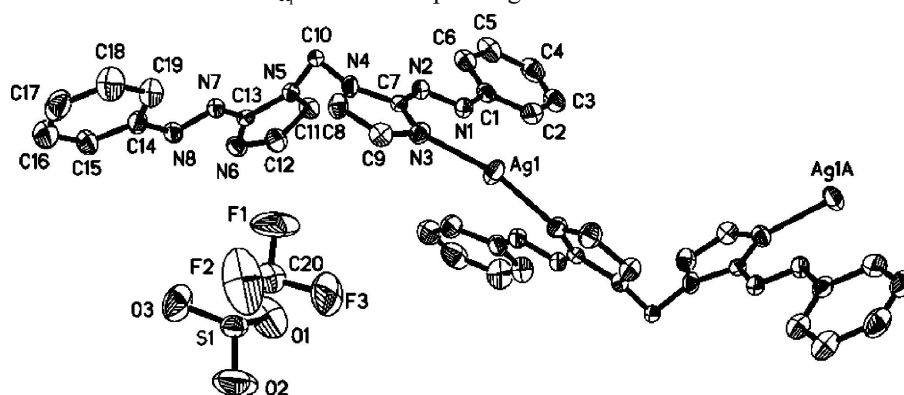


**Figure 1**

Structure of (I) showing the atom-numbering of one asymmetry unit. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

***catena*-Poly[[silver(I)-*μ*-bis{2-[(*E*)-phenyldiazenyl]- 1*H*-imidazol-1-yl}methane] trifluoromethanesulfonate]**

*Crystal data*

| | |
|---|---|
| [Ag($C_{19}H_{16}N_8$)]($CF_3SO_3$) | $F(000) = 1224$ |
| $M_r = 613.34$ | $D_x = 1.739$ Mg m$^{-3}$ |
| Orthorhombic, $Pna2_1$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: P 2c -2n | Cell parameters from 4016 reflections |
| $a = 16.0251$ (19) Å | $\theta = 2.4$–24.4° |
| $b = 8.455$ (1) Å | $\mu = 1.01$ mm$^{-1}$ |
| $c = 17.293$ (2) Å | $T = 298$ K |
| $V = 2343.0$ (5) Å$^3$ | Block, red |
| $Z = 4$ | $0.13 \times 0.10 \times 0.10$ mm |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 11674 measured reflections |
| Radiation source: fine-focus sealed tube | 4823 independent reflections |
| Graphite monochromator | 4073 reflections with $I > 2\sigma(I)$ |
| phi and $\omega$ scans | $R_{int} = 0.057$ |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $\theta_{max} = 28.3°$, $\theta_{min} = 2.4°$ |
| | $h = -21 \rightarrow 16$ |
| $T_{min} = 0.879$, $T_{max} = 0.905$ | $k = -11 \rightarrow 11$ |
| | $l = -23 \rightarrow 19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.065$ | H-atom parameters constrained |
| $wR(F^2) = 0.167$ | $w = 1/[\sigma^2(F_o^2) + (0.0908P)^2]$ |
| $S = 1.13$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 4823 reflections | $(\Delta/\sigma)_{max} = 0.023$ |
| 326 parameters | $\Delta\rho_{max} = 1.08$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -0.54$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Absolute structure: Flack (1983), 1807 Friedel pairs |
| Secondary atom site location: difference Fourier map | Absolute structure parameter: 0.54 (5) |

*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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ag1 | 0.47527 (3) | 0.90148 (7) | 0.39948 (4) | 0.0682 (2) |
| C1 | 0.3518 (4) | 1.2960 (8) | 0.3721 (3) | 0.0509 (14) |
| C2 | 0.3877 (5) | 1.3393 (13) | 0.4422 (5) | 0.078 (2) |
| H2 | 0.4239 | 1.2714 | 0.4680 | 0.093* |
| C3 | 0.3678 (5) | 1.4883 (12) | 0.4732 (5) | 0.078 (3) |
| H3 | 0.3912 | 1.5201 | 0.5199 | 0.094* |
| C4 | 0.3152 (6) | 1.5845 (10) | 0.4357 (6) | 0.075 (2) |
| H4 | 0.3035 | 1.6836 | 0.4563 | 0.090* |
| C5 | 0.2785 (6) | 1.5408 (12) | 0.3679 (5) | 0.078 (2) |
| H5 | 0.2411 | 1.6083 | 0.3434 | 0.093* |
| C6 | 0.2974 (5) | 1.3950 (8) | 0.3356 (5) | 0.0589 (16) |
| H6 | 0.2729 | 1.3647 | 0.2892 | 0.071* |
| C7 | 0.3657 (3) | 0.9567 (8) | 0.2569 (3) | 0.0423 (12) |
| C8 | 0.3670 (4) | 0.7515 (7) | 0.1808 (4) | 0.0528 (15) |
| H8 | 0.3584 | 0.6836 | 0.1392 | 0.063* |
| C9 | 0.4113 (4) | 0.7196 (8) | 0.2445 (4) | 0.0541 (15) |
| H9 | 0.4383 | 0.6243 | 0.2542 | 0.065* |
| C10 | 0.2915 (3) | 0.9926 (9) | 0.1299 (3) | 0.0516 (14) |
| H10A | 0.2600 | 0.9216 | 0.0969 | 0.062* |
| H10B | 0.2523 | 1.0625 | 0.1556 | 0.062* |
| C11 | 0.3752 (4) | 1.2323 (9) | 0.0999 (4) | 0.0630 (17) |
| H11 | 0.3593 | 1.2961 | 0.1412 | 0.076* |
| C12 | 0.4303 (5) | 1.2674 (9) | 0.0438 (4) | 0.0623 (17) |
| H12 | 0.4594 | 1.3623 | 0.0405 | 0.075* |
| C13 | 0.3883 (3) | 1.0371 (8) | 0.0180 (3) | 0.0445 (13) |
| C14 | 0.3903 (4) | 0.7183 (8) | −0.1108 (4) | 0.0544 (15) |
| C15 | 0.4215 (5) | 0.7007 (11) | −0.1837 (4) | 0.0690 (19) |
| H15 | 0.4534 | 0.7812 | −0.2053 | 0.083* |
| C16 | 0.4061 (7) | 0.5638 (13) | −0.2260 (6) | 0.088 (3) |
| H16 | 0.4262 | 0.5518 | −0.2760 | 0.106* |
| C17 | 0.3599 (7) | 0.4471 (14) | −0.1909 (7) | 0.093 (3) |
| H17 | 0.3498 | 0.3540 | −0.2179 | 0.112* |
| C18 | 0.3283 (7) | 0.4624 (11) | −0.1177 (6) | 0.090 (3) |
| H18 | 0.2972 | 0.3812 | −0.0957 | 0.108* |
| C19 | 0.3433 (6) | 0.6010 (9) | −0.0767 (5) | 0.070 (2) |

| | | | | |
|---|---|---|---|---|
| H19 | 0.3219 | 0.6143 | −0.0271 | 0.084* |
| C20 | 0.5958 (6) | −0.0608 (11) | 0.1501 (5) | 0.075 (2) |
| F1 | 0.5243 (3) | 0.0059 (14) | 0.1521 (6) | 0.152 (4) |
| F2 | 0.5931 (9) | −0.2044 (11) | 0.1290 (6) | 0.199 (6) |
| F3 | 0.6175 (6) | −0.0668 (10) | 0.2239 (4) | 0.131 (3) |
| N1 | 0.3750 (3) | 1.1435 (7) | 0.3445 (3) | 0.0501 (11) |
| N2 | 0.3443 (3) | 1.1075 (6) | 0.2807 (3) | 0.0462 (11) |
| N3 | 0.4113 (3) | 0.8465 (6) | 0.2935 (3) | 0.0484 (11) |
| N4 | 0.3370 (3) | 0.9007 (6) | 0.1878 (3) | 0.0450 (12) |
| N5 | 0.3475 (3) | 1.0842 (6) | 0.0837 (3) | 0.0427 (11) |
| N6 | 0.4379 (4) | 1.1474 (7) | −0.0069 (3) | 0.0520 (12) |
| N7 | 0.3705 (3) | 0.8891 (6) | −0.0124 (3) | 0.0465 (12) |
| N8 | 0.4090 (3) | 0.8640 (7) | −0.0747 (3) | 0.0508 (12) |
| O1 | 0.6671 (6) | 0.1988 (10) | 0.1246 (6) | 0.127 (3) |
| O2 | 0.7448 (5) | −0.0336 (14) | 0.1010 (6) | 0.149 (4) |
| O3 | 0.6378 (5) | 0.0472 (10) | 0.0180 (4) | 0.104 (2) |
| S1 | 0.67017 (10) | 0.0515 (2) | 0.09234 (12) | 0.0592 (4) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ag1 | 0.0678 (3) | 0.0891 (4) | 0.0477 (3) | −0.0057 (2) | −0.0201 (2) | 0.0008 (3) |
| C1 | 0.047 (3) | 0.059 (4) | 0.047 (3) | −0.014 (3) | 0.013 (2) | −0.013 (3) |
| C2 | 0.053 (4) | 0.117 (7) | 0.064 (5) | −0.010 (4) | 0.000 (3) | −0.016 (5) |
| C3 | 0.066 (4) | 0.104 (7) | 0.064 (5) | −0.033 (5) | 0.016 (4) | −0.048 (5) |
| C4 | 0.079 (6) | 0.069 (5) | 0.077 (6) | −0.016 (4) | 0.024 (5) | −0.027 (4) |
| C5 | 0.082 (5) | 0.077 (5) | 0.074 (5) | 0.002 (4) | 0.024 (4) | −0.006 (4) |
| C6 | 0.063 (4) | 0.056 (4) | 0.058 (4) | −0.004 (3) | 0.012 (3) | −0.006 (3) |
| C7 | 0.031 (2) | 0.065 (4) | 0.032 (3) | −0.006 (2) | 0.0032 (19) | 0.005 (2) |
| C8 | 0.070 (4) | 0.045 (3) | 0.044 (3) | −0.010 (3) | −0.001 (3) | −0.011 (3) |
| C9 | 0.059 (4) | 0.044 (3) | 0.059 (4) | −0.001 (3) | 0.001 (3) | 0.002 (3) |
| C10 | 0.033 (2) | 0.092 (5) | 0.030 (3) | 0.000 (3) | 0.001 (2) | −0.011 (3) |
| C11 | 0.058 (4) | 0.080 (5) | 0.051 (4) | 0.010 (3) | 0.006 (3) | −0.004 (3) |
| C12 | 0.071 (4) | 0.058 (4) | 0.058 (4) | −0.002 (3) | 0.007 (3) | 0.006 (3) |
| C13 | 0.032 (2) | 0.069 (4) | 0.033 (3) | 0.004 (2) | −0.004 (2) | 0.001 (2) |
| C14 | 0.057 (3) | 0.065 (4) | 0.041 (3) | 0.013 (3) | −0.007 (3) | −0.006 (3) |
| C15 | 0.069 (4) | 0.081 (5) | 0.056 (4) | 0.019 (4) | 0.005 (3) | −0.015 (4) |
| C16 | 0.084 (6) | 0.109 (8) | 0.070 (6) | 0.020 (5) | −0.004 (5) | −0.017 (5) |
| C17 | 0.098 (7) | 0.091 (7) | 0.090 (7) | 0.017 (6) | −0.030 (6) | −0.039 (6) |
| C18 | 0.117 (7) | 0.063 (5) | 0.090 (8) | −0.007 (5) | 0.000 (6) | −0.005 (5) |
| C19 | 0.085 (5) | 0.066 (5) | 0.059 (4) | −0.002 (4) | −0.001 (4) | 0.000 (3) |
| C20 | 0.076 (5) | 0.073 (5) | 0.076 (6) | −0.010 (4) | 0.007 (4) | 0.029 (4) |
| F1 | 0.051 (3) | 0.237 (9) | 0.169 (8) | −0.006 (4) | 0.022 (3) | 0.111 (8) |
| F2 | 0.347 (16) | 0.110 (5) | 0.141 (8) | −0.123 (8) | 0.069 (9) | −0.022 (5) |
| F3 | 0.159 (7) | 0.167 (7) | 0.065 (4) | 0.015 (5) | 0.009 (4) | 0.049 (4) |
| N1 | 0.050 (3) | 0.064 (3) | 0.037 (2) | −0.006 (2) | −0.001 (2) | −0.002 (2) |
| N2 | 0.043 (2) | 0.061 (3) | 0.035 (2) | −0.003 (2) | 0.0013 (19) | −0.003 (2) |
| N3 | 0.050 (3) | 0.051 (3) | 0.044 (3) | −0.005 (2) | −0.006 (2) | 0.006 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N4 | 0.051 (3) | 0.051 (3) | 0.033 (2) | −0.008 (2) | 0.002 (2) | −0.0095 (19) |
| N5 | 0.039 (2) | 0.054 (3) | 0.035 (2) | 0.0043 (18) | −0.0010 (19) | 0.001 (2) |
| N6 | 0.049 (3) | 0.061 (3) | 0.047 (3) | 0.008 (3) | 0.006 (2) | 0.008 (3) |
| N7 | 0.044 (2) | 0.062 (3) | 0.034 (2) | 0.006 (2) | 0.0006 (18) | 0.000 (2) |
| N8 | 0.051 (3) | 0.064 (3) | 0.038 (2) | 0.009 (2) | 0.0003 (19) | 0.000 (2) |
| O1 | 0.154 (8) | 0.089 (5) | 0.138 (8) | −0.037 (5) | 0.043 (6) | −0.017 (5) |
| O2 | 0.076 (4) | 0.222 (9) | 0.148 (8) | 0.060 (6) | 0.018 (5) | 0.058 (8) |
| O3 | 0.120 (6) | 0.134 (6) | 0.060 (4) | −0.030 (5) | −0.012 (4) | 0.037 (4) |
| S1 | 0.0443 (7) | 0.0712 (10) | 0.0622 (10) | −0.0010 (7) | 0.0022 (7) | 0.0131 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ag1—N3 | 2.152 (5) | C11—H11 | 0.9300 |
| Ag1—N6[i] | 2.174 (6) | C12—N6 | 1.347 (10) |
| C1—C6 | 1.364 (11) | C12—H12 | 0.9300 |
| C1—C2 | 1.390 (10) | C13—N6 | 1.298 (9) |
| C1—N1 | 1.424 (9) | C13—N5 | 1.371 (7) |
| C2—C3 | 1.406 (14) | C13—N7 | 1.387 (8) |
| C2—H2 | 0.9300 | C14—C15 | 1.364 (10) |
| C3—C4 | 1.339 (14) | C14—C19 | 1.378 (11) |
| C3—H3 | 0.9300 | C14—N8 | 1.413 (8) |
| C4—C5 | 1.363 (13) | C15—C16 | 1.391 (13) |
| C4—H4 | 0.9300 | C15—H15 | 0.9300 |
| C5—C6 | 1.386 (11) | C16—C17 | 1.374 (16) |
| C5—H5 | 0.9300 | C16—H16 | 0.9300 |
| C6—H6 | 0.9300 | C17—C18 | 1.369 (16) |
| C7—N3 | 1.342 (8) | C17—H17 | 0.9300 |
| C7—N4 | 1.365 (8) | C18—C19 | 1.390 (12) |
| C7—N2 | 1.383 (8) | C18—H18 | 0.9300 |
| C8—C9 | 1.338 (10) | C19—H19 | 0.9300 |
| C8—N4 | 1.355 (8) | C20—F2 | 1.268 (13) |
| C8—H8 | 0.9300 | C20—F1 | 1.278 (11) |
| C9—N3 | 1.366 (9) | C20—F3 | 1.322 (11) |
| C9—H9 | 0.9300 | C20—S1 | 1.822 (8) |
| C10—N5 | 1.429 (8) | N1—N2 | 1.246 (7) |
| C10—N4 | 1.463 (9) | N6—Ag1[ii] | 2.174 (6) |
| C10—H10A | 0.9700 | N7—N8 | 1.259 (7) |
| C10—H10B | 0.9700 | O1—S1 | 1.365 (9) |
| C11—C12 | 1.345 (10) | O2—S1 | 1.404 (7) |
| C11—N5 | 1.357 (9) | O3—S1 | 1.388 (7) |
| | | | |
| N3—Ag1—N6[i] | 153.9 (2) | C19—C14—N8 | 123.7 (6) |
| C6—C1—C2 | 120.4 (7) | C14—C15—C16 | 120.8 (9) |
| C6—C1—N1 | 124.6 (6) | C14—C15—H15 | 119.6 |
| C2—C1—N1 | 115.0 (7) | C16—C15—H15 | 119.6 |
| C1—C2—C3 | 118.3 (9) | C17—C16—C15 | 117.5 (9) |
| C1—C2—H2 | 120.8 | C17—C16—H16 | 121.3 |
| C3—C2—H2 | 120.8 | C15—C16—H16 | 121.3 |

| | | | |
|---|---|---|---|
| C4—C3—C2 | 120.2 (7) | C16—C17—C18 | 122.6 (9) |
| C4—C3—H3 | 119.9 | C16—C17—H17 | 118.7 |
| C2—C3—H3 | 119.9 | C18—C17—H17 | 118.7 |
| C3—C4—C5 | 121.6 (8) | C17—C18—C19 | 119.2 (10) |
| C3—C4—H4 | 119.2 | C17—C18—H18 | 120.4 |
| C5—C4—H4 | 119.2 | C19—C18—H18 | 120.4 |
| C4—C5—C6 | 119.5 (10) | C14—C19—C18 | 118.9 (8) |
| C4—C5—H5 | 120.2 | C14—C19—H19 | 120.6 |
| C6—C5—H5 | 120.2 | C18—C19—H19 | 120.6 |
| C1—C6—C5 | 120.0 (8) | F2—C20—F1 | 113.5 (11) |
| C1—C6—H6 | 120.0 | F2—C20—F3 | 104.5 (10) |
| C5—C6—H6 | 120.0 | F1—C20—F3 | 103.1 (9) |
| N3—C7—N4 | 110.8 (6) | F2—C20—S1 | 111.3 (8) |
| N3—C7—N2 | 129.4 (6) | F1—C20—S1 | 111.7 (6) |
| N4—C7—N2 | 119.8 (5) | F3—C20—S1 | 112.2 (7) |
| C9—C8—N4 | 107.5 (6) | N2—N1—C1 | 114.6 (6) |
| C9—C8—H8 | 126.2 | N1—N2—C7 | 113.0 (5) |
| N4—C8—H8 | 126.2 | C7—N3—C9 | 104.6 (5) |
| C8—C9—N3 | 110.7 (6) | C7—N3—Ag1 | 120.7 (4) |
| C8—C9—H9 | 124.7 | C9—N3—Ag1 | 134.2 (4) |
| N3—C9—H9 | 124.7 | C8—N4—C7 | 106.4 (6) |
| N5—C10—N4 | 110.9 (4) | C8—N4—C10 | 127.6 (5) |
| N5—C10—H10A | 109.5 | C7—N4—C10 | 125.6 (5) |
| N4—C10—H10A | 109.5 | C11—N5—C13 | 106.4 (5) |
| N5—C10—H10B | 109.5 | C11—N5—C10 | 126.1 (5) |
| N4—C10—H10B | 109.5 | C13—N5—C10 | 127.3 (5) |
| H10A—C10—H10B | 108.0 | C13—N6—C12 | 105.6 (6) |
| C12—C11—N5 | 105.6 (6) | C13—N6—Ag1ii | 120.2 (5) |
| C12—C11—H11 | 127.2 | C12—N6—Ag1ii | 133.3 (5) |
| N5—C11—H11 | 127.2 | N8—N7—C13 | 112.0 (5) |
| C11—C12—N6 | 111.3 (7) | N7—N8—C14 | 114.9 (6) |
| C11—C12—H12 | 124.4 | O1—S1—O3 | 112.9 (6) |
| N6—C12—H12 | 124.4 | O1—S1—O2 | 117.1 (7) |
| N6—C13—N5 | 111.0 (6) | O3—S1—O2 | 113.8 (6) |
| N6—C13—N7 | 130.4 (6) | O1—S1—C20 | 103.1 (5) |
| N5—C13—N7 | 118.5 (5) | O3—S1—C20 | 104.5 (5) |
| C15—C14—C19 | 121.1 (7) | O2—S1—C20 | 103.4 (5) |
| C15—C14—N8 | 115.2 (7) | | |
| | | | |
| C6—C1—C2—C3 | −1.4 (11) | N2—C7—N4—C8 | −179.3 (5) |
| N1—C1—C2—C3 | 179.9 (6) | N3—C7—N4—C10 | −174.5 (5) |
| C1—C2—C3—C4 | 0.3 (12) | N2—C7—N4—C10 | 7.2 (8) |
| C2—C3—C4—C5 | 1.3 (12) | N5—C10—N4—C8 | −91.0 (8) |
| C3—C4—C5—C6 | −1.7 (12) | N5—C10—N4—C7 | 81.0 (7) |
| C2—C1—C6—C5 | 1.0 (10) | C12—C11—N5—C13 | 0.3 (7) |
| N1—C1—C6—C5 | 179.5 (6) | C12—C11—N5—C10 | 176.1 (6) |
| C4—C5—C6—C1 | 0.6 (11) | N6—C13—N5—C11 | −0.8 (7) |
| N4—C8—C9—N3 | −0.3 (8) | N7—C13—N5—C11 | −179.1 (5) |

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|---|---|---|---|
| N5—C11—C12—N6 | 0.2 (9) | N6—C13—N5—C10 | −176.5 (5) |
| C19—C14—C15—C16 | 0.5 (12) | N7—C13—N5—C10 | 5.2 (9) |
| N8—C14—C15—C16 | −178.8 (7) | N4—C10—N5—C11 | −88.1 (7) |
| C14—C15—C16—C17 | −1.2 (13) | N4—C10—N5—C13 | 86.8 (7) |
| C15—C16—C17—C18 | 1.1 (15) | N5—C13—N6—C12 | 0.9 (7) |
| C16—C17—C18—C19 | −0.1 (16) | N7—C13—N6—C12 | 178.9 (6) |
| C15—C14—C19—C18 | 0.5 (12) | N5—C13—N6—Ag1ii | 171.3 (4) |
| N8—C14—C19—C18 | 179.7 (8) | N7—C13—N6—Ag1ii | −10.6 (9) |
| C17—C18—C19—C14 | −0.6 (14) | C11—C12—N6—C13 | −0.7 (8) |
| C6—C1—N1—N2 | 3.2 (9) | C11—C12—N6—Ag1ii | −169.3 (5) |
| C2—C1—N1—N2 | −178.2 (6) | N6—C13—N7—N8 | −1.3 (9) |
| C1—N1—N2—C7 | −177.8 (5) | N5—C13—N7—N8 | 176.7 (5) |
| N3—C7—N2—N1 | 2.4 (8) | C13—N7—N8—C14 | −176.8 (5) |
| N4—C7—N2—N1 | −179.7 (5) | C15—C14—N8—N7 | 170.3 (6) |
| N4—C7—N3—C9 | 0.8 (6) | C19—C14—N8—N7 | −9.0 (9) |
| N2—C7—N3—C9 | 178.9 (6) | F2—C20—S1—O1 | −177.9 (10) |
| N4—C7—N3—Ag1 | 174.6 (4) | F1—C20—S1—O1 | 54.1 (10) |
| N2—C7—N3—Ag1 | −7.3 (8) | F3—C20—S1—O1 | −61.1 (9) |
| C8—C9—N3—C7 | −0.3 (7) | F2—C20—S1—O3 | 63.9 (10) |
| C8—C9—N3—Ag1 | −172.8 (5) | F1—C20—S1—O3 | −64.1 (10) |
| N6i—Ag1—N3—C7 | −170.1 (5) | F3—C20—S1—O3 | −179.4 (8) |
| N6i—Ag1—N3—C9 | 1.5 (9) | F2—C20—S1—O2 | −55.5 (11) |
| C9—C8—N4—C7 | 0.8 (7) | F1—C20—S1—O2 | 176.5 (10) |
| C9—C8—N4—C10 | 174.1 (6) | F3—C20—S1—O2 | 61.3 (10) |
| N3—C7—N4—C8 | −1.0 (7) | | |

Symmetry codes: (i) −*x*+1, −*y*+2, *z*+1/2; (ii) −*x*+1, −*y*+2, *z*−1/2.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C10—H10*B*···O1iii | 0.97 | 2.50 | 3.285 (10) | 138 |
| C8—H8···O2iv | 0.93 | 2.31 | 3.021 (10) | 133 |

Symmetry codes: (iii) *x*−1/2, −*y*+3/2, *z*; (iv) *x*−1/2, −*y*+1/2, *z*.