

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

Aquabis[*N'*-(2-hydroxybenzylidene)-isonicotinohydrazide- κ N]silver(I) nitrate

Shahriar Ghammamy,^{a*} Hajar Sahebalzamani,^b Nina Khaligh^b and Rahmatollah Rahimi^c

^aDepartment of Chemistry, Faculty of Science, Imam Khomeini International University, Ghazvin, Iran, ^bDepartment of Chemistry, Faculty of Science, Islamic Azad University Ardebil Branch, Ardebil, Iran, and ^cFaculty of Chemistry, Iran University of Science and Technology, Tehran, Iran

Correspondence e-mail: shghamamy@yahoo.com

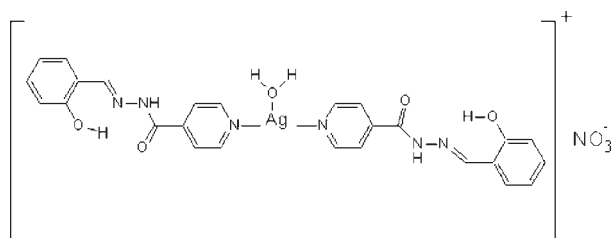
Received 15 January 2010; accepted 8 February 2010

Key indicators: single-crystal X-ray study; $T = 120$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.029; wR factor = 0.077; data-to-parameter ratio = 15.9.

In the title compound, $[\text{Ag}(\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})]\text{NO}_3$, two N atoms from two pyridine rings of two *N'*-(2-hydroxybenzylidene)isonicotinohydrazide ligands coordinate to the Ag^{I} atom, forming a nearly linear geometry with an $\text{N}-\text{Ag}-\text{N}$ angle of $171.63(6)^\circ$; a water O atom is located at the apical site, completing the T-shaped coordination. The crystal structure is stabilized by extensive $\text{O}-\text{H}\cdots\text{O}$, $\text{O}-\text{H}\cdots\text{N}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonding.

Related literature

For factors affecting the coordination geometry of silver, see: Dong *et al.* (2004); Niu *et al.* (2009a); Sumbly & Hardie (2005); Abu-Youssef *et al.* (2007). For related structures, see: Li *et al.* (2006); Näther & Beck (2004); Niu *et al.* (2009b).



Experimental

Crystal data

$[\text{Ag}(\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})]\text{NO}_3$ $b = 12.6459(6)$ Å
 $M_r = 670.39$ $c = 18.5719(9)$ Å
 Monoclinic, $P2_1/c$ $\beta = 104.738(1)^\circ$
 $a = 11.7194(6)$ Å $V = 2661.8(2)$ Å³

$Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.82$ mm⁻¹

$T = 120$ K
 $0.55 \times 0.45 \times 0.30$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1998)
 $T_{\text{min}} = 0.686$, $T_{\text{max}} = 0.791$

26832 measured reflections
 6427 independent reflections
 5518 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.026$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
 $wR(F^2) = 0.077$
 $S = 1.07$
 6427 reflections
 403 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.04$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.57$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{O1W}-\text{H1W}\cdots\text{O7}^{\text{i}}$ | 0.84 (3) | 2.01 (3) | 2.844 (2) | 171 (3) |
| $\text{O1W}-\text{H2W}\cdots\text{O2}^{\text{ii}}$ | 0.79 (3) | 2.04 (3) | 2.821 (2) | 172 (3) |
| $\text{N2}-\text{H2N}\cdots\text{O6}$ | 0.84 (3) | 2.09 (3) | 2.880 (2) | 157 (2) |
| $\text{N5}-\text{H5N}\cdots\text{O7}^{\text{iii}}$ | 0.90 (3) | 1.97 (3) | 2.863 (2) | 169 (2) |
| $\text{O2}-\text{H2O}\cdots\text{N3}$ | 0.85 (3) | 1.79 (3) | 2.560 (2) | 150 (2) |
| $\text{O4}-\text{H4O}\cdots\text{N6}$ | 0.81 (2) | 1.86 (2) | 2.607 (2) | 153 (2) |

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

Data collection: SMART (Bruker, 2007); cell refinement: SAINT-Plus (Bruker, 2007); 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.

The authors thank Dr M. Amirnasr, Dr A. R. Mahjoub and Dr N. Safari for valuable discussions.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2256).

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supporting information

Acta Cryst. (2010). E66, m294 [doi:10.1107/S1600536810005027]

Aquabis[N'-(2-hydroxybenzylidene)isonicotinohydrazide- κ N]silver(I) nitrate**Shahriar Ghammamy, Hajar Sahebalzamani, Nina Khaligh and Rahmatollah Rahimi****S1. Comment**

It is noteworthy that the coordination geometry of the silver metal center can be affected by many factors, such as coordination nature of organic ligands, temperature, counteranions, etc. (Dong *et al.*, 2004; Niu *et al.*, 2009a; Sumbly & Hardie, 2005; Abu-Youssef *et al.*, 2007). The crystal structures of bis(pyridine-4-carboxylic acid-N)silver(I) nitrate dihydrate (Li *et al.*, 2006), chlorotris(3-methylpyridine-N)silver(I) (Näther & Beck, 2004) and bis[N0-(3-cyanobenzylidene)isonicotinohydrazide]silver(I) trifluoroacetate (Niu *et al.*, 2009b) have been reported. We have synthesized a new coordination complex of silver using N'-(2-hydroxybenzylidene)isonicotinohydrazide ligand, (I), and determined its crystal structure which is presented in this article.

The central Ag atom in (I) is coordinated by two nitrogen atoms from two pyridine rings of two different ligands and a water O atom located at the apical site, defining slightly distorted linear coordination geometry (Fig. 1). The cations, anions and solvent water molecules are linked by O—H \cdots O, O—H \cdots N and N—H \cdots O hydrogen bonds into a three-dimensional network (Table 1).

S2. Experimental

A solution of N'-(2-hydroxybenzylidene)isonicotinohydrazide (0.14 g, 1 mol) in CH₃OH (10 ml) was added to an aqueous solution of AgNO₃ (0.1 g, 1 mol) in water (5 ml) with stirring at 333 K. A small amount of precipitate was removed from the resulting solution to grow crystals for crystallographic study. Prism shaped colorless crystals of (I) were obtained by slow evaporation of the solvent from a solution of (I) in CCl₄ at room temperature over a period of 3 d.

S3. Refinement

The hydrogen atoms bonded to N and O atoms were located from a difference Fourier map and were allowed to refine freely. The aryl H atoms were placed in calculated position with C—H = 0.95 Å in riding mode, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$ of the carrier C atoms. The residual electron density in the final difference map was located in the close proximity of Ag atom and was essentially meaningless.

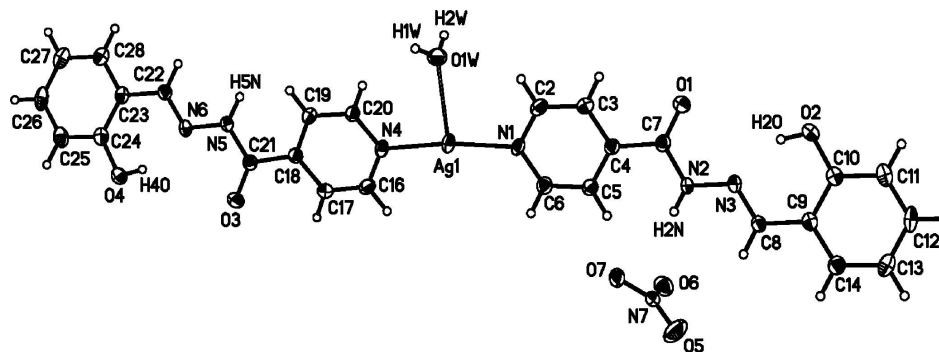


Figure 1

The asymmetric unit of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

Aquabis[*N'*-(2-hydroxybenzylidene)isonicotinohydrazide- κ N]silver(I) nitrate

Crystal data

$[\text{Ag}(\text{C}_{13}\text{H}_{11}\text{N}_3\text{O}_2)_2(\text{H}_2\text{O})]\text{NO}_3$

$M_r = 670.39$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.7194(6) \text{ \AA}$

$b = 12.6459(6) \text{ \AA}$

$c = 18.5719(9) \text{ \AA}$

$\beta = 104.738(1)^\circ$

$V = 2661.8(2) \text{ \AA}^3$

$Z = 4$

$F(000) = 1360$

$D_x = 1.673 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 530 reflections

$\theta = 3\text{--}28^\circ$

$\mu = 0.82 \text{ mm}^{-1}$

$T = 120 \text{ K}$

Prism, colourless

$0.55 \times 0.45 \times 0.30 \text{ mm}$

Data collection

Bruker SMART 1000 CCD area-detector
diffractometer

Radiation source: normal-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: multi-scan

(*SADABS*; Sheldrick, 1998)

$T_{\min} = 0.686$, $T_{\max} = 0.791$

26832 measured reflections

6427 independent reflections

5518 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\max} = 28.0^\circ$, $\theta_{\min} = 1.8^\circ$

$h = -15 \rightarrow 15$

$k = -16 \rightarrow 16$

$l = -24 \rightarrow 24$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.029$

$wR(F^2) = 0.077$

$S = 1.07$

6427 reflections

403 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

H atoms treated by a mixture of independent
and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0415P)^2 + 1.2646P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.002$

$\Delta\rho_{\max} = 1.04 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.57 \text{ e \AA}^{-3}$

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 $F^2 > 2\sigma(F^2)$ 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> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|------|---------------|---------------|---------------|----------------------------------|
| Ag1 | 0.775957 (12) | 0.740141 (11) | 0.273949 (7) | 0.02310 (6) |
| O1 | 0.34784 (12) | 0.58945 (10) | -0.05478 (8) | 0.0300 (3) |
| O2 | 0.13029 (13) | 0.62068 (10) | -0.23755 (8) | 0.0270 (3) |
| H2O | 0.174 (2) | 0.642 (2) | -0.1962 (14) | 0.039 (7)* |
| O3 | 1.18823 (12) | 0.93761 (10) | 0.59595 (8) | 0.0296 (3) |
| O4 | 1.41552 (13) | 0.91337 (11) | 0.78672 (8) | 0.0281 (3) |
| H4O | 1.373 (2) | 0.8915 (19) | 0.7484 (14) | 0.036 (7)* |
| N1 | 0.64148 (14) | 0.72810 (12) | 0.17184 (8) | 0.0205 (3) |
| N2 | 0.31651 (14) | 0.76550 (12) | -0.06954 (8) | 0.0187 (3) |
| H2N | 0.3355 (19) | 0.827 (2) | -0.0542 (12) | 0.026 (6)* |
| N3 | 0.23344 (14) | 0.74841 (11) | -0.13455 (9) | 0.0184 (3) |
| N4 | 0.91745 (13) | 0.77455 (12) | 0.37111 (8) | 0.0196 (3) |
| N5 | 1.23864 (14) | 0.76411 (12) | 0.61217 (9) | 0.0187 (3) |
| H5N | 1.239 (2) | 0.700 (2) | 0.5912 (15) | 0.045 (7)* |
| N6 | 1.31761 (13) | 0.78524 (12) | 0.67872 (8) | 0.0197 (3) |
| C2 | 0.59564 (16) | 0.63071 (15) | 0.14847 (10) | 0.0246 (4) |
| H2A | 0.6244 | 0.5710 | 0.1787 | 0.030* |
| C3 | 0.50945 (16) | 0.61508 (14) | 0.08293 (10) | 0.0235 (4) |
| H3A | 0.4807 | 0.5460 | 0.0687 | 0.028* |
| C4 | 0.46537 (15) | 0.70135 (14) | 0.03811 (9) | 0.0194 (3) |
| C5 | 0.51035 (16) | 0.80089 (14) | 0.06191 (10) | 0.0216 (3) |
| H5A | 0.4820 | 0.8618 | 0.0329 | 0.026* |
| C6 | 0.59588 (16) | 0.81041 (15) | 0.12748 (10) | 0.0229 (4) |
| H6A | 0.6248 | 0.8792 | 0.1426 | 0.027* |
| C7 | 0.37251 (15) | 0.67941 (14) | -0.03274 (10) | 0.0200 (3) |
| C8 | 0.17347 (15) | 0.82700 (14) | -0.16895 (9) | 0.0194 (3) |
| H8A | 0.1879 | 0.8968 | -0.1499 | 0.023* |
| C9 | 0.08375 (15) | 0.80705 (14) | -0.23707 (10) | 0.0200 (3) |
| C10 | 0.06388 (16) | 0.70525 (15) | -0.26912 (10) | 0.0210 (3) |
| C11 | -0.02388 (17) | 0.68925 (17) | -0.33365 (10) | 0.0273 (4) |
| H11A | -0.0355 | 0.6209 | -0.3555 | 0.033* |
| C12 | -0.09495 (17) | 0.77244 (17) | -0.36661 (11) | 0.0280 (4) |
| H12A | -0.1553 | 0.7608 | -0.4109 | 0.034* |
| C13 | -0.07862 (17) | 0.87339 (17) | -0.33525 (10) | 0.0281 (4) |
| H13A | -0.1282 | 0.9302 | -0.3575 | 0.034* |

| | | | | |
|------|--------------|--------------|---------------|------------|
| C14 | 0.01051 (16) | 0.88956 (15) | -0.27153 (10) | 0.0241 (4) |
| H14A | 0.0224 | 0.9584 | -0.2506 | 0.029* |
| C16 | 0.96229 (16) | 0.87207 (14) | 0.38692 (10) | 0.0234 (4) |
| H16A | 0.9344 | 0.9272 | 0.3522 | 0.028* |
| C17 | 1.04701 (16) | 0.89570 (14) | 0.45134 (10) | 0.0231 (4) |
| H19B | 1.0772 | 0.9655 | 0.4602 | 0.028* |
| C18 | 1.08769 (15) | 0.81621 (14) | 0.50305 (9) | 0.0194 (3) |
| C19 | 1.04189 (16) | 0.71489 (15) | 0.48736 (10) | 0.0207 (3) |
| H19A | 1.0678 | 0.6587 | 0.5215 | 0.025* |
| C20 | 0.95837 (16) | 0.69751 (14) | 0.42146 (10) | 0.0211 (3) |
| H20A | 0.9280 | 0.6280 | 0.4109 | 0.025* |
| C21 | 1.17579 (15) | 0.84614 (14) | 0.57436 (9) | 0.0200 (3) |
| C22 | 1.38215 (15) | 0.70897 (14) | 0.71241 (10) | 0.0200 (3) |
| H22A | 1.3736 | 0.6401 | 0.6913 | 0.024* |
| C23 | 1.46765 (16) | 0.72811 (14) | 0.78232 (10) | 0.0209 (3) |
| C24 | 1.48193 (16) | 0.82865 (15) | 0.81647 (10) | 0.0224 (4) |
| C25 | 1.56702 (17) | 0.84345 (16) | 0.88292 (10) | 0.0279 (4) |
| H25A | 1.5760 | 0.9109 | 0.9062 | 0.033* |
| C26 | 1.63897 (18) | 0.76048 (17) | 0.91552 (11) | 0.0303 (4) |
| H26A | 1.6972 | 0.7718 | 0.9608 | 0.036* |
| C27 | 1.62699 (17) | 0.66057 (17) | 0.88272 (11) | 0.0309 (4) |
| H27A | 1.6768 | 0.6040 | 0.9052 | 0.037* |
| C28 | 1.54123 (17) | 0.64503 (16) | 0.81680 (10) | 0.0264 (4) |
| H28A | 1.5320 | 0.5769 | 0.7945 | 0.032* |
| N7 | 0.23978 (14) | 0.99376 (11) | -0.00096 (8) | 0.0240 (3) |
| O5 | 0.14711 (16) | 1.04260 (14) | -0.02193 (9) | 0.0520 (5) |
| O6 | 0.31228 (13) | 0.98880 (11) | -0.03995 (8) | 0.0314 (3) |
| O7 | 0.26376 (13) | 0.94629 (10) | 0.06137 (7) | 0.0284 (3) |
| O1W | 0.76685 (14) | 0.54006 (11) | 0.30562 (9) | 0.0308 (3) |
| H1W | 0.759 (2) | 0.519 (2) | 0.3471 (15) | 0.039 (7)* |
| H2W | 0.801 (3) | 0.496 (2) | 0.2897 (16) | 0.055 (9)* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|-------------|--------------|-------------|
| Ag1 | 0.01855 (9) | 0.03073 (9) | 0.01712 (8) | 0.00154 (5) | -0.00076 (6) | 0.00185 (5) |
| O1 | 0.0320 (7) | 0.0221 (7) | 0.0302 (7) | 0.0029 (5) | -0.0025 (6) | -0.0047 (5) |
| O2 | 0.0318 (7) | 0.0214 (6) | 0.0253 (7) | -0.0001 (5) | 0.0029 (6) | -0.0062 (5) |
| O3 | 0.0332 (7) | 0.0218 (7) | 0.0290 (7) | 0.0022 (5) | -0.0009 (6) | -0.0058 (5) |
| O4 | 0.0323 (7) | 0.0235 (7) | 0.0249 (7) | -0.0031 (5) | 0.0005 (6) | -0.0050 (5) |
| N1 | 0.0221 (8) | 0.0266 (8) | 0.0132 (7) | 0.0085 (6) | 0.0052 (6) | 0.0035 (6) |
| N2 | 0.0184 (7) | 0.0197 (7) | 0.0154 (7) | -0.0004 (5) | -0.0008 (6) | -0.0019 (5) |
| N3 | 0.0173 (7) | 0.0232 (7) | 0.0146 (7) | -0.0013 (5) | 0.0037 (6) | -0.0008 (5) |
| N4 | 0.0150 (7) | 0.0264 (8) | 0.0164 (7) | 0.0022 (6) | 0.0021 (6) | 0.0014 (6) |
| N5 | 0.0191 (7) | 0.0195 (7) | 0.0159 (7) | -0.0015 (5) | 0.0013 (6) | -0.0021 (5) |
| N6 | 0.0180 (7) | 0.0246 (7) | 0.0152 (7) | -0.0021 (6) | 0.0020 (6) | -0.0019 (6) |
| C2 | 0.0235 (9) | 0.0239 (9) | 0.0252 (9) | 0.0064 (7) | 0.0039 (7) | 0.0050 (7) |
| C3 | 0.0244 (9) | 0.0212 (8) | 0.0238 (9) | 0.0037 (7) | 0.0040 (7) | 0.0011 (7) |

| | | | | | | |
|-----|-------------|-------------|-------------|-------------|-------------|-------------|
| C4 | 0.0196 (8) | 0.0206 (8) | 0.0185 (8) | 0.0033 (6) | 0.0057 (7) | 0.0011 (6) |
| C5 | 0.0213 (9) | 0.0209 (9) | 0.0219 (9) | 0.0012 (7) | 0.0038 (7) | 0.0013 (7) |
| C6 | 0.0219 (9) | 0.0231 (9) | 0.0223 (9) | -0.0023 (7) | 0.0029 (7) | 0.0010 (7) |
| C7 | 0.0171 (8) | 0.0233 (8) | 0.0190 (8) | 0.0028 (6) | 0.0037 (6) | -0.0002 (6) |
| C8 | 0.0198 (8) | 0.0198 (8) | 0.0178 (8) | -0.0020 (6) | 0.0034 (6) | -0.0018 (6) |
| C9 | 0.0202 (8) | 0.0222 (8) | 0.0183 (8) | -0.0035 (7) | 0.0057 (7) | -0.0006 (6) |
| C10 | 0.0201 (8) | 0.0241 (9) | 0.0200 (8) | -0.0031 (7) | 0.0071 (7) | -0.0011 (7) |
| C11 | 0.0253 (9) | 0.0357 (11) | 0.0205 (9) | -0.0067 (8) | 0.0054 (7) | -0.0057 (8) |
| C12 | 0.0178 (9) | 0.0488 (12) | 0.0149 (8) | -0.0055 (8) | -0.0005 (7) | 0.0011 (8) |
| C13 | 0.0230 (9) | 0.0377 (11) | 0.0226 (9) | 0.0023 (8) | 0.0039 (7) | 0.0087 (8) |
| C14 | 0.0269 (9) | 0.0248 (9) | 0.0206 (9) | -0.0011 (7) | 0.0062 (7) | 0.0024 (7) |
| C16 | 0.0252 (9) | 0.0213 (8) | 0.0234 (9) | 0.0046 (7) | 0.0059 (7) | 0.0044 (7) |
| C17 | 0.0263 (9) | 0.0190 (8) | 0.0237 (9) | 0.0006 (7) | 0.0054 (7) | -0.0001 (7) |
| C18 | 0.0192 (8) | 0.0207 (8) | 0.0189 (8) | 0.0020 (6) | 0.0060 (7) | -0.0010 (6) |
| C19 | 0.0197 (8) | 0.0217 (8) | 0.0197 (8) | -0.0001 (7) | 0.0034 (7) | 0.0030 (7) |
| C20 | 0.0222 (8) | 0.0200 (8) | 0.0188 (8) | -0.0012 (7) | 0.0014 (7) | 0.0012 (6) |
| C21 | 0.0196 (8) | 0.0213 (8) | 0.0192 (8) | 0.0003 (6) | 0.0053 (7) | -0.0006 (6) |
| C22 | 0.0214 (8) | 0.0198 (8) | 0.0183 (8) | -0.0023 (7) | 0.0040 (7) | -0.0009 (6) |
| C23 | 0.0191 (8) | 0.0260 (9) | 0.0174 (8) | -0.0034 (7) | 0.0042 (7) | 0.0009 (7) |
| C24 | 0.0203 (8) | 0.0262 (9) | 0.0208 (8) | -0.0057 (7) | 0.0056 (7) | 0.0002 (7) |
| C25 | 0.0262 (10) | 0.0348 (10) | 0.0219 (9) | -0.0109 (8) | 0.0046 (7) | -0.0032 (8) |
| C26 | 0.0202 (9) | 0.0496 (13) | 0.0180 (9) | -0.0098 (8) | -0.0006 (7) | 0.0044 (8) |
| C27 | 0.0241 (10) | 0.0411 (11) | 0.0261 (10) | 0.0006 (8) | 0.0036 (8) | 0.0104 (8) |
| C28 | 0.0261 (9) | 0.0283 (9) | 0.0242 (9) | 0.0001 (7) | 0.0052 (7) | 0.0046 (7) |
| N7 | 0.0332 (8) | 0.0160 (7) | 0.0185 (7) | 0.0010 (6) | -0.0012 (6) | -0.0018 (5) |
| O5 | 0.0536 (11) | 0.0551 (11) | 0.0430 (9) | 0.0335 (9) | 0.0045 (8) | 0.0096 (8) |
| O6 | 0.0413 (8) | 0.0264 (7) | 0.0276 (7) | -0.0055 (6) | 0.0108 (6) | -0.0014 (5) |
| O7 | 0.0404 (8) | 0.0210 (6) | 0.0192 (6) | -0.0051 (6) | -0.0007 (6) | 0.0023 (5) |
| O1W | 0.0431 (9) | 0.0238 (7) | 0.0281 (8) | 0.0042 (6) | 0.0138 (7) | 0.0015 (6) |

Geometric parameters (Å, °)

| | | | |
|---------|-------------|----------|-----------|
| Ag1—N1 | 2.1406 (16) | C10—C11 | 1.381 (3) |
| Ag1—N4 | 2.1616 (15) | C11—C12 | 1.384 (3) |
| Ag1—O1W | 2.6059 (14) | C11—H11A | 0.9500 |
| O1—C7 | 1.219 (2) | C12—C13 | 1.396 (3) |
| O2—C10 | 1.364 (2) | C12—H12A | 0.9500 |
| O2—H2O | 0.85 (3) | C13—C14 | 1.380 (3) |
| O3—C21 | 1.221 (2) | C13—H13A | 0.9500 |
| O4—C24 | 1.356 (2) | C14—H14A | 0.9500 |
| O4—H4O | 0.81 (3) | C16—C17 | 1.379 (3) |
| N1—C6 | 1.350 (2) | C16—H16A | 0.9500 |
| N1—C2 | 1.369 (2) | C17—C18 | 1.388 (2) |
| N2—N3 | 1.362 (2) | C17—H19B | 0.9500 |
| N2—C7 | 1.362 (2) | C18—C19 | 1.391 (3) |
| N2—H2N | 0.83 (2) | C18—C21 | 1.506 (2) |
| N3—C8 | 1.289 (2) | C19—C20 | 1.377 (2) |
| N4—C16 | 1.343 (2) | C19—H19A | 0.9500 |

| | | | |
|------------|-------------|--------------|-------------|
| N4—C20 | 1.351 (2) | C20—H20A | 0.9500 |
| N5—C21 | 1.360 (2) | C22—C23 | 1.444 (3) |
| N5—N6 | 1.369 (2) | C22—H22A | 0.9500 |
| N5—H5N | 0.90 (3) | C23—C28 | 1.406 (3) |
| N6—C22 | 1.286 (2) | C23—C24 | 1.412 (3) |
| C2—C3 | 1.384 (3) | C24—C25 | 1.388 (3) |
| C2—H2A | 0.9500 | C25—C26 | 1.385 (3) |
| C3—C4 | 1.390 (2) | C25—H25A | 0.9500 |
| C3—H3A | 0.9500 | C26—C27 | 1.394 (3) |
| C4—C5 | 1.393 (3) | C26—H26A | 0.9500 |
| C4—C7 | 1.505 (2) | C27—C28 | 1.386 (3) |
| C5—C6 | 1.372 (2) | C27—H27A | 0.9500 |
| C5—H5A | 0.9500 | C28—H28A | 0.9500 |
| C6—H6A | 0.9500 | N7—O5 | 1.224 (2) |
| C8—C9 | 1.447 (2) | N7—O6 | 1.250 (2) |
| C8—H8A | 0.9500 | N7—O7 | 1.2705 (19) |
| C9—C14 | 1.398 (2) | O1W—H1W | 0.84 (3) |
| C9—C10 | 1.412 (3) | O1W—H2W | 0.79 (3) |
| | | | |
| N1—Ag1—N4 | 171.63 (6) | C13—C12—H12A | 119.8 |
| N1—Ag1—O1W | 93.88 (5) | C14—C13—C12 | 119.12 (18) |
| N4—Ag1—O1W | 94.23 (5) | C14—C13—H13A | 120.4 |
| C10—O2—H2O | 106.6 (17) | C12—C13—H13A | 120.4 |
| C24—O4—H4O | 104.5 (18) | C13—C14—C9 | 121.63 (18) |
| C6—N1—C2 | 115.94 (16) | C13—C14—H14A | 119.2 |
| C6—N1—Ag1 | 125.00 (13) | C9—C14—H14A | 119.2 |
| C2—N1—Ag1 | 119.07 (11) | N4—C16—C17 | 122.94 (16) |
| N3—N2—C7 | 117.57 (15) | N4—C16—H16A | 118.5 |
| N3—N2—H2N | 121.2 (15) | C17—C16—H16A | 118.5 |
| C7—N2—H2N | 121.1 (15) | C16—C17—C18 | 119.21 (17) |
| C8—N3—N2 | 119.60 (14) | C16—C17—H19B | 120.4 |
| C16—N4—C20 | 117.42 (16) | C18—C17—H19B | 120.4 |
| C16—N4—Ag1 | 122.79 (12) | C17—C18—C19 | 118.41 (16) |
| C20—N4—Ag1 | 119.63 (12) | C17—C18—C21 | 117.67 (16) |
| C21—N5—N6 | 118.07 (15) | C19—C18—C21 | 123.88 (16) |
| C21—N5—H5N | 121.6 (17) | C20—C19—C18 | 118.85 (17) |
| N6—N5—H5N | 119.4 (17) | C20—C19—H19A | 120.6 |
| C22—N6—N5 | 118.16 (15) | C18—C19—H19A | 120.6 |
| N1—C2—C3 | 123.16 (16) | N4—C20—C19 | 123.17 (17) |
| N1—C2—H2A | 118.4 | N4—C20—H20A | 118.4 |
| C3—C2—H2A | 118.4 | C19—C20—H20A | 118.4 |
| C2—C3—C4 | 119.45 (17) | O3—C21—N5 | 123.33 (16) |
| C2—C3—H3A | 120.3 | O3—C21—C18 | 121.66 (16) |
| C4—C3—H3A | 120.3 | N5—C21—C18 | 115.00 (15) |
| C3—C4—C5 | 117.81 (17) | N6—C22—C23 | 119.96 (16) |
| C3—C4—C7 | 117.06 (16) | N6—C22—H22A | 120.0 |
| C5—C4—C7 | 125.13 (16) | C23—C22—H22A | 120.0 |
| C6—C5—C4 | 119.55 (17) | C28—C23—C24 | 118.66 (17) |

| | | | |
|----------------|--------------|-----------------|--------------|
| C6—C5—H5A | 120.2 | C28—C23—C22 | 119.27 (17) |
| C4—C5—H5A | 120.2 | C24—C23—C22 | 122.05 (17) |
| N1—C6—C5 | 124.09 (17) | O4—C24—C25 | 117.62 (17) |
| N1—C6—H6A | 118.0 | O4—C24—C23 | 122.56 (16) |
| C5—C6—H6A | 118.0 | C25—C24—C23 | 119.82 (18) |
| O1—C7—N2 | 122.33 (16) | C26—C25—C24 | 120.42 (19) |
| O1—C7—C4 | 121.53 (16) | C26—C25—H25A | 119.8 |
| N2—C7—C4 | 116.13 (15) | C24—C25—H25A | 119.8 |
| N3—C8—C9 | 118.84 (16) | C25—C26—C27 | 120.87 (19) |
| N3—C8—H8A | 120.6 | C25—C26—H26A | 119.6 |
| C9—C8—H8A | 120.6 | C27—C26—H26A | 119.6 |
| C14—C9—C10 | 118.10 (16) | C28—C27—C26 | 118.96 (19) |
| C14—C9—C8 | 119.67 (16) | C28—C27—H27A | 120.5 |
| C10—C9—C8 | 122.18 (16) | C26—C27—H27A | 120.5 |
| O2—C10—C11 | 118.38 (17) | C27—C28—C23 | 121.28 (19) |
| O2—C10—C9 | 121.24 (16) | C27—C28—H28A | 119.4 |
| C11—C10—C9 | 120.38 (18) | C23—C28—H28A | 119.4 |
| C10—C11—C12 | 120.25 (19) | O5—N7—O6 | 121.33 (16) |
| C10—C11—H11A | 119.9 | O5—N7—O7 | 120.08 (17) |
| C12—C11—H11A | 119.9 | O6—N7—O7 | 118.59 (15) |
| C11—C12—C13 | 120.50 (18) | H1W—O1W—H2W | 108 (3) |
| C11—C12—H12A | 119.8 | | |
| O1W—Ag1—N1—C6 | 175.36 (14) | C12—C13—C14—C9 | -0.9 (3) |
| O1W—Ag1—N1—C2 | -4.07 (14) | C10—C9—C14—C13 | -0.3 (3) |
| O1W—Ag1—N4—C16 | -178.91 (14) | C8—C9—C14—C13 | -177.92 (17) |
| O1W—Ag1—N4—C20 | -3.61 (14) | C20—N4—C16—C17 | 0.1 (3) |
| C7—N2—N3—C8 | 175.98 (16) | Ag1—N4—C16—C17 | 175.52 (14) |
| C21—N5—N6—C22 | -175.93 (16) | N4—C16—C17—C18 | -0.7 (3) |
| C6—N1—C2—C3 | 1.2 (3) | C16—C17—C18—C19 | 0.6 (3) |
| Ag1—N1—C2—C3 | -179.31 (14) | C16—C17—C18—C21 | -177.08 (16) |
| N1—C2—C3—C4 | -0.5 (3) | C17—C18—C19—C20 | 0.0 (3) |
| C2—C3—C4—C5 | -0.3 (3) | C21—C18—C19—C20 | 177.56 (17) |
| C2—C3—C4—C7 | 179.53 (16) | C16—N4—C20—C19 | 0.6 (3) |
| C3—C4—C5—C6 | 0.4 (3) | Ag1—N4—C20—C19 | -174.99 (14) |
| C7—C4—C5—C6 | -179.42 (17) | C18—C19—C20—N4 | -0.6 (3) |
| C2—N1—C6—C5 | -1.1 (3) | N6—N5—C21—O3 | 1.7 (3) |
| Ag1—N1—C6—C5 | 179.44 (14) | N6—N5—C21—C18 | -177.92 (14) |
| C4—C5—C6—N1 | 0.3 (3) | C17—C18—C21—O3 | 19.3 (3) |
| N3—N2—C7—O1 | -2.5 (3) | C19—C18—C21—O3 | -158.27 (18) |
| N3—N2—C7—C4 | 178.87 (15) | C17—C18—C21—N5 | -161.04 (16) |
| C3—C4—C7—O1 | -9.2 (3) | C19—C18—C21—N5 | 21.4 (2) |
| C5—C4—C7—O1 | 170.63 (17) | N5—N6—C22—C23 | 179.24 (16) |
| C3—C4—C7—N2 | 169.47 (16) | N6—C22—C23—C28 | -177.15 (17) |
| C5—C4—C7—N2 | -10.7 (3) | N6—C22—C23—C24 | 1.2 (3) |
| N2—N3—C8—C9 | -178.63 (15) | C28—C23—C24—O4 | 179.40 (17) |
| N3—C8—C9—C14 | 174.16 (16) | C22—C23—C24—O4 | 1.0 (3) |
| N3—C8—C9—C10 | -3.3 (3) | C28—C23—C24—C25 | -0.3 (3) |

| | | | |
|-----------------|--------------|-----------------|--------------|
| C14—C9—C10—O2 | -178.56 (16) | C22—C23—C24—C25 | -178.70 (17) |
| C8—C9—C10—O2 | -1.0 (3) | O4—C24—C25—C26 | -178.97 (17) |
| C14—C9—C10—C11 | 1.5 (3) | C23—C24—C25—C26 | 0.8 (3) |
| C8—C9—C10—C11 | 179.04 (17) | C24—C25—C26—C27 | -0.4 (3) |
| O2—C10—C11—C12 | 178.61 (16) | C25—C26—C27—C28 | -0.3 (3) |
| C9—C10—C11—C12 | -1.5 (3) | C26—C27—C28—C23 | 0.8 (3) |
| C10—C11—C12—C13 | 0.2 (3) | C24—C23—C28—C27 | -0.4 (3) |
| C11—C12—C13—C14 | 1.0 (3) | C22—C23—C28—C27 | 177.98 (17) |

Hydrogen-bond geometry (Å, °)

| <i>D</i> —H... <i>A</i> | <i>D</i> —H | H... <i>A</i> | <i>D</i> ... <i>A</i> | <i>D</i> —H... <i>A</i> |
|--|-------------|---------------|-----------------------|-------------------------|
| O1 <i>W</i> —H1 <i>W</i> ...O7 ⁱ | 0.84 (3) | 2.01 (3) | 2.844 (2) | 171 (3) |
| O1 <i>W</i> —H2 <i>W</i> ...O2 ⁱⁱ | 0.79 (3) | 2.04 (3) | 2.821 (2) | 172 (3) |
| N2—H2 <i>N</i> ...O6 | 0.84 (3) | 2.09 (3) | 2.880 (2) | 157 (2) |
| N5—H5 <i>N</i> ...O7 ⁱⁱⁱ | 0.90 (3) | 1.97 (3) | 2.863 (2) | 169 (2) |
| O2—H2 <i>O</i> ...N3 | 0.85 (3) | 1.79 (3) | 2.560 (2) | 150 (2) |
| O4—H4 <i>O</i> ...N6 | 0.81 (2) | 1.86 (2) | 2.607 (2) | 153 (2) |

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