

# catena-Poly[ammonium [aquabis( $\mu$ -2,3,5,6-tetraoxo-4-nitropyridin-4-ido)-argentate(I)]]

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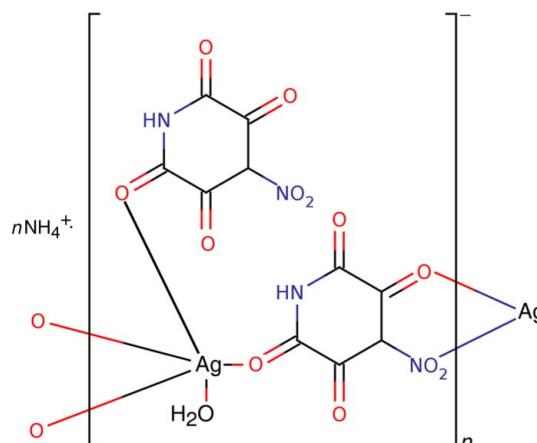
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.021;  $wR$  factor = 0.066; data-to-parameter ratio = 9.8.

In the title compound,  $\{(\text{NH}_4)[\text{Ag}(\text{C}_5\text{HN}_2\text{O}_6)_2(\text{H}_2\text{O})]\}_n$ , the  $\text{Ag}^{\text{I}}$  cation is seven-coordinated and is surrounded by four oxo O atoms of the 2,3,5,6-tetraoxo-4-nitropyridin-4-ide species [ $\text{Ag}-\text{O} = 2.3848$  (19), 2.4931 (18), 2.5361 (18) and 2.573 (2) Å], two nitro O atoms [ $\text{Ag}-\text{O} = 2.644$  (2) and 2.661 (2) Å], and one water molecule [ $\text{Ag}-\text{O} = 2.3133$  (19) Å]. The pyridin-4-ide mono-anions act as polydentate bridging ligands and form a three-dimensional network that is stabilized through  $\text{O}-\text{H}\cdots\text{O}$  and  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds involving the coordinating water molecule and the imide function as donor groups. The ammonium cations are located in the cavities of the framework and are also involved in hydrogen bonding to O atoms of the ligand.

## Related literature

For reviews of 1,2-dicarbonyl compounds, see: Aldoshin (2008); Ohba & Okawa (2000). The synthesis and crystal structures of ammonium and sodium 2,3,5,6-tetraoxo-4-nitropyridinates have been reported previously (Palkina *et al.*, 2000; Kuzmina *et al.*, 2004). The structure of the organic anion in its hexaqua metal salts is described by Kovalchukova *et al.* (2003 and 2013). For references to related structures of metal complexes with cyclic polyoxo compounds, see: Coronado *et al.* (2007); Kitagawa & Kawata (2002).



## Experimental

### Crystal data

$(\text{NH}_4)[\text{Ag}(\text{C}_5\text{HN}_2\text{O}_6)_2(\text{H}_2\text{O})]$

$M_r = 514.08$

Monoclinic,  $P2_1/c$

$a = 8.784$  (2) Å

$b = 18.551$  (4) Å

$c = 9.195$  (2) Å

$\beta = 90.70$  (3)°

$V = 1498.2$  (5) Å<sup>3</sup>

$Z = 4$

Mo  $K\alpha$  radiation

$\mu = 1.44$  mm<sup>-1</sup>

$T = 293$  K

$0.35 \times 0.31 \times 0.08$  mm

### Data collection

Enraf Nonius CAD-4

diffractometer

Absorption correction: part of the

refinement model ( $\Delta F$ )

(Walker & Stuart, 1983)

$T_{\text{min}} = 0.406$ ,  $T_{\text{max}} = 0.798$

2952 measured reflections

2768 independent reflections

2094 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.014$

3 standard reflections every 60 min

intensity decay: none

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.021$

$wR(F^2) = 0.066$

$S = 1.09$

2768 reflections

283 parameters

11 restraints

H atoms treated by a mixture of

independent and constrained

refinement

$\Delta\rho_{\text{max}} = 0.42$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.58$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N4}-\text{H4}\cdots\text{O11}^{\text{i}}$	0.86	2.18	2.979 (3)	155
$\text{N10}-\text{H10}\cdots\text{O2}$	0.86	2.26	2.945 (3)	137
$\text{N10}-\text{H10}\cdots\text{O3}$	0.86	2.29	3.030 (3)	144
$\text{O1}-\text{H11}\cdots\text{O131}^{\text{ii}}$	0.80 (3)	2.06 (3)	2.851 (3)	177 (5)
$\text{O1}-\text{H12}\cdots\text{O8}^{\text{iii}}$	0.80 (3)	2.02 (3)	2.781 (2)	160 (3)
$\text{N2}-\text{H21}\cdots\text{O6}^{\text{iv}}$	0.83 (2)	2.16 (2)	2.962 (3)	163 (3)
$\text{N2}-\text{H22}\cdots\text{O72}^{\text{v}}$	0.83 (2)	2.20 (2)	2.998 (3)	160 (3)

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

Data collection: *CAD-4-PC* (Enraf-Nonius, 1993); cell refinement: *CAD-4-PC*; data reduction: *CAD-4-PC*; 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: *CIFTAB97* and *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PJ2004).

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## supporting information

*Acta Cryst.* (2013). E69, m477–m478 [doi:10.1107/S1600536813020631]

## **catena-Poly[ammonium [aquabis( $\mu$ -2,3,5,6-tetraoxo-4-nitropyridin-4-ido)argentate(I)]]**

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### **S1. Comment**

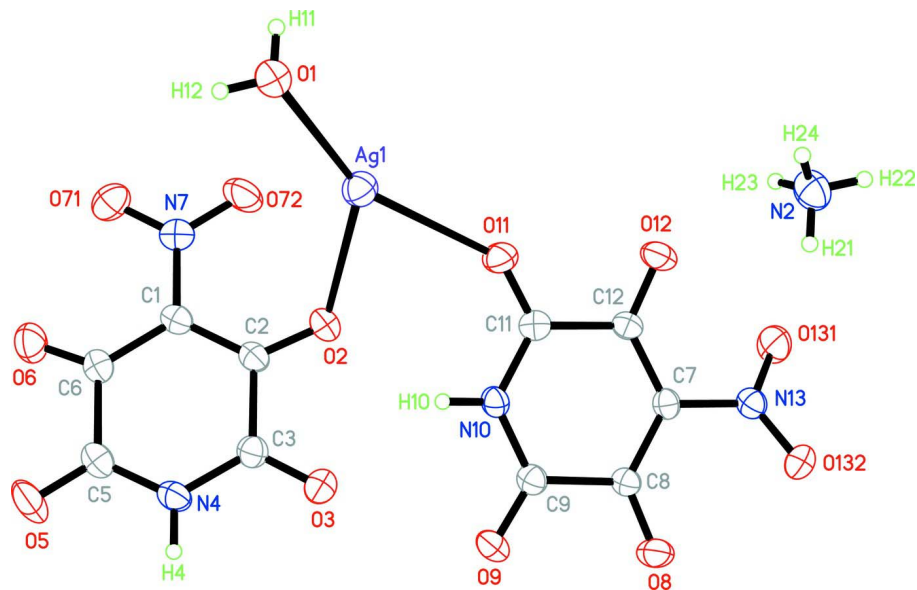
1,2-dicarbonyl compounds attract great interest because of the features of their structure and high reactivity. One of the simplest representatives of them is oxalic acid. As described by S. Aldoshin (Aldoshin, 2008), bimetallic coordination polymers based on oxalate and thiooxalate bridging ligands possess different types of magnetic activity and can intercalate complex organic molecules and ions. These have been extensively used as building units in supramolecular coordination systems (Ohba & Okawa, 2000). The replacement of oxalate anions by other 1,2-dicarbonyl cyclic compounds may be of interest from the synthetic and practical point of view. As an example (Coronado *et al.* 2007), the paramagnetic and chiral anion  $[\text{Fe}(\text{C}_5\text{O}_5)_3]^{3-}$  has been combined with the organic donor BEDT-TTF DET (bis(ethylenedithio)tetrathiafulvalene) to synthesize a novel paramagnetic semiconductor with the first chirality-induced  $\alpha$ -phase,  $\alpha$ -(BEDT-TTF)5 $[\text{Fe}(\text{C}_5\text{O}_5)_3]$ ·5H<sub>2</sub>O, and one of the few known paramagnetic molecular metals,  $\beta$ -(BEDT-TTF)5 $[\text{Fe}(\text{C}_5\text{O}_5)_3]$ ·C<sub>6</sub>H<sub>5</sub>CN. The variety of coordination modes, some geometric characteristics as well as electrical, magnetic and other properties of coordinate compounds of dibenzoquinone-1,4 derivatives of a general formula H<sub>2</sub>C<sub>6</sub>O<sub>4</sub>X<sub>2</sub> are summarised by S. Kitagawa and S. Kawata (Kitagawa & Kawata, 2002). The present paper deals with the crystal structure determination of ammonium-silver 2,3,5,6-tetraoxo-4-nitropyridinate monohydrate (NH<sub>4</sub>) $[\text{Ag}(\text{C}_5\text{HN}_2\text{O}_6)_2(\text{H}_2\text{O})]$ . The molecular structure of the above substance consists of Ag(I) and ammonium cations, two crystallographically nonequivalent 2,3,5,6-tetraoxo-4-nitropyridinate mono anions, and one coordinated water molecule. Each of the Ag(I) cation displays sevenfold coordination by O2, O5, O8, and O11 of the keto-groups of the organic species. The Ag—O distances are 2.3848 (19); 2.4931 (18); 2.5361 (18); and 2.573 (2) Å. Two coordinate bonds involve the O atoms of the nitro-group of the organic anion (2.644 (2) and 2.661 (2) Å). The shortest distance in the coordination sphere of Ag(I) involves the coordinated water molecule (2.3133 (19) Å). The 2,3,5,6-tetraoxo-4-nitropyridinate anions act as polydentate bridging ligands. This coordination mode leads to formation of polymer chains. The coordination does not change significantly the C—O distances of the ligand comparing with its ammonium and sodium salts (Palkina *et al.*, 2000; Kuzmina *et al.*, 2004). The corresponding bond lengths are in the range 1.224 (3) to 1.220 (3) Å for the nitro-diketone fragment, and 1.210 (4) to 1.215 (4) Å for the amide fragment. These two fragments of the organic mono anion are connected by an almost single C—C bonds (C2—C3 length is 1.531 (4), and C5—C6 length is 1.544 (4) Å). The ammonium cation has the outer sphere character, and forms bridging H-bonds with the O atoms of the organic anions linking the polymer chains into three-dimensional structure. The H atoms of the coordinated water molecules are also involved into the H-bonding.

## S2. Experimental

Single crystals of  $C_{10}H_8AgN_5O_{13}$  were grown by the slow evaporation of the ethanol solution of the 1-to-1 molar mixture of silver nitrate and ammonium 2,3,5,6-tetraoxo-4-nitropyridinate.

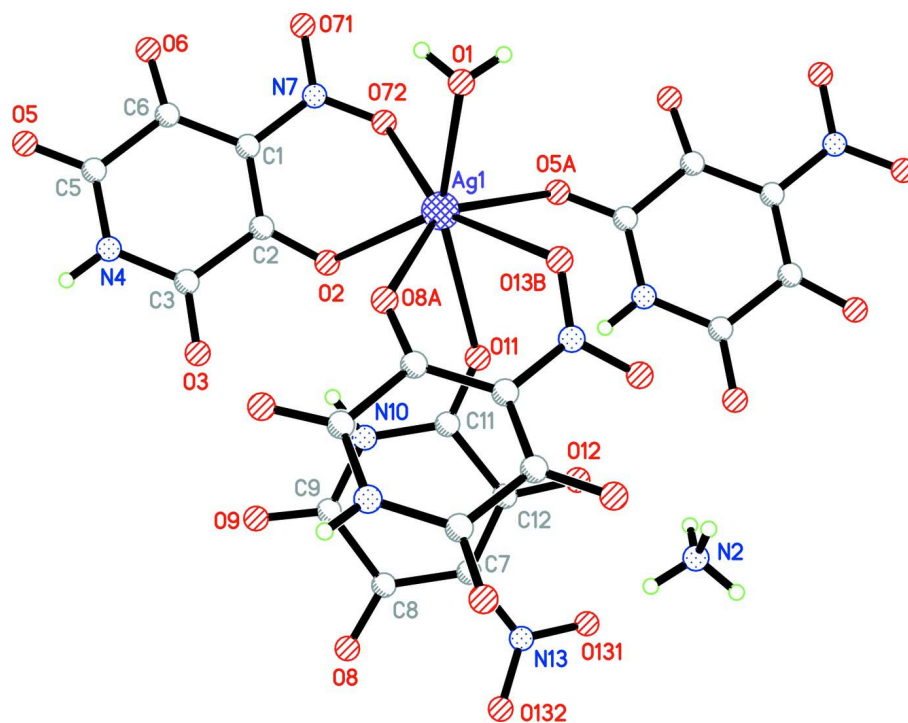
## S3. Refinement

The structure of  $(NH_4)[Ag(C_5HN_2O_6)_2(H_2O)]$  was solved by direct method and all non-hydrogen atoms were located and refined in anisotropically. All the hydrogen atoms were located in difference electron density syntheses and their positions refined subject to chemically reasonable restraints.

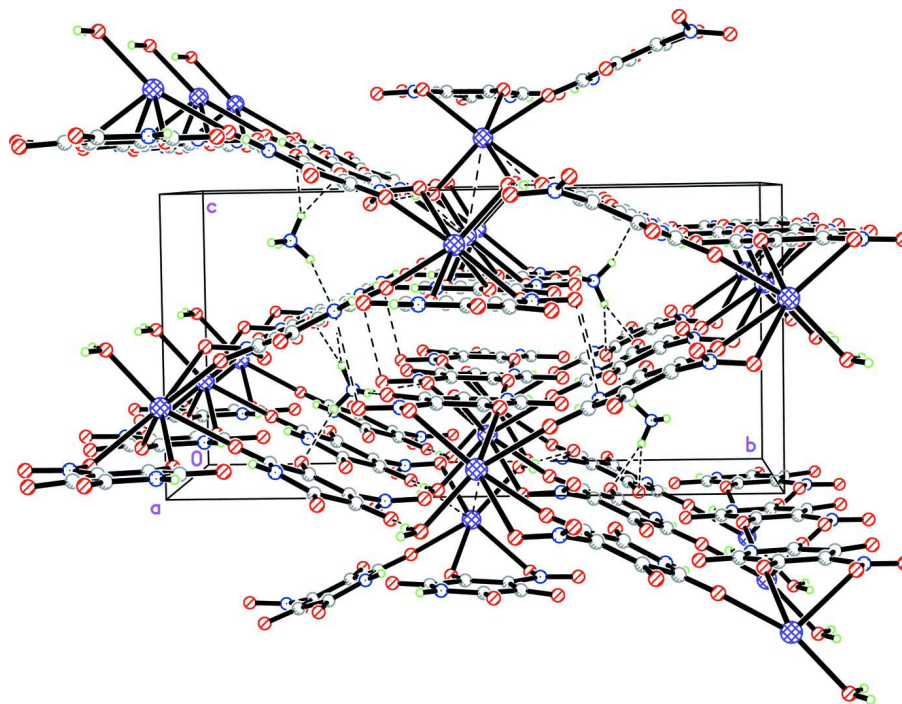


**Figure 1**

ORTEP view of  $(NH_4)[Ag(C_5HN_2O_6)_2(H_2O)]$  with atom labeling scheme (displacement ellipsoids are drawn at the 50% probability level for non-hydrogen atoms).

**Figure 2**

Structure of the coordination sphere of Ag(I).

**Figure 3**

Molecular packing in the crystal of the complex along the crystallographic axis c.

**catena-Poly[ammonium [aquabis( $\mu$ -2,3,5,6-tetraoxo-4-nitropyridin-4-ido)argentate(I)]]***Crystal data*(NH<sub>4</sub>)[Ag(C<sub>5</sub>HN<sub>2</sub>O<sub>6</sub>)<sub>2</sub>(H<sub>2</sub>O)] $M_r = 514.08$ Monoclinic,  $P2_1/c$ 

Hall symbol: -P 2ybc

 $a = 8.784$  (2) Å $b = 18.551$  (4) Å $c = 9.195$  (2) Å $\beta = 90.70$  (3)° $V = 1498.2$  (5) Å<sup>3</sup> $Z = 4$  $F(000) = 1016$  $D_x = 2.279$  Mg m<sup>-3</sup>Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 25 reflections

 $\theta = 9.3$ – $11.8$ ° $\mu = 1.44$  mm<sup>-1</sup> $T = 293$  K

Plate, dark yellow

 $0.35 \times 0.31 \times 0.08$  mm*Data collection*

Enraf Nonius CAD-4

diffractometer

Radiation source: fine-focus sealed tube

 $\beta$ -filter monochromator $\omega/2\theta$  scans

Absorption correction: part of the refinement

model ( $\Delta F$ )

Walker &amp; Stuart (1983)

 $T_{\min} = 0.406$ ,  $T_{\max} = 0.798$ 

2952 measured reflections

2768 independent reflections

2094 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.014$  $\theta_{\max} = 25.5$ °,  $\theta_{\min} = 2.2$ ° $h = 0 \rightarrow 10$  $k = 0 \rightarrow 22$  $l = -11 \rightarrow 11$ 

3 standard reflections every 60 min

intensity decay: none

*Refinement*Refinement on  $F^2$ 

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.021$  $wR(F^2) = 0.066$  $S = 1.09$ 

2768 reflections

283 parameters

11 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

 $w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 0.0506P]$ where  $P = (F_o^2 + 2F_c^2)/3$  $(\Delta/\sigma)_{\max} = 0.001$  $\Delta\rho_{\max} = 0.42$  e Å<sup>-3</sup> $\Delta\rho_{\min} = -0.58$  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 (Å<sup>2</sup>)*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.68914 (2)	0.518350 (10)	0.16959 (2)	0.03092 (9)
O1	0.6981 (2)	0.43383 (10)	-0.0151 (2)	0.0367 (4)
O2	0.49428 (18)	0.55092 (10)	0.3355 (2)	0.0337 (4)

O3	0.2721 (2)	0.64390 (10)	0.3252 (3)	0.0437 (5)
O5	-0.0852 (2)	0.46912 (11)	0.3204 (2)	0.0430 (5)
O6	0.1206 (2)	0.36677 (10)	0.3468 (2)	0.0380 (4)
O71	0.4081 (2)	0.33294 (10)	0.3308 (2)	0.0374 (4)
O72	0.5781 (2)	0.41601 (11)	0.3380 (3)	0.0434 (5)
O8	0.59699 (19)	0.87943 (10)	0.5161 (2)	0.0346 (4)
O9	0.40503 (19)	0.77524 (10)	0.4454 (2)	0.0371 (4)
O11	0.7861 (2)	0.62851 (10)	0.3053 (2)	0.0335 (4)
O12	0.99467 (19)	0.72206 (10)	0.3830 (2)	0.0361 (4)
O131	1.0495 (2)	0.83839 (10)	0.5427 (3)	0.0440 (5)
O132	0.8913 (2)	0.92310 (9)	0.4915 (2)	0.0337 (4)
N2	1.1853 (2)	0.79954 (14)	0.1619 (3)	0.0356 (5)
N4	0.0902 (2)	0.55773 (12)	0.3224 (2)	0.0277 (4)
H4	0.0200	0.5900	0.3174	0.033*
N7	0.4426 (2)	0.39746 (11)	0.3354 (2)	0.0255 (4)
N10	0.5921 (2)	0.70207 (10)	0.3659 (2)	0.0234 (4)
H10	0.5263	0.6718	0.3324	0.028*
N13	0.9224 (2)	0.85893 (11)	0.5015 (2)	0.0250 (4)
C1	0.3262 (2)	0.45034 (14)	0.3364 (2)	0.0232 (5)
C2	0.3668 (3)	0.52426 (12)	0.3337 (2)	0.0230 (4)
C3	0.2389 (3)	0.58051 (13)	0.3276 (3)	0.0267 (5)
C5	0.0468 (3)	0.48715 (13)	0.3246 (3)	0.0264 (5)
C6	0.1700 (3)	0.42790 (13)	0.3368 (2)	0.0243 (5)
C7	0.8114 (2)	0.80583 (12)	0.4653 (2)	0.0219 (4)
C8	0.6544 (2)	0.82305 (12)	0.4741 (2)	0.0212 (4)
C9	0.5389 (3)	0.76440 (13)	0.4277 (2)	0.0236 (5)
C11	0.7427 (3)	0.68490 (12)	0.3543 (2)	0.0222 (4)
C12	0.8630 (3)	0.74009 (12)	0.4048 (2)	0.0222 (4)
H11	0.768 (3)	0.4067 (17)	-0.019 (5)	0.074 (6)*
H12	0.624 (3)	0.4089 (17)	-0.015 (5)	0.074 (6)*
H21	1.109 (3)	0.8260 (14)	0.166 (4)	0.074 (6)*
H22	1.263 (3)	0.8246 (14)	0.176 (4)	0.074 (6)*
H23	1.182 (4)	0.7675 (14)	0.225 (3)	0.074 (6)*
H24	1.190 (4)	0.7813 (16)	0.080 (2)	0.074 (6)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Ag1	0.03248 (13)	0.03008 (13)	0.03023 (13)	-0.00021 (7)	0.00124 (8)	-0.00114 (8)
O1	0.0281 (9)	0.0371 (10)	0.0449 (11)	-0.0023 (8)	0.0016 (8)	-0.0077 (8)
O2	0.0202 (8)	0.0337 (9)	0.0471 (11)	-0.0027 (7)	0.0010 (7)	-0.0058 (8)
O3	0.0299 (9)	0.0264 (9)	0.0747 (15)	0.0000 (8)	-0.0052 (9)	-0.0102 (9)
O5	0.0197 (9)	0.0485 (11)	0.0607 (13)	-0.0068 (8)	-0.0051 (8)	0.0142 (10)
O6	0.0330 (9)	0.0325 (10)	0.0485 (11)	-0.0067 (7)	-0.0014 (8)	0.0053 (8)
O71	0.0462 (11)	0.0284 (9)	0.0374 (10)	0.0044 (8)	-0.0032 (8)	0.0019 (8)
O72	0.0233 (9)	0.0408 (10)	0.0662 (14)	0.0076 (8)	0.0017 (9)	0.0079 (10)
O8	0.0241 (8)	0.0340 (9)	0.0455 (11)	0.0061 (7)	-0.0065 (8)	-0.0150 (8)
O9	0.0189 (9)	0.0374 (10)	0.0551 (12)	-0.0008 (7)	0.0040 (8)	-0.0096 (9)

O11	0.0280 (9)	0.0327 (10)	0.0398 (10)	0.0029 (7)	-0.0013 (7)	-0.0140 (8)
O12	0.0204 (9)	0.0394 (10)	0.0484 (11)	0.0035 (7)	0.0034 (8)	-0.0105 (8)
O131	0.0251 (9)	0.0359 (10)	0.0707 (14)	-0.0020 (8)	-0.0166 (9)	-0.0045 (9)
O132	0.0338 (9)	0.0223 (9)	0.0451 (11)	-0.0026 (7)	0.0010 (8)	-0.0044 (7)
N2	0.0285 (11)	0.0406 (13)	0.0376 (13)	-0.0039 (9)	-0.0015 (9)	-0.0011 (10)
N4	0.0200 (9)	0.0316 (10)	0.0313 (11)	0.0040 (8)	-0.0017 (8)	0.0003 (9)
N7	0.0291 (10)	0.0305 (11)	0.0168 (9)	0.0042 (8)	-0.0014 (7)	0.0022 (8)
N10	0.0193 (9)	0.0257 (10)	0.0253 (10)	-0.0024 (7)	-0.0025 (7)	-0.0033 (8)
N13	0.0232 (9)	0.0284 (10)	0.0234 (10)	-0.0014 (8)	-0.0005 (7)	-0.0030 (8)
C1	0.0214 (11)	0.0304 (12)	0.0178 (11)	0.0023 (9)	-0.0015 (8)	-0.0002 (9)
C2	0.0195 (10)	0.0311 (12)	0.0183 (10)	-0.0002 (9)	0.0004 (8)	-0.0034 (9)
C3	0.0244 (11)	0.0291 (13)	0.0266 (12)	-0.0007 (10)	-0.0020 (9)	-0.0059 (9)
C5	0.0234 (11)	0.0356 (13)	0.0202 (11)	-0.0018 (10)	-0.0018 (8)	0.0029 (10)
C6	0.0245 (11)	0.0300 (12)	0.0184 (11)	-0.0022 (9)	-0.0013 (9)	0.0011 (9)
C7	0.0211 (11)	0.0239 (10)	0.0204 (11)	-0.0023 (9)	-0.0028 (8)	0.0001 (9)
C8	0.0197 (10)	0.0250 (11)	0.0187 (10)	0.0006 (8)	-0.0022 (8)	-0.0022 (9)
C9	0.0221 (11)	0.0269 (11)	0.0218 (11)	-0.0003 (9)	-0.0013 (9)	-0.0024 (9)
C11	0.0250 (11)	0.0257 (11)	0.0157 (10)	0.0020 (9)	-0.0015 (8)	-0.0002 (9)
C12	0.0202 (11)	0.0257 (11)	0.0207 (10)	0.0020 (9)	0.0001 (8)	0.0005 (9)

*Geometric parameters (Å, °)*

Ag1—O1	2.3133 (19)	O132—N13	1.225 (3)
Ag1—O2	2.3848 (19)	O132—Ag1 <sup>iv</sup>	2.661 (2)
Ag1—O8 <sup>i</sup>	2.4931 (18)	N2—H21	0.832 (19)
Ag1—O11	2.5361 (18)	N2—H22	0.83 (2)
Ag1—O5 <sup>ii</sup>	2.573 (2)	N2—H23	0.830 (19)
Ag1—O72	2.644 (2)	N2—H24	0.827 (19)
Ag1—O132 <sup>i</sup>	2.661 (2)	N4—C5	1.364 (3)
O1—H11	0.80 (3)	N4—C3	1.373 (3)
O1—H12	0.80 (3)	N4—H4	0.8600
O2—C2	1.224 (3)	N7—C1	1.417 (3)
O3—C3	1.212 (3)	N10—C11	1.366 (3)
O5—C5	1.206 (3)	N10—C9	1.373 (3)
O5—Ag1 <sup>iii</sup>	2.573 (2)	N10—H10	0.8600
O6—C6	1.218 (3)	N13—C7	1.423 (3)
O71—N7	1.235 (3)	C1—C2	1.417 (3)
O72—N7	1.239 (3)	C1—C6	1.434 (3)
O8—C8	1.225 (3)	C2—C3	1.534 (3)
O8—Ag1 <sup>iv</sup>	2.4931 (18)	C5—C6	1.546 (3)
O9—C9	1.206 (3)	C7—C12	1.417 (3)
O11—C11	1.203 (3)	C7—C8	1.419 (3)
O12—C12	1.223 (3)	C8—C9	1.544 (3)
O131—N13	1.235 (3)	C11—C12	1.539 (3)
O1—Ag1—O2	132.26 (6)	C5—N4—H4	117.9
O1—Ag1—O2	132.26 (6)	C3—N4—H4	117.9
O2—Ag1—O2	0.00 (5)	O71—N7—O72	120.3 (2)



O1—Ag1—O8 <sup>i</sup>	96.52 (7)	O71—N7—C1	119.6 (2)
O2—Ag1—O8 <sup>i</sup>	86.50 (7)	O72—N7—C1	120.0 (2)
O2—Ag1—O8 <sup>i</sup>	86.50 (7)	C11—N10—C9	124.3 (2)
O1—Ag1—O11	153.27 (7)	C11—N10—H10	117.8
O2—Ag1—O11	73.76 (6)	C9—N10—H10	117.8
O2—Ag1—O11	73.76 (6)	O132—N13—O131	121.6 (2)
O8 <sup>i</sup> —Ag1—O11	76.73 (7)	O132—N13—C7	120.24 (19)
O1—Ag1—O5 <sup>ii</sup>	97.02 (7)	O131—N13—C7	118.21 (19)
O2—Ag1—O5 <sup>ii</sup>	107.42 (7)	N7—C1—C2	119.23 (19)
O2—Ag1—O5 <sup>ii</sup>	107.42 (7)	N7—C1—C6	119.3 (2)
O8 <sup>i</sup> —Ag1—O5 <sup>ii</sup>	144.87 (6)	C2—C1—C6	121.5 (2)
O11—Ag1—O5 <sup>ii</sup>	76.64 (7)	O2—C2—O2	0.00 (16)
O1—Ag1—O72	87.67 (7)	O2—C2—C1	128.4 (2)
O2—Ag1—O72	62.25 (7)	O2—C2—C1	128.4 (2)
O2—Ag1—O72	62.25 (7)	O2—C2—C3	113.3 (2)
O8 <sup>i</sup> —Ag1—O72	139.31 (6)	O2—C2—C3	113.3 (2)
O11—Ag1—O72	114.48 (7)	C1—C2—C3	118.3 (2)
O5 <sup>ii</sup> —Ag1—O72	73.55 (6)	O3—C3—O3	0.0 (2)
O1—Ag1—O132 <sup>i</sup>	78.24 (6)	O3—C3—N4	121.8 (2)
O2—Ag1—O132 <sup>i</sup>	141.23 (6)	O3—C3—N4	121.8 (2)
O2—Ag1—O132 <sup>i</sup>	141.23 (6)	O3—C3—C2	119.0 (2)
O8 <sup>i</sup> —Ag1—O132 <sup>i</sup>	63.63 (6)	O3—C3—C2	119.0 (2)
O11—Ag1—O132 <sup>i</sup>	75.60 (6)	N4—C3—C2	119.2 (2)
O5 <sup>ii</sup> —Ag1—O132 <sup>i</sup>	87.76 (6)	O5—C5—N4	122.3 (2)
O72—Ag1—O132 <sup>i</sup>	155.09 (5)	O5—C5—C6	118.5 (2)
Ag1—O1—H11	120 (3)	N4—C5—C6	119.2 (2)
Ag1—O1—H12	111 (3)	O6—C6—C1	127.8 (2)
H11—O1—H12	105.3 (9)	O6—C6—C5	114.7 (2)
O2—O2—C2	0 (10)	C1—C6—C5	117.6 (2)
O2—O2—Ag1	0 (6)	C12—C7—C8	122.1 (2)
C2—O2—Ag1	123.54 (16)	C12—C7—N13	117.8 (2)
O3—O3—C3	0 (10)	C8—C7—N13	119.65 (19)
C5—O5—Ag1 <sup>iii</sup>	130.73 (17)	O8—C8—C7	127.9 (2)
N7—O72—Ag1	123.30 (16)	O8—C8—C9	114.66 (19)
C8—O8—Ag1 <sup>iv</sup>	134.07 (15)	C7—C8—C9	117.45 (19)
C11—O11—Ag1	141.17 (16)	O9—C9—N10	122.3 (2)
N13—O132—Ag1 <sup>iv</sup>	120.06 (15)	O9—C9—C8	118.9 (2)
H21—N2—H22	108.8 (9)	N10—C9—C8	118.83 (19)
H21—N2—H23	111 (3)	O11—C11—N10	122.9 (2)
H22—N2—H23	109.0 (9)	O11—C11—C12	118.2 (2)
H21—N2—H24	109.7 (9)	N10—C11—C12	118.9 (2)
H22—N2—H24	108 (3)	O12—C12—C7	127.4 (2)
H23—N2—H24	110.0 (9)	O12—C12—C11	114.6 (2)
C5—N4—C3	124.1 (2)	C7—C12—C11	118.00 (19)

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

*Hydrogen-bond geometry (Å, °)*

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N4—H4 $\cdots$ O11 <sup>iii</sup>	0.86	2.18	2.979 (3)	155
N10—H10 $\cdots$ O2	0.86	2.26	2.945 (3)	137
N10—H10 $\cdots$ O3	0.86	2.29	3.030 (3)	144
O1—H11 $\cdots$ O131 <sup>v</sup>	0.80 (3)	2.06 (3)	2.851 (3)	177 (5)
O1—H12 $\cdots$ O8 <sup>vi</sup>	0.80 (3)	2.02 (3)	2.781 (2)	160 (3)
N2—H21 $\cdots$ O6 <sup>vii</sup>	0.83 (2)	2.16 (2)	2.962 (3)	163 (3)
N2—H22 $\cdots$ O72 <sup>viii</sup>	0.83 (2)	2.20 (2)	2.998 (3)	160 (3)

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