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# *catena*-Poly[[[aqua(pyridine-4-carboxylato-$\kappa N$)silver(I)]-$\mu$-hexamethylenetetraamine-$\kappa^2 N:N'$] dihydrate]

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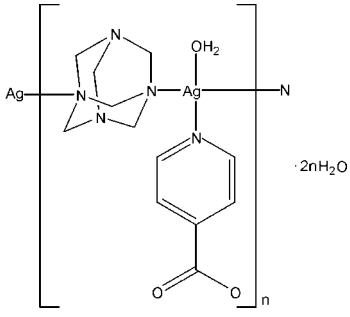
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.016; $wR$ factor = 0.041; data-to-parameter ratio = 10.5.

In the title compound, $\{[Ag(C_6H_4NO_2)(C_6H_{12}N_4)(H_2O)]\cdot 2H_2O\}_n$, the $Ag^I$ atom shows a distorted triangular pyramidal geometry,, formed by two N atoms from two hexamethylenetetraamine (hmt) ligands and one N atom from a pyridine-4-carboxylate (4-pdc) ligand and one water molecule. The hmt ligands bridge the Ag atoms, forming a chain along [001]. The carboxylate group of the 4-pdc ligand is uncoordinated. O—H···O hydrogen bonds between the water molecules and carboxylate groups stabilize the structure.

## Related literature

For general background to the design and synthesis of coordination polymers, see: Eddaoudi *et al.* (2001).




## Experimental

### *Crystal data*

$[Ag(C_6H_4NO_2)(C_6H_{12}N_4)(H_2O)]\cdot 2H_2O$
$M_r$ = 424.22
Orthorhombic, $Pna2_1$
$a$ = 11.8271 (5) Å
$b$ = 13.2122 (5) Å
$c$ = 10.2560 (4) Å
$V$ = 1602.62 (11) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 1.29 mm$^{-1}$
$T$ = 293 K
0.24 × 0.20 × 0.19 mm

### *Data collection*

Bruker APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.747, $T_{max}$ = 0.792
7849 measured reflections
2380 independent reflections
2347 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.041
$S$ = 1.08
2380 reflections
226 parameters
10 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.55 e Å$^{-3}$
Absolute structure: Flack (1983), 876 Friedel pairs
Flack parameter: 0.01 (2)

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

| | | | |
|---|---|---|---|
| Ag1—N1 | 2.287 (2) | Ag1—N5$^{i}$ | 2.306 (2) |
| Ag1—N2 | 2.256 (2) | Ag1—O1*W* | 2.673 (2) |

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

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1*W*—H1*A*···O2*W*$^{ii}$ | 0.85 (3) | 1.91 (3) | 2.743 (3) | 169 (3) |
| O1*W*—H1*B*···O1$^{iii}$ | 0.85 (1) | 1.91 (2) | 2.714 (2) | 157 (3) |
| O2*W*—H2*A*···O2 | 0.84 (1) | 1.88 (1) | 2.722 (3) | 173 (3) |
| O2*W*—H2*B*···O3*W*$^{iv}$ | 0.84 (3) | 1.99 (3) | 2.787 (3) | 161 (3) |
| O3*W*—H3*A*···O1*W*$^{v}$ | 0.85 (1) | 1.95 (1) | 2.788 (3) | 169 (3) |
| O3*W*—H3*B*···O1 | 0.85 (1) | 1.89 (1) | 2.728 (2) | 169 (3) |

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

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2384).

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# supporting information

*Acta Cryst.* (2011). E**67**, m47 [https://doi.org/10.1107/S1600536810050452]

## *catena*-Poly[[[aqua(pyridine-4-carboxylato-$\kappa N$)silver(I)]-$\mu$-hexamethylenetetramine-$\kappa^2N$:$N'$] dihydrate]

**Dajun Sun, Liying Han and Hu Zang**

### S1. Comment

The design and synthesis of coordination polymers have been a research field of rapid expansion not only because of their fascinating structures, but also owing to their interesting properties as new functional materials of tremendous potential applications in molecular recognition, ion-exchange, and catalysis for reactions (Eddaoudi *et al.*, 2001). In this work, the reaction of pyridine-4-carboxylatic acid (4-Hpdc) and hexamethylenetetraamine (hmt) with $Ag^I$ ion yielded a new coordination polymer.

As shown in Fig. 1, the asymmetric unit of the title compound contains one $Ag^I$ atom, one 4-pdc ligand, one hmt ligand, one coordinated water molecule and two uncoordinated water molecules. The Ag1 atom shows a distorted triangle pyramidal geometry, completed by three N atoms from two hmt ligands and one 4-pdc ligand and one O atom from a water molecule. The hmt ligands bridge the Ag atoms, forming a one-dimensional chain. The carboxylate group of the 4-pdc ligand is uncoordinated. O—H···O hydrogen bonds between the water molecules and carboxylate groups stabilize the structure.

### S2. Experimental

A mixture of 4-Hpdc (0.615 g, 0.5 mmol), $Ag(NO_3)_2$ (0.085 g, 0.5 mmol) and hmt (0.070 g, 0.5 mmol) in water was heated at 150°C in a Teflon-lined stainless steel autoclave for 5 d. The reaction system was then slowly cooled to room temperature. Crystals suitable for X-ray diffraction analysis were collected by filtration.

### S3. Refinement

C-bound H atoms were positioned geometrically and refined using a riding mode, with C—H = 0.93 and 0.97 Å and $U_{iso}$(H) = 1.2$U_{eq}$(C). The water H atoms were located in a difference Fourier map and refined with restraints of O—H = 0.85 (1) and H···H = 1.38 (1) Å and $U_{iso}$(H) = 1.5$U_{eq}$(O).

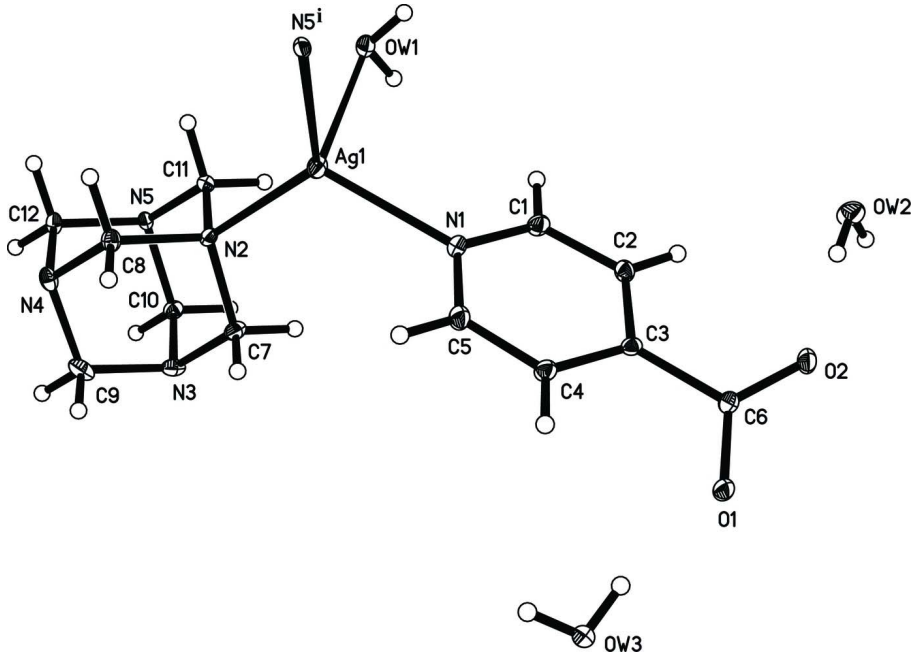


**Figure 1**

The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (i) -*x*, -*y*, *z*+1/2].

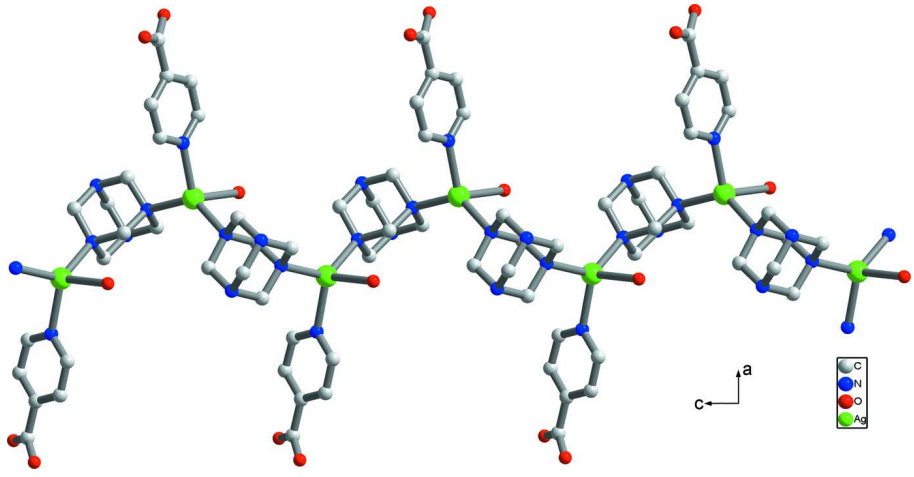


**Figure 2**

View of the chain structure in the title compound.

***catena*-Poly[[[aqua(pyridine-4-carboxylato-$\kappa N$)silver(I)]-$\mu$-hexamethylenetetraamine-$\kappa^2N:N'$] dihydrate]**

*Crystal data*

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$M_r = 424.22$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 11.8271\ (5)$ Å
$b = 13.2122\ (5)$ Å
$c = 10.2560\ (4)$ Å
$V = 1602.62\ (11)$ Å$^3$
$Z = 4$
$F(000) = 864$
$D_x = 1.758$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2380 reflections
$\theta = 3.0$–$26.1°$

$\mu$ = 1.29 mm$^{-1}$
$T$ = 293 K

Block, colorless
0.24 × 0.20 × 0.19 mm

*Data collection*

Bruker APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.747, $T_{max}$ = 0.792

7849 measured reflections
2380 independent reflections
2347 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.3°
$h$ = −13→14
$k$ = −15→15
$l$ = −10→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.016
$wR(F^2)$ = 0.041
$S$ = 1.08
2380 reflections
226 parameters
10 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0231P)^2 + 0.3127P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.55 e Å$^{-3}$
Absolute structure: Flack (1983), 876 Friedel pairs
Absolute structure parameter: 0.01 (2)

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Ag1 | 0.128363 (13) | 0.013803 (11) | 0.15278 (4) | 0.02268 (7) |
| C1 | 0.3975 (2) | 0.04853 (19) | 0.1327 (3) | 0.0235 (6) |
| H1 | 0.3756 | 0.0961 | 0.0708 | 0.028* |
| C2 | 0.51160 (18) | 0.03798 (16) | 0.1607 (3) | 0.0213 (5) |
| H2 | 0.5645 | 0.0788 | 0.1190 | 0.026* |
| C3 | 0.5467 (2) | −0.03375 (17) | 0.2511 (2) | 0.0180 (5) |
| C4 | 0.4633 (2) | −0.09081 (18) | 0.3108 (3) | 0.0226 (5) |
| H4 | 0.4826 | −0.1395 | 0.3724 | 0.027* |
| C5 | 0.3513 (2) | −0.0753 (2) | 0.2786 (3) | 0.0253 (6) |
| H5 | 0.2968 | −0.1145 | 0.3200 | 0.030* |
| C6 | 0.6705 (2) | −0.04864 (19) | 0.2834 (2) | 0.0195 (5) |
| C7 | 0.1034 (2) | −0.1856 (2) | −0.0106 (3) | 0.0232 (6) |
| H7A | 0.1690 | −0.1589 | −0.0556 | 0.028* |
| H7B | 0.1299 | −0.2228 | 0.0651 | 0.028* |
| C8 | −0.0697 (2) | −0.14419 (19) | 0.0997 (2) | 0.0214 (5) |
| H8A | −0.0454 | −0.1812 | 0.1764 | 0.026* |
| H8B | −0.1189 | −0.0898 | 0.1281 | 0.026* |
| C9 | −0.0568 (2) | −0.29341 (18) | −0.0278 (3) | 0.0298 (6) |
| H9A | −0.0977 | −0.3395 | −0.0842 | 0.036* |
| H9B | −0.0321 | −0.3312 | 0.0482 | 0.036* |
| C10 | 0.0045 (2) | −0.19809 (17) | −0.2111 (2) | 0.0216 (5) |

| | | | | |
|---|---|---|---|---|
| H10A | −0.0355 | −0.2433 | −0.2696 | 0.026* |
| H10B | 0.0696 | −0.1715 | −0.2573 | 0.026* |
| C11 | −0.0086 (2) | −0.04628 (17) | −0.0847 (3) | 0.0188 (5) |
| H11A | −0.0572 | 0.0093 | −0.0586 | 0.023* |
| H11B | 0.0560 | −0.0179 | −0.1301 | 0.023* |
| C12 | −0.1700 (2) | −0.15591 (19) | −0.1010 (3) | 0.0207 (5) |
| H12A | −0.2195 | −0.1012 | −0.0741 | 0.025* |
| H12B | −0.2126 | −0.2005 | −0.1579 | 0.025* |
| N1 | 0.31739 (18) | −0.00721 (15) | 0.1914 (2) | 0.0226 (6) |
| N2 | 0.03133 (16) | −0.10028 (15) | 0.0333 (2) | 0.0175 (4) |
| N3 | 0.04299 (17) | −0.25501 (15) | −0.0976 (2) | 0.0238 (4) |
| N4 | −0.13283 (16) | −0.21224 (17) | 0.0138 (2) | 0.0225 (5) |
| N5 | −0.07120 (15) | −0.11312 (15) | −0.1745 (2) | 0.0165 (4) |
| O1 | 0.69699 (14) | −0.13139 (13) | 0.33372 (19) | 0.0263 (4) |
| O2 | 0.73760 (15) | 0.02175 (13) | 0.2588 (2) | 0.0294 (5) |
| O1W | 0.11516 (14) | 0.16451 (15) | −0.0205 (2) | 0.0254 (4) |
| H1A | 0.145 (2) | 0.2117 (19) | 0.024 (3) | 0.038* |
| H1B | 0.161 (2) | 0.147 (2) | −0.080 (2) | 0.038* |
| O2W | 0.73929 (16) | 0.19124 (15) | 0.1080 (2) | 0.0344 (5) |
| H2A | 0.736 (2) | 0.1415 (17) | 0.159 (2) | 0.052* |
| H2B | 0.777 (3) | 0.176 (2) | 0.042 (2) | 0.052* |
| O3W | 0.60916 (15) | −0.31522 (14) | 0.4000 (3) | 0.0330 (5) |
| H3A | 0.5402 (12) | −0.313 (2) | 0.423 (3) | 0.049* |
| H3B | 0.629 (2) | −0.2569 (14) | 0.373 (4) | 0.049* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Ag1 | 0.01850 (10) | 0.02679 (10) | 0.02274 (11) | −0.00070 (6) | −0.00291 (10) | −0.00824 (17) |
| C1 | 0.0231 (11) | 0.0237 (11) | 0.0236 (19) | 0.0030 (9) | −0.0032 (12) | 0.0047 (12) |
| C2 | 0.0200 (10) | 0.0214 (10) | 0.0226 (12) | −0.0030 (8) | 0.0014 (14) | 0.0042 (15) |
| C3 | 0.0193 (12) | 0.0163 (11) | 0.0185 (13) | 0.0030 (9) | −0.0024 (10) | −0.0034 (10) |
| C4 | 0.0203 (12) | 0.0220 (12) | 0.0256 (14) | 0.0024 (9) | 0.0013 (11) | 0.0062 (11) |
| C5 | 0.0201 (12) | 0.0263 (14) | 0.0295 (15) | −0.0025 (10) | 0.0028 (11) | 0.0048 (12) |
| C6 | 0.0177 (12) | 0.0225 (12) | 0.0184 (13) | 0.0003 (10) | 0.0004 (10) | 0.0004 (10) |
| C7 | 0.0202 (12) | 0.0234 (14) | 0.0262 (16) | 0.0054 (10) | −0.0018 (12) | −0.0043 (12) |
| C8 | 0.0206 (12) | 0.0248 (13) | 0.0188 (12) | −0.0023 (10) | 0.0012 (10) | 0.0021 (10) |
| C9 | 0.0414 (16) | 0.0176 (13) | 0.0305 (15) | −0.0053 (11) | −0.0100 (13) | 0.0024 (11) |
| C10 | 0.0216 (12) | 0.0223 (12) | 0.0208 (13) | 0.0025 (9) | −0.0006 (11) | −0.0039 (10) |
| C11 | 0.0179 (12) | 0.0157 (10) | 0.0228 (13) | −0.0002 (9) | 0.0000 (10) | 0.0016 (10) |
| C12 | 0.0154 (12) | 0.0257 (13) | 0.0208 (13) | −0.0046 (10) | −0.0008 (11) | 0.0032 (11) |
| N1 | 0.0158 (10) | 0.0237 (10) | 0.0284 (16) | 0.0010 (8) | −0.0010 (9) | −0.0004 (8) |
| N2 | 0.0132 (9) | 0.0191 (10) | 0.0202 (11) | 0.0020 (8) | −0.0010 (8) | −0.0002 (8) |
| N3 | 0.0290 (11) | 0.0179 (10) | 0.0244 (11) | 0.0055 (9) | −0.0075 (10) | −0.0041 (9) |
| N4 | 0.0232 (11) | 0.0252 (12) | 0.0190 (12) | −0.0077 (8) | −0.0014 (9) | 0.0053 (9) |
| N5 | 0.0150 (10) | 0.0167 (10) | 0.0178 (11) | −0.0032 (8) | 0.0000 (8) | 0.0014 (8) |
| O1 | 0.0186 (8) | 0.0235 (9) | 0.0366 (11) | −0.0002 (7) | −0.0035 (8) | 0.0104 (8) |
| O2 | 0.0190 (9) | 0.0265 (10) | 0.0427 (13) | −0.0057 (7) | −0.0055 (9) | 0.0098 (8) |

| | | | | | | |
|---|---|---|---|---|---|---|
| O1W | 0.0196 (9) | 0.0265 (11) | 0.0300 (12) | −0.0025 (7) | 0.0035 (8) | −0.0021 (9) |
| O2W | 0.0317 (10) | 0.0319 (10) | 0.0396 (12) | 0.0047 (8) | 0.0038 (9) | 0.0147 (8) |
| O3W | 0.0219 (9) | 0.0206 (10) | 0.0564 (15) | −0.0012 (7) | −0.0013 (10) | 0.0072 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Ag1—N1 | 2.287 (2) | C8—H8B | 0.9700 |
| Ag1—N2 | 2.256 (2) | C9—N4 | 1.463 (3) |
| Ag1—N5$^{i}$ | 2.306 (2) | C9—N3 | 1.470 (4) |
| Ag1—O1W | 2.673 (2) | C9—H9A | 0.9700 |
| C1—N1 | 1.342 (3) | C9—H9B | 0.9700 |
| C1—C2 | 1.387 (3) | C10—N3 | 1.459 (3) |
| C1—H1 | 0.9300 | C10—N5 | 1.484 (3) |
| C2—C3 | 1.390 (4) | C10—H10A | 0.9700 |
| C2—H2 | 0.9300 | C10—H10B | 0.9700 |
| C3—C4 | 1.384 (3) | C11—N5 | 1.476 (3) |
| C3—C6 | 1.513 (3) | C11—N2 | 1.482 (3) |
| C4—C5 | 1.380 (3) | C11—H11A | 0.9700 |
| C4—H4 | 0.9300 | C11—H11B | 0.9700 |
| C5—N1 | 1.330 (3) | C12—N4 | 1.461 (3) |
| C5—H5 | 0.9300 | C12—N5 | 1.501 (3) |
| C6—O2 | 1.249 (3) | C12—H12A | 0.9700 |
| C6—O1 | 1.249 (3) | C12—H12B | 0.9700 |
| C7—N3 | 1.465 (3) | O1W—H1A | 0.85 (3) |
| C7—N2 | 1.483 (3) | O1W—H1B | 0.85 (1) |
| C7—H7A | 0.9700 | O2W—H2A | 0.84 (1) |
| C7—H7B | 0.9700 | O2W—H2B | 0.84 (3) |
| C8—N4 | 1.464 (3) | O3W—H3A | 0.85 (1) |
| C8—N2 | 1.492 (3) | O3W—H3B | 0.85 (1) |
| C8—H8A | 0.9700 | | |

| | | | |
|---|---|---|---|
| N2—Ag1—N1 | 120.67 (7) | N3—C10—N5 | 112.10 (19) |
| N2—Ag1—N5$^{i}$ | 130.41 (7) | N3—C10—H10A | 109.2 |
| N1—Ag1—N5$^{i}$ | 102.86 (7) | N5—C10—H10A | 109.2 |
| N2—Ag1—O1W | 96.13 (7) | N3—C10—H10B | 109.2 |
| N1—Ag1—O1W | 105.23 (6) | N5—C10—H10B | 109.2 |
| N5$^{i}$—Ag1—O1W | 94.00 (7) | H10A—C10—H10B | 107.9 |
| N1—C1—C2 | 122.6 (3) | N5—C11—N2 | 112.42 (18) |
| N1—C1—H1 | 118.7 | N5—C11—H11A | 109.1 |
| C2—C1—H1 | 118.7 | N2—C11—H11A | 109.1 |
| C1—C2—C3 | 119.8 (2) | N5—C11—H11B | 109.1 |
| C1—C2—H2 | 120.1 | N2—C11—H11B | 109.1 |
| C3—C2—H2 | 120.1 | H11A—C11—H11B | 107.9 |
| C4—C3—C2 | 116.9 (2) | N4—C12—N5 | 111.27 (19) |
| C4—C3—C6 | 121.5 (2) | N4—C12—H12A | 109.4 |
| C2—C3—C6 | 121.6 (2) | N5—C12—H12A | 109.4 |
| C5—C4—C3 | 119.8 (2) | N4—C12—H12B | 109.4 |
| C5—C4—H4 | 120.1 | N5—C12—H12B | 109.4 |

| | | | |
|---|---|---|---|
| C3—C4—H4 | 120.1 | H12A—C12—H12B | 108.0 |
| N1—C5—C4 | 123.4 (2) | C5—N1—C1 | 117.3 (2) |
| N1—C5—H5 | 118.3 | C5—N1—Ag1 | 119.57 (17) |
| C4—C5—H5 | 118.3 | C1—N1—Ag1 | 123.05 (17) |
| O2—C6—O1 | 125.1 (2) | C11—N2—C7 | 107.5 (2) |
| O2—C6—C3 | 118.3 (2) | C11—N2—C8 | 107.76 (18) |
| O1—C6—C3 | 116.6 (2) | C7—N2—C8 | 107.63 (19) |
| N3—C7—N2 | 112.35 (19) | C11—N2—Ag1 | 106.48 (14) |
| N3—C7—H7A | 109.1 | C7—N2—Ag1 | 112.35 (14) |
| N2—C7—H7A | 109.1 | C8—N2—Ag1 | 114.77 (15) |
| N3—C7—H7B | 109.1 | C10—N3—C7 | 108.4 (2) |
| N2—C7—H7B | 109.1 | C10—N3—C9 | 108.41 (19) |
| H7A—C7—H7B | 107.9 | C7—N3—C9 | 108.1 (2) |
| N4—C8—N2 | 111.90 (19) | C12—N4—C9 | 108.8 (2) |
| N4—C8—H8A | 109.2 | C12—N4—C8 | 109.0 (2) |
| N2—C8—H8A | 109.2 | C9—N4—C8 | 108.17 (19) |
| N4—C8—H8B | 109.2 | C11—N5—C10 | 107.94 (17) |
| N2—C8—H8B | 109.2 | C11—N5—C12 | 107.64 (19) |
| H8A—C8—H8B | 107.9 | C10—N5—C12 | 108.15 (19) |
| N4—C9—N3 | 112.48 (19) | C11—N5—Ag1$^{ii}$ | 106.63 (14) |
| N4—C9—H9A | 109.1 | C10—N5—Ag1$^{ii}$ | 114.39 (15) |
| N3—C9—H9A | 109.1 | C12—N5—Ag1$^{ii}$ | 111.83 (14) |
| N4—C9—H9B | 109.1 | H1A—O1W—H1B | 108.9 (15) |
| N3—C9—H9B | 109.1 | H2A—O2W—H2B | 110.2 (16) |
| H9A—C9—H9B | 107.8 | H3A—O3W—H3B | 108.7 (15) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1*W*—H1*A*···O2*W*$^{iii}$ | 0.85 (3) | 1.91 (3) | 2.743 (3) | 169 (3) |
| O1*W*—H1*B*···O1$^{iv}$ | 0.85 (1) | 1.91 (2) | 2.714 (2) | 157 (3) |
| O2*W*—H2*A*···O2 | 0.84 (1) | 1.88 (1) | 2.722 (3) | 173 (3) |
| O2*W*—H2*B*···O3*W*$^{v}$ | 0.84 (3) | 1.99 (3) | 2.787 (3) | 161 (3) |
| O3*W*—H3*A*···O1*W*$^{vi}$ | 0.85 (1) | 1.95 (1) | 2.788 (3) | 169 (3) |
| O3*W*—H3*B*···O1 | 0.85 (1) | 1.89 (1) | 2.728 (2) | 169 (3) |

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