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catena-Poly[[[aquisilver(I)]- μ -4,4'-bipyridine- κ^2 N:N'] 4-aminobenzoate nitrate hydrate]

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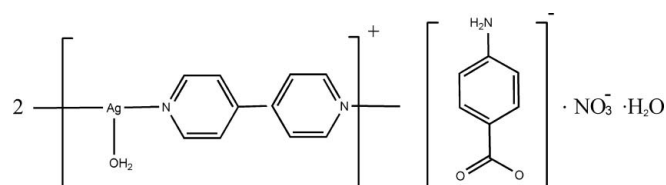
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 Key indicators: single-crystal X-ray study; $T = 293$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.023; wR factor = 0.059; data-to-parameter ratio = 12.4.

In the structure of the title compound, $2[\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})](\text{C}_7\text{H}_6\text{NO}_2)(\text{NO}_3)\cdot\text{H}_2\text{O}$, the Ag^{I} atom is three-coordinated in a T-shaped configuration by two N atoms from two symmetry-related 4,4'-bipyridine (bipy) ligands at short distances and by one water O atom at a longer distance. Each bipy ligand bridges two neighbouring Ag^{I} atoms, forming a chain structure extending parallel to [101]. The complete 4-aminobenzoate anion, the nitrate anion and the uncoordinated water molecule are located on mirror planes: together with the coordinated water molecule, they form $\text{N}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{O}$ and $\text{O}-\text{H}\cdots\text{N}$ hydrogen bonds, stabilizing the crystal structure.

Related literature

 For a related structure, see: Zhang *et al.* (2008).


Experimental

Crystal data

 $2[\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})](\text{C}_7\text{H}_6\text{NO}_2)(\text{NO}_3)\cdot\text{H}_2\text{O}$
 $M_r = 780.29$

 Monoclinic, $P2_1/m$
 $a = 8.2595$ (4) Å

 $b = 17.3531$ (8) Å

 $c = 9.9267$ (4) Å

 $\beta = 103.231$ (1)°

 $V = 1385.01$ (11) Å³
 $Z = 2$

 Mo $K\alpha$ radiation

 $\mu = 1.48$ mm⁻¹
 $T = 293$ K

 $0.24 \times 0.21 \times 0.17$ mm

Data collection

Bruker APEX CCD area-detector diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

 $T_{\text{min}} = 0.54$, $T_{\text{max}} = 0.83$

7782 measured reflections

2847 independent reflections

 2390 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.024$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.023$
 $wR(F^2) = 0.059$
 $S = 1.07$

2847 reflections

230 parameters

8 restraints

H atoms treated by a mixture of independent and constrained refinement

 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.38$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|--|-------------|--------------------------|-------------|
| Ag1—N3 ⁱ | 2.139 (2) | Ag1—O1W ⁱⁱ | 2.6799 (17) |
| Ag1—N2 | 2.1444 (19) | | |
| N3 ⁱ —Ag1—N2 | 172.70 (7) | N2—Ag1—O1W ⁱⁱ | 90.84 (6) |
| N3 ⁱ —Ag1—O1W ⁱⁱ | 92.88 (6) | | |

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

Table 2

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| N1—H1A ⁱⁱⁱ ···O2W ⁱⁱⁱ | 0.85 (4) | 2.34 (2) | 3.160 (5) | 163 |
| N1—H1B ^{iv} ···O2 ^{iv} | 0.85 (4) | 2.10 (4) | 2.932 (4) | 167 |
| O1W—HW11···O1 | 0.85 (3) | 1.91 (3) | 2.747 (2) | 172 (3) |
| O1W—HW12···O4 | 0.83 (3) | 2.15 (3) | 2.927 (3) | 154 (3) |
| O2W—HW21···O1 | 0.85 (3) | 2.14 (3) | 2.979 (4) | 169 (3) |
| O2W—HW22···O5 ^v | 0.86 (3) | 2.30 (2) | 3.084 (3) | 151 |
| O2W—HW22···O5 ^{vi} | 0.86 (3) | 2.30 (2) | 3.084 (3) | 151 |
| O2W—HW22···N4 ^v | 0.86 (3) | 2.63 (3) | 3.476 (4) | 167 |

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

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); 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); software used to prepare material for publication: SHELXTL.

The authors thank Anshan Normal University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2305).

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 Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.
 Zhang, Y.-M., Hou, D.-Y., Li, T.-C. & Xin, G. (2008). Acta Cryst. E64, m224.

supporting information

Acta Cryst. (2010). E66, m287 [doi:10.1107/S1600536810005052]

catena-Poly[[[aquisilver(I)]- μ -4,4'-bipyridine- κ^2 N:N'] 4-aminobenzoate nitrate hydrate]

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S1. Comment

Silver coordination polymers have received intense interests because of their interesting structural features and potential applications (Zhang *et al.*, 2008). We report here the synthesis and structure of the title compound,

[Ag₂(C₁₀H₈N₂)₂(H₂O)₂](C₇H₆NO₂).NO₃.H₂O, (I).

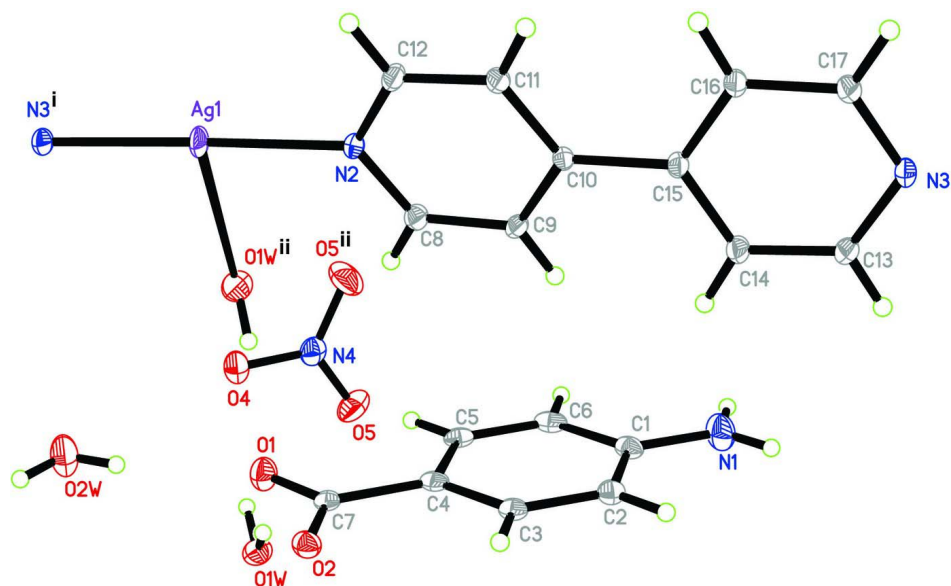
In the crystal structure of compound (I), the Ag^I atom is three-coordinated by two nitrogen atoms from two symmetry-related bipy (bipy = 4,4'-bipyridine) ligands and one water water molecule in a T-shaped coordination configuration (Fig. 1). Each bipy ligand bridges two neighboring Ag^I atoms to form a chain structure along [101]. Further, *L* anions (*L* = 4-aminobenzoate), the nitrate anion, and the uncoordinated water molecule form N—H \cdots O and O—H \cdots O hydrogen bonds, stabilizing the structure of (I).

S2. Experimental

A mixture of AgNO₃ (1 mmol), NaOH (0.040 g, 1 mmol) and 4-aminobenzoic acid (1 mmol) in water (15 ml) was stirred for 10 min at room temperature. Then 4,4'-bipyridine (1 mmol) was added to the solution with stirring for 30 min and a white precipitate was obtained. The precipitate was dissolved by dropwise addition of ammonia (5 M). Single crystals were obtained by slow evaporation of the solution at room temperature.

S3. Refinement

All H atoms on C atoms were positioned geometrically (C—H = 0.93 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(carrier). The amino and water H atoms were located in a difference Fourier map, and were refined with a distance restraints of N—H = O—H = 0.85 Å.

**Figure 1**

The structure of (I), showing the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry codes: (i) $x-1, y, z-1$; (ii) $x, 1.5-y, z$]

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Crystal data

$2[\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})](\text{C}_7\text{H}_6\text{NO}_2)(\text{NO}_3)\cdot\text{H}_2\text{O}$

$M_r = 780.29$

Monoclinic, $P2_1/m$

Hall symbol: $-P\ 2y$

$a = 8.2595$ (4) Å

$b = 17.3531$ (8) Å

$c = 9.9267$ (4) Å

$\beta = 103.231$ (1)°

$V = 1385.01$ (11) Å³

$Z = 2$

$F(000) = 780$

$D_x = 1.871$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 2847 reflections

$\theta = 2.1\text{--}26.1^\circ$

$\mu = 1.48$ mm⁻¹

$T = 293$ K

Block, colourless

$0.24 \times 0.21 \times 0.17$ mm

Data collection

Bruker APEX CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

φ and ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1996)

$T_{\min} = 0.54, T_{\max} = 0.83$

7782 measured reflections

2847 independent reflections

2390 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.024$

$\theta_{\max} = 26.1^\circ, \theta_{\min} = 2.1^\circ$

$h = -10 \rightarrow 7$

$k = -21 \rightarrow 17$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.059$

$S = 1.07$

2847 reflections

230 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 atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0284P)^2 + 0.2523P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.003$
 $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.38 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|------------|--------------|------------|----------------------------------|
| C1 | 0.9046 (4) | 0.7500 | 0.9999 (4) | 0.0234 (8) |
| C2 | 0.7795 (4) | 0.7500 | 1.0736 (4) | 0.0216 (7) |
| H2 | 0.8082 | 0.7500 | 1.1698 | 0.026* |
| C3 | 0.6139 (4) | 0.7500 | 1.0056 (4) | 0.0201 (7) |
| H3 | 0.5331 | 0.7500 | 1.0573 | 0.024* |
| C4 | 0.5645 (4) | 0.7500 | 0.8621 (3) | 0.0198 (7) |
| C5 | 0.6902 (4) | 0.7500 | 0.7886 (4) | 0.0215 (7) |
| H5 | 0.6610 | 0.7500 | 0.6924 | 0.026* |
| C6 | 0.8556 (4) | 0.7500 | 0.8547 (4) | 0.0240 (8) |
| H6 | 0.9361 | 0.7500 | 0.8027 | 0.029* |
| C7 | 0.3820 (4) | 0.7500 | 0.7909 (3) | 0.0198 (7) |
| C8 | 0.6051 (3) | 0.95341 (14) | 0.7979 (2) | 0.0211 (5) |
| H8 | 0.5907 | 0.9099 | 0.7417 | 0.025* |
| C9 | 0.7206 (3) | 0.95076 (14) | 0.9219 (2) | 0.0203 (5) |
| H9 | 0.7822 | 0.9061 | 0.9477 | 0.024* |
| C10 | 0.7458 (3) | 1.01485 (13) | 1.0091 (2) | 0.0156 (5) |
| C11 | 0.6492 (3) | 1.07948 (14) | 0.9627 (2) | 0.0204 (5) |
| H11 | 0.6611 | 1.1238 | 1.0166 | 0.025* |
| C12 | 0.5365 (3) | 1.07780 (14) | 0.8371 (2) | 0.0219 (5) |
| H12 | 0.4739 | 1.1218 | 0.8082 | 0.026* |
| C13 | 1.0736 (3) | 0.94885 (15) | 1.3175 (2) | 0.0235 (5) |
| H13 | 1.1264 | 0.9031 | 1.3512 | 0.028* |
| C14 | 0.9522 (3) | 0.94648 (14) | 1.1975 (2) | 0.0238 (5) |
| H14 | 0.9241 | 0.8998 | 1.1523 | 0.029* |
| C15 | 0.8700 (3) | 1.01438 (13) | 1.1424 (2) | 0.0172 (5) |
| C16 | 0.9155 (3) | 1.08119 (14) | 1.2193 (2) | 0.0210 (5) |
| H16 | 0.8627 | 1.1276 | 1.1897 | 0.025* |
| C17 | 1.0384 (3) | 1.07876 (14) | 1.3392 (2) | 0.0231 (5) |
| H17 | 1.0664 | 1.1243 | 1.3883 | 0.028* |
| N1 | 1.0689 (4) | 0.7500 | 1.0676 (4) | 0.0366 (8) |

| | | | | |
|------|-------------|---------------|---------------|-------------|
| N2 | 0.5122 (2) | 1.01603 (11) | 0.7543 (2) | 0.0180 (4) |
| N3 | 1.1201 (2) | 1.01423 (11) | 1.3889 (2) | 0.0206 (4) |
| N4 | 0.6731 (4) | 0.7500 | 0.3860 (3) | 0.0293 (7) |
| O1 | 0.3438 (3) | 0.7500 | 0.6599 (3) | 0.0305 (6) |
| O2 | 0.2780 (3) | 0.7500 | 0.8655 (2) | 0.0234 (5) |
| O1W | 0.4203 (2) | 0.62838 (10) | 0.50869 (19) | 0.0327 (4) |
| O2W | 0.0951 (4) | 0.7500 | 0.3901 (3) | 0.0499 (8) |
| O4 | 0.5190 (3) | 0.7500 | 0.3396 (3) | 0.0365 (7) |
| O5 | 0.7501 (3) | 0.68814 (12) | 0.4064 (2) | 0.0511 (6) |
| Ag1 | 0.32721 (2) | 1.014048 (12) | 0.563502 (18) | 0.02456 (8) |
| H1A | 1.099 (5) | 0.7500 | 1.155 (2) | 0.046 (14)* |
| H1B | 1.143 (4) | 0.7500 | 1.021 (4) | 0.044 (13)* |
| HW11 | 0.400 (4) | 0.6633 (16) | 0.562 (3) | 0.065* |
| HW12 | 0.448 (4) | 0.6508 (18) | 0.443 (2) | 0.065* |
| HW21 | 0.154 (4) | 0.7500 | 0.472 (3) | 0.065* |
| HW22 | -0.004 (3) | 0.7500 | 0.404 (4) | 0.065* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|--------------|--------------|--------------|
| C1 | 0.0206 (18) | 0.0152 (18) | 0.035 (2) | 0.000 | 0.0080 (15) | 0.000 |
| C2 | 0.0238 (18) | 0.0190 (18) | 0.0225 (18) | 0.000 | 0.0064 (14) | 0.000 |
| C3 | 0.0230 (18) | 0.0137 (17) | 0.0254 (18) | 0.000 | 0.0093 (14) | 0.000 |
| C4 | 0.0234 (18) | 0.0109 (17) | 0.0267 (19) | 0.000 | 0.0089 (15) | 0.000 |
| C5 | 0.032 (2) | 0.0118 (17) | 0.0234 (18) | 0.000 | 0.0116 (15) | 0.000 |
| C6 | 0.0270 (19) | 0.0154 (18) | 0.034 (2) | 0.000 | 0.0171 (16) | 0.000 |
| C7 | 0.0244 (18) | 0.0092 (16) | 0.0246 (19) | 0.000 | 0.0033 (15) | 0.000 |
| C8 | 0.0243 (13) | 0.0189 (13) | 0.0175 (12) | 0.0005 (10) | -0.0003 (10) | -0.0022 (10) |
| C9 | 0.0244 (13) | 0.0145 (12) | 0.0187 (12) | 0.0019 (10) | -0.0022 (10) | 0.0011 (10) |
| C10 | 0.0140 (11) | 0.0174 (12) | 0.0146 (11) | -0.0019 (9) | 0.0012 (9) | 0.0016 (9) |
| C11 | 0.0233 (13) | 0.0156 (12) | 0.0194 (12) | 0.0004 (9) | -0.0013 (10) | -0.0031 (9) |
| C12 | 0.0222 (12) | 0.0192 (13) | 0.0208 (12) | 0.0054 (10) | -0.0027 (10) | 0.0010 (10) |
| C13 | 0.0256 (13) | 0.0180 (13) | 0.0228 (13) | 0.0017 (10) | -0.0030 (10) | 0.0021 (10) |
| C14 | 0.0274 (13) | 0.0177 (13) | 0.0211 (12) | 0.0012 (10) | -0.0051 (10) | -0.0023 (10) |
| C15 | 0.0140 (11) | 0.0198 (12) | 0.0166 (12) | -0.0008 (9) | 0.0007 (9) | 0.0013 (9) |
| C16 | 0.0205 (12) | 0.0180 (13) | 0.0207 (12) | 0.0017 (10) | -0.0034 (10) | -0.0013 (10) |
| C17 | 0.0256 (13) | 0.0179 (13) | 0.0217 (13) | -0.0005 (10) | -0.0031 (10) | -0.0025 (10) |
| N1 | 0.0192 (17) | 0.051 (2) | 0.039 (2) | 0.000 | 0.0064 (17) | 0.000 |
| N2 | 0.0179 (10) | 0.0195 (10) | 0.0145 (10) | -0.0001 (8) | -0.0007 (8) | 0.0017 (8) |
| N3 | 0.0199 (10) | 0.0223 (11) | 0.0161 (10) | -0.0004 (9) | -0.0029 (8) | -0.0005 (8) |
| N4 | 0.0349 (19) | 0.035 (2) | 0.0175 (15) | 0.000 | 0.0045 (14) | 0.000 |
| O1 | 0.0278 (14) | 0.0388 (16) | 0.0232 (14) | 0.000 | 0.0024 (11) | 0.000 |
| O2 | 0.0211 (13) | 0.0210 (13) | 0.0287 (14) | 0.000 | 0.0071 (11) | 0.000 |
| O1W | 0.0407 (12) | 0.0278 (11) | 0.0273 (11) | -0.0025 (9) | 0.0030 (9) | 0.0029 (8) |
| O2W | 0.0302 (16) | 0.062 (2) | 0.051 (2) | 0.000 | -0.0047 (14) | 0.000 |
| O4 | 0.0275 (15) | 0.0436 (17) | 0.0352 (16) | 0.000 | 0.0005 (12) | 0.000 |
| O5 | 0.0491 (13) | 0.0414 (14) | 0.0585 (14) | 0.0149 (11) | 0.0034 (11) | 0.0173 (11) |
| Ag1 | 0.02136 (12) | 0.03052 (13) | 0.01619 (11) | 0.00025 (8) | -0.00732 (8) | -0.00028 (8) |

Geometric parameters (Å, °)

| | | | |
|--|-------------|---------------------|-----------|
| Ag1—N3 ⁱ | 2.139 (2) | C17—H17 | 0.9300 |
| Ag1—N2 | 2.1444 (19) | O1—C7 | 1.266 (4) |
| Ag1—O1W ⁱⁱ | 2.6799 (17) | O2—C7 | 1.255 (4) |
| N2—C12 | 1.337 (3) | N1—C1 | 1.369 (4) |
| N2—C8 | 1.344 (3) | N1—H1A | 0.85 (4) |
| N3—C17 | 1.342 (3) | N1—H1B | 0.85 (4) |
| N3—C13 | 1.346 (3) | C1—C2 | 1.396 (5) |
| N3—Ag1 ⁱⁱⁱ | 2.139 (2) | C1—C6 | 1.405 (5) |
| C8—C9 | 1.374 (3) | C2—C3 | 1.380 (4) |
| C8—H8 | 0.9300 | C2—H2 | 0.9300 |
| C9—C10 | 1.396 (3) | C3—C4 | 1.389 (5) |
| C9—H9 | 0.9300 | C3—H3 | 0.9300 |
| C10—C11 | 1.392 (3) | C4—C5 | 1.399 (4) |
| C10—C15 | 1.477 (3) | C4—C7 | 1.511 (4) |
| C11—C12 | 1.375 (3) | C5—C6 | 1.373 (5) |
| C11—H11 | 0.9300 | C5—H5 | 0.9300 |
| C12—H12 | 0.9300 | C6—H6 | 0.9300 |
| C13—C14 | 1.371 (3) | O4—N4 | 1.251 (4) |
| C13—H13 | 0.9300 | O5—N4 | 1.240 (2) |
| C14—C15 | 1.407 (3) | N4—O5 ⁱⁱ | 1.240 (2) |
| C14—H14 | 0.9300 | O1W—HW11 | 0.85 (2) |
| C15—C16 | 1.392 (3) | O1W—HW12 | 0.85 (2) |
| C16—C17 | 1.377 (3) | O2W—HW21 | 0.85 (2) |
| C16—H16 | 0.9300 | O2W—HW22 | 0.85 (2) |
| N3 ⁱ —Ag1—N2 | 172.70 (7) | C17—C16—H16 | 120.0 |
| N3 ⁱ —Ag1—O1W ⁱⁱ | 92.88 (6) | C15—C16—H16 | 120.0 |
| N2—Ag1—O1W ⁱⁱ | 90.84 (6) | N3—C17—C16 | 123.6 (2) |
| C12—N2—C8 | 117.1 (2) | N3—C17—H17 | 118.2 |
| C12—N2—Ag1 | 122.13 (15) | C16—C17—H17 | 118.2 |
| C8—N2—Ag1 | 120.71 (16) | C1—N1—H1A | 122 (3) |
| C17—N3—C13 | 116.8 (2) | C1—N1—H1B | 119 (3) |
| C17—N3—Ag1 ⁱⁱⁱ | 122.74 (16) | H1A—N1—H1B | 119 (3) |
| C13—N3—Ag1 ⁱⁱⁱ | 120.27 (16) | N1—C1—C2 | 120.8 (3) |
| N2—C8—C9 | 122.9 (2) | N1—C1—C6 | 121.6 (3) |
| N2—C8—H8 | 118.5 | C2—C1—C6 | 117.6 (3) |
| C9—C8—H8 | 118.5 | C3—C2—C1 | 120.9 (3) |
| C8—C9—C10 | 120.2 (2) | C3—C2—H2 | 119.5 |
| C8—C9—H9 | 119.9 | C1—C2—H2 | 119.5 |
| C10—C9—H9 | 119.9 | C2—C3—C4 | 121.8 (3) |
| C11—C10—C9 | 116.4 (2) | C2—C3—H3 | 119.1 |
| C11—C10—C15 | 121.9 (2) | C4—C3—H3 | 119.1 |
| C9—C10—C15 | 121.7 (2) | C3—C4—C5 | 117.1 (3) |
| C12—C11—C10 | 120.1 (2) | C3—C4—C7 | 120.4 (3) |
| C12—C11—H11 | 120.0 | C5—C4—C7 | 122.5 (3) |
| C10—C11—H11 | 120.0 | C6—C5—C4 | 121.8 (3) |

| | | | |
|--------------------------------|--------------|--------------------------------|-------------|
| N2—C12—C11 | 123.3 (2) | C6—C5—H5 | 119.1 |
| N2—C12—H12 | 118.3 | C4—C5—H5 | 119.1 |
| C11—C12—H12 | 118.3 | C5—C6—C1 | 120.8 (3) |
| N3—C13—C14 | 123.1 (2) | C5—C6—H6 | 119.6 |
| N3—C13—H13 | 118.4 | C1—C6—H6 | 119.6 |
| C14—C13—H13 | 118.4 | O2—C7—O1 | 124.2 (3) |
| C13—C14—C15 | 120.3 (2) | O2—C7—C4 | 117.9 (3) |
| C13—C14—H14 | 119.8 | O1—C7—C4 | 117.9 (3) |
| C15—C14—H14 | 119.8 | O5—N4—O5 ⁱⁱ | 119.9 (3) |
| C16—C15—C14 | 116.1 (2) | O5—N4—O4 | 120.02 (16) |
| C16—C15—C10 | 122.1 (2) | O5 ⁱⁱ —N4—O4 | 120.02 (16) |
| C14—C15—C10 | 121.8 (2) | HW11—O1W—HW12 | 107 (3) |
| C17—C16—C15 | 120.1 (2) | HW21—O2W—HW22 | 102 (3) |
| | | | |
| N3 ⁱ —Ag1—N2—C12 | -61.6 (6) | C9—C10—C15—C14 | -9.2 (4) |
| N3 ⁱ —Ag1—N2—C8 | 116.0 (6) | C14—C15—C16—C17 | 2.1 (4) |
| C12—N2—C8—C9 | 0.4 (3) | C10—C15—C16—C17 | -176.4 (2) |
| Ag1—N2—C8—C9 | -177.37 (18) | C13—N3—C17—C16 | -1.8 (4) |
| N2—C8—C9—C10 | 0.0 (4) | Ag1 ⁱⁱⁱ —N3—C17—C16 | 173.52 (19) |
| C8—C9—C10—C11 | -0.3 (3) | C15—C16—C17—N3 | -0.1 (4) |
| C8—C9—C10—C15 | -179.3 (2) | N1—C1—C2—C3 | 180.000 (2) |
| C9—C10—C11—C12 | 0.1 (3) | C6—C1—C2—C3 | 0.000 (2) |
| C15—C10—C11—C12 | 179.2 (2) | C1—C2—C3—C4 | 0.000 (2) |
| C8—N2—C12—C11 | -0.6 (4) | C2—C3—C4—C5 | 0.000 (2) |
| Ag1—N2—C12—C11 | 177.15 (18) | C2—C3—C4—C7 | 180.000 (2) |
| C10—C11—C12—N2 | 0.3 (4) | C3—C4—C5—C6 | 0.000 (2) |
| C17—N3—C13—C14 | 1.6 (4) | C7—C4—C5—C6 | 180.000 (1) |
| Ag1 ⁱⁱⁱ —N3—C13—C14 | -173.80 (19) | C4—C5—C6—C1 | 0.000 (2) |
| N3—C13—C14—C15 | 0.4 (4) | N1—C1—C6—C5 | 180.000 (2) |
| C13—C14—C15—C16 | -2.3 (4) | C2—C1—C6—C5 | 0.000 (2) |
| C13—C14—C15—C10 | 176.3 (2) | C3—C4—C7—O2 | 0.000 (1) |
| C11—C10—C15—C16 | -9.7 (4) | C5—C4—C7—O2 | 180.000 (1) |
| C9—C10—C15—C16 | 169.3 (2) | C3—C4—C7—O1 | 180.000 (1) |
| C11—C10—C15—C14 | 171.8 (2) | C5—C4—C7—O1 | 0.000 (1) |

Symmetry codes: (i) $x-1, y, z-1$; (ii) $x, -y+3/2, z$; (iii) $x+1, y, z+1$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------------------|----------|-------------|-------------|---------------|
| N1—H1A \cdots O2W ⁱⁱⁱ | 0.85 (4) | 2.34 (2) | 3.160 (5) | 163 |
| N1—H1B \cdots O2 ^{iv} | 0.85 (4) | 2.10 (4) | 2.932 (4) | 167 |
| O1W—HW11 \cdots O1 | 0.85 (3) | 1.91 (3) | 2.747 (2) | 172 (3) |
| O1W—HW12 \cdots O4 | 0.83 (3) | 2.15 (3) | 2.927 (3) | 154 (3) |
| O2W—HW21 \cdots O1 | 0.85 (3) | 2.14 (3) | 2.979 (4) | 169 (3) |
| O2W—HW22 \cdots O5 ^v | 0.86 (3) | 2.30 (2) | 3.084 (3) | 151 |

| | | | | |
|-----------------------------|----------|----------|-----------|-----|
| O2W—HW22···O5 ^{vi} | 0.86 (3) | 2.30 (2) | 3.084 (3) | 151 |
| O2W—HW22···N4 ^v | 0.86 (3) | 2.63 (3) | 3.476 (4) | 167 |

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