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## Structure Reports

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Bis[4-(4-pyridylmethoxy)phenol- $\kappa$ N]-silver nitrate monohydrate

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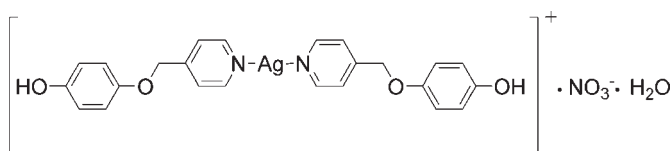
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Key indicators: single-crystal X-ray study;  $T = 291$  K; mean  $\sigma(\text{C}-\text{C}) = 0.006$  Å;  $R$  factor = 0.054;  $wR$  factor = 0.115; data-to-parameter ratio = 16.7.

In the title compound,  $[\text{Ag}(\text{C}_{12}\text{H}_{11}\text{NO}_2)_2]\text{NO}_3 \cdot \text{H}_2\text{O}$ , the  $\text{Ag}^{\text{I}}$  ion is coordinated by two N atoms from two different 4-(4-pyridylmethoxy)phenol ligands, generating a nearly linear coordination geometry with an  $\text{N}-\text{Ag}-\text{N}$  angle of  $167.1$  ( $1$ ) $^\circ$ . A three-dimensional supramolecular network is built from the uncoordinated nitrate anion, the water molecule and the cation through  $\text{O}-\text{H} \cdots \text{O}$  hydrogen bonds.

## Related literature

For the synthesis of the title ligand, see: Gao *et al.* (2006); Zou *et al.* (2009). For background to metal-organic complexes with flexible pyridyl-based ligands, see: Fun *et al.* (1999); Liu *et al.* (2010); You *et al.* (2009).



## Experimental

## Crystal data

 $[\text{Ag}(\text{C}_{12}\text{H}_{11}\text{NO}_2)_2]\text{NO}_3 \cdot \text{H}_2\text{O}$  $M_r = 590.33$ Monoclinic,  $P2_1/c$  $a = 9.458$  (4) Å $b = 13.507$  (7) Å $c = 20.274$  (7) Å $\beta = 111.986$  (18) $^\circ$  $V = 2401.6$  (18) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 0.89$  mm<sup>-1</sup> $T = 291$  K $0.21 \times 0.19 \times 0.18$  mm

## Data collection

Rigaku R-Axis RAPID  
diffractometer  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\text{min}} = 0.832$ ,  $T_{\text{max}} = 0.857$

22423 measured reflections  
5442 independent reflections  
2900 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.058$

## Refinement

$R[F^2 > 2\sigma(F^2)] = 0.054$   
 $wR(F^2) = 0.115$   
 $S = 1.04$   
5442 reflections

325 parameters  
H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.38$  e Å<sup>-3</sup>

Table 1

Hydrogen-bond geometry (Å,  $^\circ$ ).

| $D-\text{H} \cdots A$                               | $D-\text{H}$ | $\text{H} \cdots A$ | $D \cdots A$ | $D-\text{H} \cdots A$ |
|-----------------------------------------------------|--------------|---------------------|--------------|-----------------------|
| $\text{O1}-\text{H1A} \cdots \text{O8}^{\text{i}}$  | 0.82         | 1.90                | 2.661 (4)    | 155                   |
| $\text{O3}-\text{H3} \cdots \text{O7}$              | 0.82         | 1.88                | 2.698 (5)    | 176                   |
| $\text{O8}-\text{H31} \cdots \text{O7}$             | 0.85         | 2.05                | 2.885 (5)    | 167                   |
| $\text{O8}-\text{H32} \cdots \text{O3}^{\text{ii}}$ | 0.85         | 2.00                | 2.833 (4)    | 165                   |

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

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSK, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2780).

## References

- Fun, H.-K., Raj, S. S. S., Xiong, J.-L., Zuo, J.-L., Yu, Z. & You, X.-Z. (1999). *J. Chem. Soc. Dalton Trans.* pp. 1915–1916.
- Gao, J.-S., Liu, Y., Hou, G.-F., Yu, Y.-H. & Yan, P.-F. (2006). *Acta Cryst.* **E62**, o5645–o5646.
- Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
- Liu, Y., Yan, P.-F., Yu, Y.-H., Hou, G.-F. & Gao, J.-S. (2010). *Cryst. Growth Des.* **10**, 1559–1568.
- Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
- Rigaku/MSK (2002). *CrystalClear*. Rigaku/MSK Inc., The Woodlands, Texas, USA.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- You, Z.-L., Zhang, L., Shi, D.-H. & Ni, L.-L. (2009). *Inorg. Chem. Commun.* **12**, 1231–1233.
- Zou, P., Liu, Y., Zhang, S., Wang, X. & Gao, J.-S. (2009). *Acta Cryst.* **E65**, o2570.

## supporting information

*Acta Cryst.* (2010). E66, m754 [doi:10.1107/S1600536810020945]

## Bis[4-(4-pyridylmethoxy)phenol- $\kappa$ N]silver nitrate monohydrate

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### S1. Comment

The metal-organic compounds constructed by the pyridine-containing ligands have attracted more attention for their novel and virous structures and potential applications (Fun *et al.* 1999; Liu *et al.* 2010]. A polynuclear silver(I) complex with 2-hydroxypyridine was synthesized, and the complex maybe served as an efficient urease inhibitor (You *et al.* 2009). Based on above researches, the title compound was synthesized by reacting pyridine-containing ligand with the  $\text{AgNO}_3$ .

X-ray single-crystal analysis of title compound shows that the  $\text{Ag}^{\text{I}}$  is coordinated by two N atoms from two different 4-(4-pyridylmethoxy)-phenol ligands to generate a linear coordination geometry with the N—Ag—N angle of  $167.06(14)^\circ$  (Figure 1, Table 1). In each asymmetrical unit, the planes of the pyridine rings and benzene rings are nearly parallel and make dihedral angles of  $8.462(4)^\circ$  and  $7.165(21)^\circ$ . But the two ligands are vertical with the dihedral angle of two pyridine rings being  $86.779(11)^\circ$ .

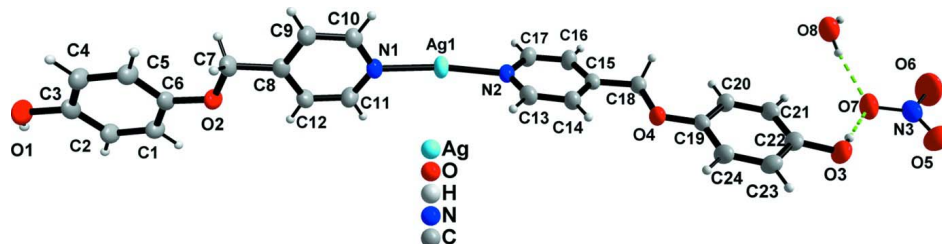
Two terminal hydroxyl groups, one uncoordinate water and one nitrate ion are linked together to form a three dimensional network through intermolecular O—H $\cdots$ O hydrogen bonds (Figure 2, Table 2).

### S2. Experimental

The synthesis of ligand see the literature (Gao *et al.* 2006; Zou *et al.* 2009). A solution of  $\text{AgNO}_3$  (0.017 g, 0.10 mmol) in water (2 ml) was dropped slowly into a methanol solution (5 ml) of ligand (0.040 g, 2 mmol) to give a clear solution. Colourless block crystals of title were obtained by slow evaporation of the clear solution under room temperature after a week.

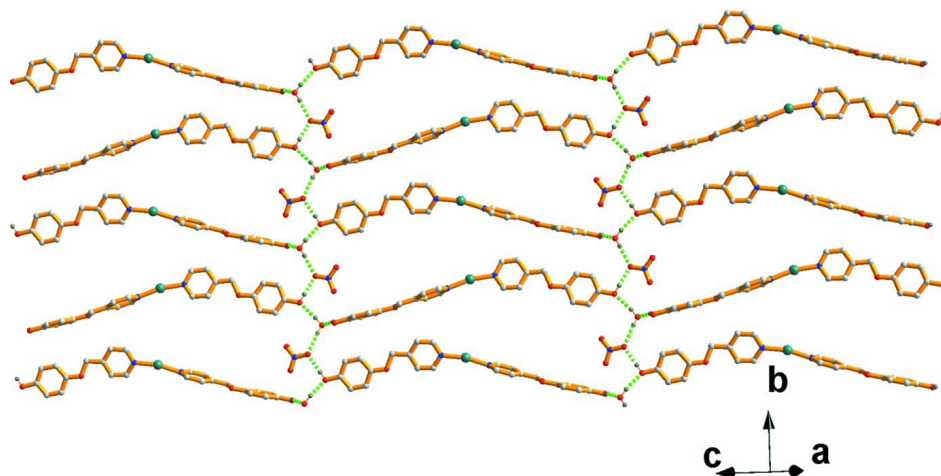
### S3. Refinement

H atoms bound to C atoms and hydroxyl groups were placed in calculated positions and treated as riding on their parent atoms, with C—H = 0.93 Å (aromatic C), C—H = 0.97 Å (methene C), and with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ . The H atoms of water molecule were initially located in a difference Fourier map, but they were treated as riding on their parent atoms with O—H = 0.85 Å and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ .



**Figure 1**

The molecular structure of title compound, showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level.



**Figure 2**

The crystal packing diagram of title compound, viewed along *a* axis. Dashed lines indicate hydrogen bonds, noninvolving hydrogen atoms are omitted for clarity.

### Bis[4-(4-pyridylmethoxy)phenol-*κ*N]silver nitrate monohydrate

#### Crystal data

[Ag(C<sub>12</sub>H<sub>11</sub>NO<sub>2</sub>)<sub>2</sub>]NO<sub>3</sub>·H<sub>2</sub>O

*M<sub>r</sub>* = 590.33

Monoclinic, *P*2<sub>1</sub>/*c*

Hall symbol: -*P* 2ybc

*a* = 9.458 (4) Å

*b* = 13.507 (7) Å

*c* = 20.274 (7) Å

β = 111.986 (18)°

*V* = 2401.6 (18) Å<sup>3</sup>

*Z* = 4

*F*(000) = 1200

*D<sub>x</sub>* = 1.633 Mg m<sup>-3</sup>

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 11930 reflections

θ = 3.0–27.5°

μ = 0.89 mm<sup>-1</sup>

*T* = 291 K

Block, colorless

0.21 × 0.19 × 0.18 mm

#### Data collection

Rigaku R-Axis RAPID  
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scan

Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)

*T<sub>min</sub>* = 0.832, *T<sub>max</sub>* = 0.857

22423 measured reflections

5442 independent reflections

2900 reflections with *I* > 2σ(*I*)

*R<sub>int</sub>* = 0.058

θ<sub>max</sub> = 27.5°, θ<sub>min</sub> = 3.0°

*h* = -12→12

*k* = -17→17

*l* = -23→26

#### Refinement

Refinement on *F*<sup>2</sup>

Least-squares matrix: full

*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.054

*wR*(*F*<sup>2</sup>) = 0.115

*S* = 1.04

5442 reflections

325 parameters

0 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/[σ<sup>2</sup>(*F<sub>o</sub>*<sup>2</sup>) + (0.0406*P*)<sup>2</sup> + 0.9527*P*]

where *P* = (*F<sub>o</sub>*<sup>2</sup> + 2*F<sub>c</sub>*<sup>2</sup>)/3

(Δ/σ)<sub>max</sub> = 0.001

Δρ<sub>max</sub> = 0.28 e Å<sup>-3</sup>

Δρ<sub>min</sub> = -0.38 e Å<sup>-3</sup>

*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 ( $\text{\AA}^2$ )*

|     | <i>x</i>    | <i>y</i>    | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|-------------|---------------|----------------------------------|
| Ag1 | 0.90730 (4) | 0.49819 (3) | 0.766410 (16) | 0.07746 (16)                     |
| O1  | 2.1641 (3)  | 0.7496 (2)  | 1.22381 (14)  | 0.0838 (9)                       |
| H1A | 2.2314      | 0.7453      | 1.2076        | 0.126*                           |
| O2  | 1.6021 (3)  | 0.6618 (2)  | 1.01902 (13)  | 0.0673 (7)                       |
| O3  | -0.3575 (3) | 0.6172 (2)  | 0.27642 (14)  | 0.0818 (9)                       |
| H3  | -0.3967     | 0.5657      | 0.2566        | 0.123*                           |
| O4  | 0.2108 (3)  | 0.5574 (2)  | 0.48365 (13)  | 0.0648 (7)                       |
| N1  | 1.0938 (4)  | 0.5514 (3)  | 0.85577 (17)  | 0.0599 (8)                       |
| N2  | 0.7030 (4)  | 0.4783 (3)  | 0.67566 (16)  | 0.0605 (9)                       |
| C1  | 1.8626 (4)  | 0.6955 (3)  | 1.0520 (2)    | 0.0616 (10)                      |
| H1  | 1.8487      | 0.6892      | 1.0043        | 0.074*                           |
| C2  | 2.0045 (4)  | 0.7167 (3)  | 1.1011 (2)    | 0.0622 (10)                      |
| H2  | 2.0861      | 0.7248      | 1.0866        | 0.075*                           |
| C3  | 2.0268 (4)  | 0.7261 (3)  | 1.1721 (2)    | 0.0596 (10)                      |
| C4  | 1.9048 (5)  | 0.7140 (3)  | 1.1922 (2)    | 0.0662 (11)                      |
| H4  | 1.9188      | 0.7203      | 1.2399        | 0.079*                           |
| C5  | 1.7617 (4)  | 0.6927 (3)  | 1.14314 (19)  | 0.0625 (11)                      |
| H5  | 1.6802      | 0.6847      | 1.1578        | 0.075*                           |
| C6  | 1.7397 (4)  | 0.6832 (3)  | 1.07254 (19)  | 0.0557 (10)                      |
| C7  | 1.4773 (4)  | 0.6405 (3)  | 1.03879 (19)  | 0.0600 (10)                      |
| H7A | 1.4508      | 0.6985      | 1.0600        | 0.072*                           |
| H7B | 1.5037      | 0.5873      | 1.0735        | 0.072*                           |
| C8  | 1.3450 (4)  | 0.6102 (3)  | 0.97345 (19)  | 0.0528 (9)                       |
| C9  | 1.2098 (4)  | 0.5805 (3)  | 0.9801 (2)    | 0.0617 (11)                      |
| H9  | 1.2015      | 0.5800      | 1.0244        | 0.074*                           |
| C10 | 1.0896 (4)  | 0.5522 (3)  | 0.9206 (2)    | 0.0625 (10)                      |
| H10 | 1.0001      | 0.5323      | 0.9257        | 0.075*                           |
| C11 | 1.2229 (5)  | 0.5806 (3)  | 0.8502 (2)    | 0.0723 (12)                      |
| H11 | 1.2284      | 0.5804      | 0.8053        | 0.087*                           |
| C12 | 1.3483 (4)  | 0.6109 (3)  | 0.9068 (2)    | 0.0631 (11)                      |
| H12 | 1.4354      | 0.6318      | 0.8998        | 0.076*                           |
| C13 | 0.6144 (5)  | 0.5569 (4)  | 0.6534 (2)    | 0.0676 (11)                      |
| H13 | 0.6493      | 0.6168      | 0.6763        | 0.081*                           |
| C14 | 0.4742 (4)  | 0.5559 (3)  | 0.5987 (2)    | 0.0620 (10)                      |
| H14 | 0.4168      | 0.6136      | 0.5854        | 0.074*                           |

|      |             |            |              |             |
|------|-------------|------------|--------------|-------------|
| C15  | 0.4202 (4)  | 0.4684 (3) | 0.56382 (18) | 0.0508 (9)  |
| C16  | 0.5105 (5)  | 0.3864 (3) | 0.5868 (2)   | 0.0653 (11) |
| H16  | 0.4781      | 0.3255     | 0.5650       | 0.078*      |
| C17  | 0.6492 (5)  | 0.3944 (4) | 0.6421 (2)   | 0.0677 (11) |
| H17  | 0.7085      | 0.3376     | 0.6568       | 0.081*      |
| C18  | 0.2680 (4)  | 0.4611 (3) | 0.50477 (19) | 0.0562 (10) |
| H18A | 0.2775      | 0.4262     | 0.4648       | 0.067*      |
| H18B | 0.1983      | 0.4245     | 0.5206       | 0.067*      |
| C19  | 0.0684 (4)  | 0.5651 (3) | 0.43111 (18) | 0.0536 (9)  |
| C20  | -0.0174 (4) | 0.4872 (3) | 0.3943 (2)   | 0.0585 (10) |
| H20  | 0.0204      | 0.4230     | 0.4042       | 0.070*      |
| C21  | -0.1600 (4) | 0.5033 (3) | 0.34252 (19) | 0.0604 (10) |
| H21  | -0.2179     | 0.4500     | 0.3178       | 0.072*      |
| C22  | -0.2163 (4) | 0.5970 (4) | 0.32752 (19) | 0.0611 (11) |
| C23  | -0.1309 (5) | 0.6762 (3) | 0.3639 (2)   | 0.0657 (11) |
| H23  | -0.1688     | 0.7403     | 0.3537       | 0.079*      |
| C24  | 0.0111 (5)  | 0.6598 (3) | 0.4155 (2)   | 0.0644 (11) |
| H24  | 0.0690      | 0.7132     | 0.4402       | 0.077*      |
| O5   | -0.6790 (5) | 0.5495 (3) | 0.15883 (18) | 0.1028 (11) |
| O6   | -0.7139 (5) | 0.3980 (4) | 0.1501 (3)   | 0.169 (2)   |
| O7   | -0.4972 (4) | 0.4493 (3) | 0.21269 (17) | 0.0924 (10) |
| N3   | -0.6322 (5) | 0.4659 (4) | 0.1726 (2)   | 0.0748 (11) |
| O8   | -0.4291 (3) | 0.2671 (2) | 0.29281 (18) | 0.0947 (10) |
| H31  | -0.4422     | 0.3165     | 0.2651       | 0.142*      |
| H32  | -0.4804     | 0.2184     | 0.2694       | 0.142*      |

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

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$      | $U^{13}$     | $U^{23}$      |
|-----|-------------|-------------|-------------|---------------|--------------|---------------|
| Ag1 | 0.0540 (2)  | 0.1015 (3)  | 0.0613 (2)  | -0.01044 (19) | 0.00368 (15) | -0.00670 (19) |
| O1  | 0.0576 (18) | 0.114 (3)   | 0.0640 (17) | -0.0152 (17)  | 0.0045 (15)  | -0.0085 (16)  |
| O2  | 0.0477 (16) | 0.094 (2)   | 0.0534 (15) | -0.0097 (15)  | 0.0109 (13)  | 0.0040 (14)   |
| O3  | 0.0646 (18) | 0.097 (2)   | 0.0640 (17) | 0.0063 (17)   | 0.0008 (15)  | 0.0130 (16)   |
| O4  | 0.0518 (17) | 0.0639 (19) | 0.0626 (16) | -0.0080 (14)  | 0.0031 (14)  | 0.0036 (14)   |
| N1  | 0.049 (2)   | 0.061 (2)   | 0.059 (2)   | -0.0014 (17)  | 0.0082 (16)  | -0.0005 (16)  |
| N2  | 0.050 (2)   | 0.078 (3)   | 0.0505 (18) | -0.0069 (18)  | 0.0148 (16)  | -0.0006 (17)  |
| C1  | 0.060 (3)   | 0.071 (3)   | 0.054 (2)   | -0.004 (2)    | 0.021 (2)    | 0.0004 (19)   |
| C2  | 0.050 (2)   | 0.070 (3)   | 0.062 (2)   | -0.003 (2)    | 0.016 (2)    | 0.000 (2)     |
| C3  | 0.048 (2)   | 0.056 (3)   | 0.061 (2)   | -0.0021 (19)  | 0.005 (2)    | 0.0006 (19)   |
| C4  | 0.063 (3)   | 0.080 (3)   | 0.049 (2)   | -0.004 (2)    | 0.015 (2)    | -0.004 (2)    |
| C5  | 0.055 (2)   | 0.076 (3)   | 0.054 (2)   | -0.002 (2)    | 0.017 (2)    | 0.001 (2)     |
| C6  | 0.048 (2)   | 0.055 (3)   | 0.054 (2)   | -0.0013 (18)  | 0.0072 (19)  | 0.0030 (18)   |
| C7  | 0.046 (2)   | 0.071 (3)   | 0.057 (2)   | -0.004 (2)    | 0.0127 (19)  | -0.0061 (19)  |
| C8  | 0.051 (2)   | 0.044 (2)   | 0.057 (2)   | 0.0041 (18)   | 0.0119 (18)  | -0.0015 (17)  |
| C9  | 0.054 (2)   | 0.074 (3)   | 0.054 (2)   | -0.003 (2)    | 0.017 (2)    | 0.001 (2)     |
| C10 | 0.049 (2)   | 0.072 (3)   | 0.061 (2)   | -0.004 (2)    | 0.014 (2)    | 0.002 (2)     |
| C11 | 0.066 (3)   | 0.096 (4)   | 0.052 (2)   | -0.008 (3)    | 0.018 (2)    | -0.002 (2)    |
| C12 | 0.055 (2)   | 0.075 (3)   | 0.057 (2)   | -0.012 (2)    | 0.017 (2)    | -0.003 (2)    |

|     |           |           |             |              |             |              |
|-----|-----------|-----------|-------------|--------------|-------------|--------------|
| C13 | 0.066 (3) | 0.067 (3) | 0.062 (2)   | -0.015 (2)   | 0.015 (2)   | -0.009 (2)   |
| C14 | 0.054 (3) | 0.061 (3) | 0.063 (2)   | -0.005 (2)   | 0.013 (2)   | 0.001 (2)    |
| C15 | 0.046 (2) | 0.063 (3) | 0.0435 (19) | -0.0065 (18) | 0.0169 (17) | -0.0004 (17) |
| C16 | 0.060 (3) | 0.063 (3) | 0.061 (2)   | 0.002 (2)    | 0.010 (2)   | -0.010 (2)   |
| C17 | 0.062 (3) | 0.074 (3) | 0.057 (2)   | 0.005 (2)    | 0.012 (2)   | -0.001 (2)   |
| C18 | 0.052 (2) | 0.065 (3) | 0.049 (2)   | -0.005 (2)   | 0.0150 (19) | -0.0022 (18) |
| C19 | 0.046 (2) | 0.065 (3) | 0.048 (2)   | -0.009 (2)   | 0.0151 (18) | 0.0033 (19)  |
| C20 | 0.055 (2) | 0.058 (3) | 0.057 (2)   | 0.001 (2)    | 0.0141 (19) | -0.0002 (19) |
| C21 | 0.059 (2) | 0.071 (3) | 0.0472 (19) | -0.010 (2)   | 0.0144 (18) | -0.006 (2)   |
| C22 | 0.056 (3) | 0.079 (3) | 0.044 (2)   | 0.000 (2)    | 0.0134 (19) | 0.008 (2)    |
| C23 | 0.072 (3) | 0.057 (3) | 0.063 (2)   | 0.006 (2)    | 0.019 (2)   | 0.011 (2)    |
| C24 | 0.065 (3) | 0.061 (3) | 0.057 (2)   | -0.009 (2)   | 0.010 (2)   | 0.002 (2)    |
| O5  | 0.110 (3) | 0.107 (3) | 0.076 (2)   | 0.020 (3)    | 0.017 (2)   | 0.013 (2)    |
| O6  | 0.090 (3) | 0.114 (4) | 0.244 (6)   | -0.034 (3)   | -0.006 (3)  | -0.019 (4)   |
| O7  | 0.054 (2) | 0.119 (3) | 0.088 (2)   | 0.0052 (19)  | 0.0086 (18) | -0.010 (2)   |
| N3  | 0.056 (3) | 0.097 (4) | 0.066 (2)   | -0.005 (2)   | 0.017 (2)   | -0.007 (2)   |
| O8  | 0.072 (2) | 0.089 (2) | 0.115 (3)   | -0.0035 (18) | 0.0242 (19) | -0.0212 (19) |

*Geometric parameters (Å, °)*

|        |           |          |           |
|--------|-----------|----------|-----------|
| Ag1—N1 | 2.126 (3) | C10—H10  | 0.9300    |
| Ag1—N2 | 2.128 (3) | C11—C12  | 1.368 (5) |
| O1—C3  | 1.366 (4) | C11—H11  | 0.9300    |
| O1—H1A | 0.8200    | C12—H12  | 0.9300    |
| O2—C6  | 1.377 (4) | C13—C14  | 1.374 (5) |
| O2—C7  | 1.411 (4) | C13—H13  | 0.9300    |
| O3—C22 | 1.377 (4) | C14—C15  | 1.374 (5) |
| O3—H3  | 0.8201    | C14—H14  | 0.9300    |
| O4—C19 | 1.373 (4) | C15—C16  | 1.370 (5) |
| O4—C18 | 1.411 (5) | C15—C18  | 1.491 (5) |
| N1—C11 | 1.328 (5) | C16—C17  | 1.375 (5) |
| N1—C10 | 1.330 (5) | C16—H16  | 0.9300    |
| N2—C17 | 1.321 (5) | C17—H17  | 0.9300    |
| N2—C13 | 1.323 (5) | C18—H18A | 0.9700    |
| C1—C2  | 1.369 (5) | C18—H18B | 0.9700    |
| C1—C6  | 1.384 (5) | C19—C20  | 1.368 (5) |
| C1—H1  | 0.9300    | C19—C24  | 1.379 (5) |
| C2—C3  | 1.380 (5) | C20—C21  | 1.382 (5) |
| C2—H2  | 0.9300    | C20—H20  | 0.9300    |
| C3—C4  | 1.371 (5) | C21—C22  | 1.362 (5) |
| C4—C5  | 1.376 (5) | C21—H21  | 0.9300    |
| C4—H4  | 0.9300    | C22—C23  | 1.377 (6) |
| C5—C6  | 1.373 (5) | C23—C24  | 1.376 (5) |
| C5—H5  | 0.9300    | C23—H23  | 0.9300    |
| C7—C8  | 1.499 (5) | C24—H24  | 0.9300    |
| C7—H7A | 0.9700    | O5—N3    | 1.206 (5) |
| C7—H7B | 0.9700    | O6—N3    | 1.176 (5) |
| C8—C12 | 1.364 (5) | O7—N3    | 1.251 (5) |

|            |             |               |           |
|------------|-------------|---------------|-----------|
| C8—C9      | 1.394 (5)   | O8—H31        | 0.8500    |
| C9—C10     | 1.367 (5)   | O8—H32        | 0.8499    |
| C9—H9      | 0.9300      |               |           |
| N1—Ag1—N2  | 167.10 (13) | C8—C12—C11    | 119.7 (4) |
| C3—O1—H1A  | 109.5       | C8—C12—H12    | 120.2     |
| C6—O2—C7   | 117.6 (3)   | C11—C12—H12   | 120.2     |
| C22—O3—H3  | 109.5       | N2—C13—C14    | 124.3 (4) |
| C19—O4—C18 | 117.3 (3)   | N2—C13—H13    | 117.8     |
| C11—N1—C10 | 116.8 (3)   | C14—C13—H13   | 117.8     |
| C11—N1—Ag1 | 121.6 (3)   | C15—C14—C13   | 119.0 (4) |
| C10—N1—Ag1 | 121.5 (3)   | C15—C14—H14   | 120.5     |
| C17—N2—C13 | 116.1 (4)   | C13—C14—H14   | 120.5     |
| C17—N2—Ag1 | 127.1 (3)   | C16—C15—C14   | 117.1 (4) |
| C13—N2—Ag1 | 116.6 (3)   | C16—C15—C18   | 120.7 (4) |
| C2—C1—C6   | 120.8 (4)   | C14—C15—C18   | 122.1 (4) |
| C2—C1—H1   | 119.6       | C15—C16—C17   | 119.9 (4) |
| C6—C1—H1   | 119.6       | C15—C16—H16   | 120.1     |
| C1—C2—C3   | 120.2 (4)   | C17—C16—H16   | 120.1     |
| C1—C2—H2   | 119.9       | N2—C17—C16    | 123.5 (4) |
| C3—C2—H2   | 119.9       | N2—C17—H17    | 118.2     |
| O1—C3—C4   | 117.6 (3)   | C16—C17—H17   | 118.2     |
| O1—C3—C2   | 123.5 (4)   | O4—C18—C15    | 109.1 (3) |
| C4—C3—C2   | 118.8 (4)   | O4—C18—H18A   | 109.9     |
| C3—C4—C5   | 121.3 (4)   | C15—C18—H18A  | 109.9     |
| C3—C4—H4   | 119.3       | O4—C18—H18B   | 109.9     |
| C5—C4—H4   | 119.3       | C15—C18—H18B  | 109.9     |
| C6—C5—C4   | 119.8 (4)   | H18A—C18—H18B | 108.3     |
| C6—C5—H5   | 120.1       | C20—C19—O4    | 125.0 (4) |
| C4—C5—H5   | 120.1       | C20—C19—C24   | 119.1 (4) |
| C5—C6—O2   | 124.8 (3)   | O4—C19—C24    | 115.8 (4) |
| C5—C6—C1   | 119.1 (4)   | C19—C20—C21   | 120.3 (4) |
| O2—C6—C1   | 116.2 (3)   | C19—C20—H20   | 119.9     |
| O2—C7—C8   | 108.4 (3)   | C21—C20—H20   | 119.9     |
| O2—C7—H7A  | 110.0       | C22—C21—C20   | 120.4 (4) |
| C8—C7—H7A  | 110.0       | C22—C21—H21   | 119.8     |
| O2—C7—H7B  | 110.0       | C20—C21—H21   | 119.8     |
| C8—C7—H7B  | 110.0       | C21—C22—C23   | 120.0 (4) |
| H7A—C7—H7B | 108.4       | C21—C22—O3    | 122.7 (4) |
| C12—C8—C9  | 117.4 (4)   | C23—C22—O3    | 117.3 (4) |
| C12—C8—C7  | 123.5 (4)   | C24—C23—C22   | 119.5 (4) |
| C9—C8—C7   | 119.0 (3)   | C24—C23—H23   | 120.2     |
| C10—C9—C8  | 119.0 (4)   | C22—C23—H23   | 120.2     |
| C10—C9—H9  | 120.5       | C23—C24—C19   | 120.7 (4) |
| C8—C9—H9   | 120.5       | C23—C24—H24   | 119.6     |
| N1—C10—C9  | 123.5 (4)   | C19—C24—H24   | 119.6     |
| N1—C10—H10 | 118.2       | O6—N3—O5      | 120.7 (5) |
| C9—C10—H10 | 118.2       | O6—N3—O7      | 118.3 (5) |

|             |           |            |           |
|-------------|-----------|------------|-----------|
| N1—C11—C12  | 123.6 (4) | O5—N3—O7   | 121.0 (5) |
| N1—C11—H11  | 118.2     | H31—O8—H32 | 109.0     |
| C12—C11—H11 | 118.2     |            |           |

*Hydrogen-bond geometry (Å, °)*

| <i>D—H...A</i>            | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|---------------------------|------------|--------------|--------------|----------------|
| O1—H1A...O8 <sup>i</sup>  | 0.82       | 1.90         | 2.661 (4)    | 155            |
| O3—H3...O7                | 0.82       | 1.88         | 2.698 (5)    | 176            |
| O8—H31...O7               | 0.85       | 2.05         | 2.885 (5)    | 167            |
| O8—H32...O3 <sup>ii</sup> | 0.85       | 2.00         | 2.833 (4)    | 165            |

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