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Bis[diamminesilver(I)] 5-nitroisophthalate monohydrate

Di Sun, Geng-Geng Luo, Na Zhang and Rong-Bin Huang*

Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, People's Republic of China
Correspondence e-mail: rbhuang@xmu.edu.cn

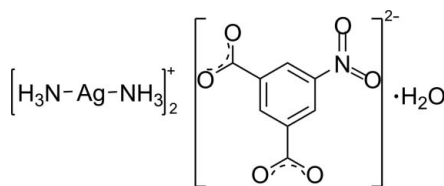
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Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.046; wR factor = 0.114; data-to-parameter ratio = 12.9.

In the title compound, $[\text{Ag}(\text{NH}_3)_2]_2(\text{C}_8\text{H}_3\text{NO}_6) \cdot \text{H}_2\text{O}$, the cations have an almost linear coordination geometry with two ammine ligands and interact with the water molecules $[\text{Ag} \cdots \text{O}_{\text{water}} = 2.725$ (4) and 2.985 (4) Å]. In the crystal, $\text{N}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds, combined with weak (lone pair) $\cdots \pi$ [$\text{O} \cdots$ centroid distance = 3.401 (4) Å] and $\pi-\pi$ stacking [centroid-centroid distance = 3.975 (3) Å] interactions, stabilize the three-dimensional supramolecular network.

Related literature

For general background to crystal engineering and supramolecular chemistry, see: Batten & Robson (1998); Blake *et al.* (1999); Yaghi *et al.* (2003). For general background to non-covalent interactions, see: Biswas *et al.* (2009); Egli & Arkhel (2007); Jeffrey *et al.* (1985); Mooibroek *et al.* (2006); Nishio *et al.* (1998); Rahman *et al.* (2003). For related structures, see: Sun, Luo, Huang *et al.* (2009); Sun, Luo, Xu *et al.* (2009); Sun, Luo, Zhang *et al.* (2009); You & Zhu (2004); You *et al.* (2004); Zheng *et al.* (2002, 2007).



Experimental

Crystal data

 $[\text{Ag}(\text{NH}_3)_2]_2(\text{C}_8\text{H}_3\text{NO}_6) \cdot \text{H}_2\text{O}$ $M_r = 511.01$ Monoclinic, $P2_1/c$ $a = 7.692$ (2) Å $b = 12.229$ (3) Å $c = 16.379$ (4) Å $\beta = 102.100$ (4)° $V = 1506.5$ (7) Å³ $Z = 4$ Mo $K\alpha$ radiation $\mu = 2.64$ mm⁻¹ $T = 298$ K

0.11 × 0.10 × 0.08 mm

Data collection

Oxford Diffraction Gemini S Ultra diffractometer

Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2006) $T_{\text{min}} = 0.760$, $T_{\text{max}} = 0.817$

7118 measured reflections

2627 independent reflections

2500 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.036$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.046$ $wR(F^2) = 0.114$ $S = 1.22$

2627 reflections

204 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 0.97$ e Å⁻³ $\Delta\rho_{\text{min}} = -0.98$ e Å⁻³

Table 1

Selected bond lengths (Å).

Ag1—N1	2.112 (5)	Ag2—N3	2.088 (4)
Ag1—N2	2.105 (5)	Ag2—N4	2.094 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1WA \cdots O1 ⁱ	0.85	1.96	2.807 (5)	177
O1W—H1WB \cdots O3	0.85	1.88	2.684 (5)	156
N1—H1B \cdots O4 ⁱⁱ	0.89	2.35	3.082 (6)	140
N1—H1C \cdots O1	0.89	2.10	2.905 (6)	149
N2—H2A \cdots O3 ⁱⁱⁱ	0.89	2.09	2.954 (6)	164
N2—H2B \cdots O4 ^{iv}	0.89	2.36	3.218 (6)	163
N2—H2C \cdots O1W ⁱⁱ	0.89	2.28	3.059 (6)	147
N2—H2C \cdots O6	0.89	2.57	2.990 (6)	110
N3—H3A \cdots O2 ^v	0.89	2.08	2.937 (6)	163
N3—H3B \cdots O1 ^{iv}	0.89	2.06	2.930 (6)	167
N3—H3C \cdots O4	0.89	2.02	2.901 (5)	173
N4—H4A \cdots O4 ^{vi}	0.89	2.23	3.088 (6)	163
N4—H4B \cdots O3 ^{vii}	0.89	2.14	3.024 (6)	176
N4—H4C \cdots O2 ⁱⁱ	0.89	2.15	3.036 (5)	175

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 1999) and *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* and *PUBLICIF* (Westrip, 2010).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2282).

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supporting information

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Bis[diamminesilver(I)] 5-nitroisophthalate monohydrate**Di Sun, Geng-Geng Luo, Na Zhang and Rong-Bin Huang****S1. Comment**

Renaissance in crystal engineering and supramolecular chemistry is due to the diverse and aesthetic structural topologies and potential use in optical, electrical, catalytic, gas storage and even drug delivery as functional solid materials (Batten & Robson, 1998; Blake *et al.*, 1999; Yaghi *et al.*, 2003). In addition to coordination bonds, noncovalent interactions such as hydrogen bond, π - π stacking, C—H $\cdots\pi$, anion $\cdots\pi$, cation $\cdots\pi$ and lone-pair(lp) $\cdots\pi$ interactions between molecules also play a pivotal role in the stability of molecule packing and govern the physicochemical properties of molecular systems in the condensed phase (Mooibroek *et al.*, 2006; Nishio *et al.*, 1998). Although Ag^I ion under ammoniacal conditions can form {[Ag(NH₃)₂]⁺}_n (n = 1 or 2) (Zheng *et al.*, 2007), which can be stabilized by supramolecular interactions, only limited [Ag(NH₃)₂]-containing compounds were documented due to the weak Ag—N_{amine} coordination bond (You *et al.*, 2004; Zheng *et al.*, 2002). Recently, we have pursued systematic investigations about the self-assembly of Ag^I ion with different bipodal N-donor ligands and multicarboxylates under ammoniacal conditions (Sun, Luo, Huang *et al.*, 2009; Sun, Luo, Xu *et al.*, 2009; Sun, Luo, Zhang *et al.*, 2009). In an attempt to exploit the Ag^I/aminopyrazine/H₂nipa system (H₂nipa = 5-nitroisophthalic acid), we surprisingly obtained the title compound.

The title compound comprises two [Ag(NH₃)₂]⁺ cations, one nipa anion and one uncoordinated water molecule in the asymmetric unit (Fig. 1). Each Ag^I ion is in an almost linear coordination environment, coordinated by two ammonia molecules, forming a cationic [Ag(NH₃)₂]⁺ monomer. The Ag—N bond lengths range from 2.088 (4) to 2.112 (5) Å (Table 1), which are comparable to the corresponding values observed in other silver(I) compounds (You & Zhu, 2004). The N1—Ag1—N2 [169.90 (19)°] and N3—Ag2—N4 [174.05 (16)°] angles deviate from the ideal 180°, as a result of weak interactions between the Ag^I ions and water molecules. The Ag1 \cdots O1Wⁱⁱⁱ and Ag2 \cdots O1W^v distances are 2.725 (4) and 2.985 (4) Å, respectively, which suggest anything other than a secondary interaction [symmetry codes: (iii) x, y+1, z; (v) x+1, -y+1/2, z+1/2]. The shortest centroid–centroid distance between neighboring phenyl rings of nipa anions is 3.975 (3) Å, with a large slippage of 2.129 Å, which suggests the existence of a weak offset π - π stacking interaction. On the other hand, one striking feature of the title compound is an lp $\cdots\pi$ interaction (Biswas *et al.*, 2009; Egli & Arkhel, 2007). A weak lp $\cdots\pi$ interaction is observed between the nitro O5 atom and phenyl ring of the nipa anion. The distance between the ring centroid and O5 atom is 3.401 (4) Å. This lp(O) $\cdots\pi$ interaction distance falls in the range of few experimental examples so far reported (Rahman *et al.*, 2003). The angle θ (which corresponds to the angle between the O atom, the ring centroid and the aromatic plane) is 83.7 (3)°, reflecting a significant lp $\cdots\pi$ interaction. Every two nipa anions arrange in a parallel manner, forming a dimer through lp(O) $\cdots\pi$ interactions, and the neighboring dimers pack together through weak π - π stacking interactions into columns running along the *a* axis (Fig. 2).

One of the ammonia molecules forms a bifurcated hydrogen bond (Jeffrey *et al.*, 1985) [N2—H2C \cdots O1Wⁱⁱ and N2—H2C \cdots O6, symmetry code: (ii) -x, -y+1, -z+1]. In addition, the [Ag(NH₃)₂]⁺ cations, nipa anions and water molecules interact *via* N—H \cdots O and O—H \cdots O hydrogen bonds (Table 2) [average N \cdots O = 3.010 (6), O \cdots O = 2.746 (5) Å] to consolidate the three-dimensional supramolecular network (Fig. 3).

S2. Experimental

All reagents and solvents were used as obtained commercially without further purification. A mixture of Ag_2O (116 mg, 0.5 mmol), 2-aminopyrazine (95 mg, 1 mmol) and H_2nipa (211 mg, 1 mmol) were stirred in $\text{CH}_3\text{CN}/\text{H}_2\text{O}$ mixed solvent (8 ml, v/v = 1:1). Then aqueous NH_3 solution (25%) was dropped into the mixture to give a clear solution under ultrasonic treatment. The resultant solution was allowed to evaporate slowly in darkness at room temperature for several days to give colorless crystals of the title compound (yield 61%). They were washed with a small volume of cold CH_3CN and diethyl ether. Analysis calculated for $\text{C}_8\text{H}_{17}\text{Ag}_2\text{N}_5\text{O}_7$: C 18.80, H 3.35, N 13.71%; found: C 18.86, H 3.39, N 13.64%.

S3. Refinement

C- and N-bound H atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93 and N—H = 0.89 Å and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C,N})$. H atoms of water molecule were located in a difference Fourier map and refined as riding, with O—H = 0.85 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{O})$.

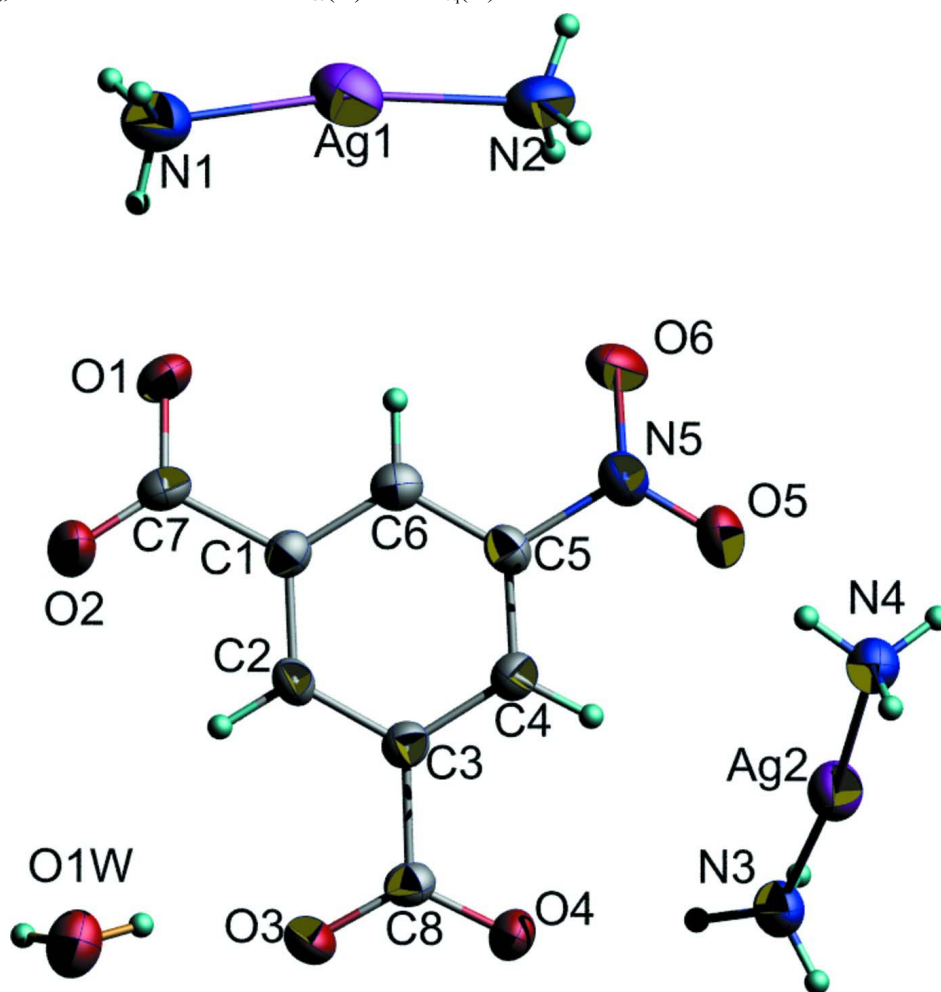
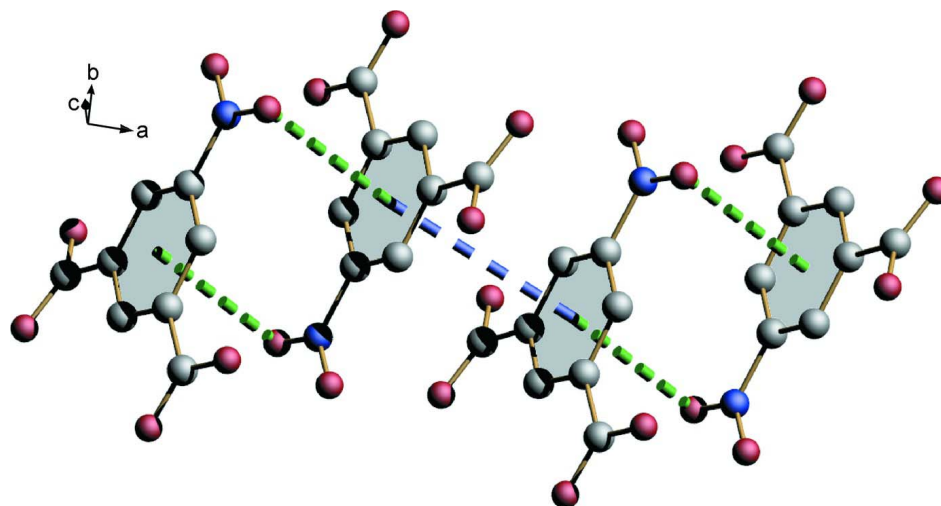
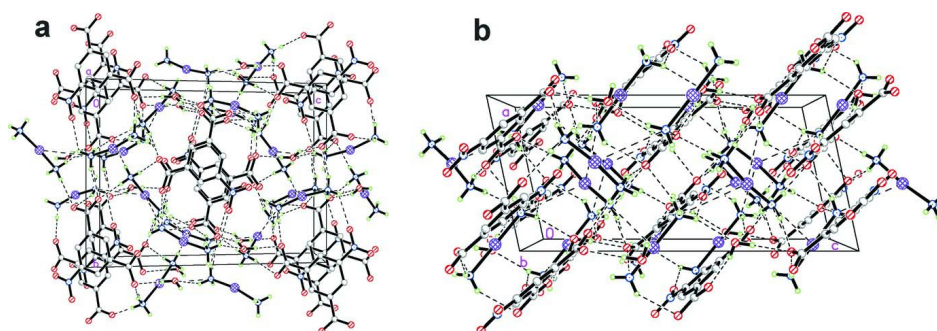


Figure 1

Molecular structure of the title compound, showing the coordination environment around the Ag^{I} center. Displacement ellipsoids are drawn at the 50% probability level.

**Figure 2**

A ball-stick perspective view of the $lp(O)\cdots\pi$ (green dashed lines) and $\pi\text{-}\pi$ (blue dashed lines) interactions in the title compound. H atoms and $[Ag(NH_3)_2]^+$ cations have been omitted for clarity.

**Figure 3**

Perspective views of the three-dimensional supramolecular network incorporating $N\text{-}H\cdots O$ and $O\text{-}H\cdots O$ hydrogen bonds (dashed lines) viewed along two different directions.

Bis[diamminesilver(I)] 5-nitroisophthalate monohydrate

Crystal data

$[Ag(NH_3)_2]_2(C_8H_5NO_6)\cdot H_2O$

$M_r = 511.01$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 7.692\ (2)\ \text{\AA}$

$b = 12.229\ (3)\ \text{\AA}$

$c = 16.379\ (4)\ \text{\AA}$

$\beta = 102.100\ (4)^\circ$

$V = 1506.5\ (7)\ \text{\AA}^3$

$Z = 4$

$F(000) = 1000$

$D_x = 2.253\ \text{Mg m}^{-3}$

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

Cell parameters from 4729 reflections

$\theta = 5.1\text{-}57.2^\circ$

$\mu = 2.64\ \text{mm}^{-1}$

$T = 298\ \text{K}$

Block, colorless

$0.11 \times 0.10 \times 0.08\ \text{mm}$

Data collection

Oxford Diffraction Gemini S Ultra
diffractometer
Radiation source: sealed tube
Graphite monochromator
Detector resolution: 16.1903 pixels mm⁻¹
 ω scans
Absorption correction: multi-scan
(*CrysAlis RED*; Oxford Diffraction, 2006)
 $T_{\min} = 0.760$, $T_{\max} = 0.817$

7118 measured reflections
2627 independent reflections
2500 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$
 $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.1^\circ$
 $h = -9 \rightarrow 9$
 $k = -8 \rightarrow 14$
 $l = -17 \rightarrow 19$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.046$
 $wR(F^2) = 0.114$
 $S = 1.22$
2627 reflections
204 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
 $w = 1/[\sigma^2(F_o^2) + (0.0451P)^2 + 2.1461P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.97 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.98 \text{ e } \text{\AA}^{-3}$
Extinction correction: *SHELXL97* (Sheldrick,
2008), $F_c^* = kFc[1 + 0.001x\text{Fc}^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0264 (13)

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	0.01233 (6)	0.87015 (4)	0.39354 (3)	0.0561 (2)
Ag2	0.56988 (5)	0.37352 (3)	0.78293 (3)	0.0444 (2)
C1	0.1106 (5)	0.4687 (4)	0.4096 (3)	0.0272 (9)
C2	0.1513 (6)	0.3606 (4)	0.4283 (3)	0.0277 (9)
H2	0.0955	0.3065	0.3922	0.033*
C3	0.2729 (5)	0.3307 (4)	0.4993 (3)	0.0273 (9)
C4	0.3475 (6)	0.4110 (4)	0.5543 (3)	0.0294 (10)
H4	0.4278	0.3929	0.6032	0.035*
C5	0.3022 (6)	0.5176 (4)	0.5362 (3)	0.0281 (9)
C6	0.1878 (6)	0.5481 (4)	0.4639 (3)	0.0294 (10)
H6	0.1631	0.6216	0.4521	0.035*
C7	-0.0153 (6)	0.4982 (4)	0.3292 (3)	0.0308 (10)
C8	0.3273 (6)	0.2131 (4)	0.5152 (3)	0.0293 (10)
N1	-0.1928 (7)	0.8046 (4)	0.3002 (3)	0.0544 (12)
H1A	-0.1867	0.8333	0.2509	0.065*
H1B	-0.2977	0.8205	0.3120	0.065*
H1C	-0.1805	0.7323	0.2983	0.065*
N2	0.2262 (6)	0.9066 (4)	0.4929 (3)	0.0499 (11)
H2A	0.2441	0.9786	0.4954	0.060*
H2B	0.3239	0.8733	0.4846	0.060*
H2C	0.2011	0.8835	0.5406	0.060*
N3	0.7101 (6)	0.2725 (4)	0.7167 (3)	0.0411 (10)
H3A	0.7576	0.2171	0.7490	0.049*

H3B	0.7962	0.3108	0.7012	0.049*
H3C	0.6364	0.2466	0.6716	0.049*
N4	0.4096 (5)	0.4767 (4)	0.8378 (2)	0.0395 (10)
H4A	0.4737	0.5333	0.8615	0.047*
H4B	0.3677	0.4399	0.8764	0.047*
H4C	0.3192	0.5008	0.7988	0.047*
N5	0.3862 (6)	0.6021 (4)	0.5942 (2)	0.0358 (9)
O1	-0.0137 (5)	0.5948 (3)	0.3058 (2)	0.0405 (8)
O1W	-0.0469 (5)	0.0861 (3)	0.3572 (2)	0.0502 (9)
H1WA	-0.0315	0.0871	0.3073	0.060*
H1WB	0.0474	0.1189	0.3813	0.060*
O2	-0.1083 (5)	0.4259 (3)	0.2916 (2)	0.0502 (10)
O3	0.2508 (5)	0.1444 (3)	0.4657 (3)	0.0494 (10)
O4	0.4452 (5)	0.1927 (3)	0.5764 (2)	0.0412 (8)
O5	0.4957 (5)	0.5735 (3)	0.6553 (2)	0.0509 (10)
O6	0.3436 (6)	0.6952 (3)	0.5786 (2)	0.0567 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0498 (3)	0.0475 (3)	0.0734 (4)	-0.00206 (19)	0.0184 (2)	-0.0061 (2)
Ag2	0.0446 (3)	0.0460 (3)	0.0402 (3)	0.00187 (17)	0.00340 (18)	-0.00385 (17)
C1	0.027 (2)	0.030 (2)	0.025 (2)	0.0008 (18)	0.0062 (16)	0.0021 (18)
C2	0.032 (2)	0.026 (2)	0.024 (2)	-0.0037 (18)	0.0049 (17)	-0.0045 (17)
C3	0.024 (2)	0.028 (2)	0.030 (2)	0.0005 (18)	0.0057 (17)	0.0014 (19)
C4	0.030 (2)	0.031 (2)	0.027 (2)	0.0013 (19)	0.0049 (17)	0.0026 (19)
C5	0.030 (2)	0.028 (2)	0.027 (2)	-0.0044 (19)	0.0088 (17)	-0.0030 (18)
C6	0.028 (2)	0.029 (2)	0.032 (2)	0.0017 (19)	0.0104 (18)	0.0025 (19)
C7	0.030 (2)	0.028 (3)	0.034 (2)	0.005 (2)	0.0069 (18)	0.006 (2)
C8	0.031 (2)	0.027 (2)	0.031 (2)	0.0054 (19)	0.0082 (19)	0.0019 (19)
N1	0.061 (3)	0.048 (3)	0.055 (3)	0.006 (2)	0.016 (2)	0.001 (2)
N2	0.052 (3)	0.038 (3)	0.062 (3)	0.006 (2)	0.015 (2)	0.009 (2)
N3	0.038 (2)	0.038 (2)	0.043 (2)	-0.0028 (19)	-0.0014 (18)	-0.0036 (19)
N4	0.039 (2)	0.039 (2)	0.039 (2)	-0.0006 (19)	0.0032 (17)	0.0000 (19)
N5	0.042 (2)	0.035 (2)	0.031 (2)	-0.0080 (19)	0.0082 (18)	-0.0020 (18)
O1	0.044 (2)	0.0333 (19)	0.0391 (19)	0.0038 (16)	-0.0021 (15)	0.0113 (16)
O1W	0.045 (2)	0.059 (3)	0.043 (2)	0.0005 (19)	0.0004 (16)	-0.0007 (19)
O2	0.054 (2)	0.037 (2)	0.047 (2)	-0.0080 (18)	-0.0167 (17)	0.0017 (18)
O3	0.060 (2)	0.0287 (19)	0.049 (2)	0.0045 (17)	-0.0119 (18)	-0.0091 (17)
O4	0.0412 (18)	0.0344 (19)	0.0393 (18)	0.0044 (15)	-0.0112 (15)	0.0000 (15)
O5	0.060 (2)	0.046 (2)	0.039 (2)	-0.0077 (19)	-0.0089 (17)	-0.0042 (17)
O6	0.088 (3)	0.027 (2)	0.049 (2)	0.002 (2)	-0.001 (2)	-0.0022 (17)

Geometric parameters (Å, °)

Ag1—N1	2.112 (5)	C7—O1	1.243 (6)
Ag1—N2	2.105 (5)	C8—O3	1.228 (6)
Ag2—N3	2.088 (4)	C8—O4	1.229 (5)

Ag2—N4	2.094 (4)	N1—H1A	0.8900
Ag1—O1W ⁱ	2.725 (4)	N1—H1B	0.8900
Ag2—O1W ⁱⁱ	2.985 (4)	N1—H1C	0.8900
C1—C6	1.367 (6)	N2—H2A	0.8900
C1—C2	1.378 (6)	N2—H2B	0.8900
C1—C7	1.505 (6)	N2—H2C	0.8900
C2—C3	1.380 (6)	N3—H3A	0.8900
C2—H2	0.9300	N3—H3B	0.8900
C3—C4	1.374 (6)	N3—H3C	0.8900
C3—C8	1.505 (6)	N4—H4A	0.8900
C4—C5	1.366 (6)	N4—H4B	0.8900
C4—H4	0.9300	N4—H4C	0.8900
C5—C6	1.370 (6)	N5—O6	1.198 (6)
C5—N5	1.460 (6)	N5—O5	1.217 (5)
C6—H6	0.9300	O1W—H1WA	0.8501
C7—O2	1.220 (6)	O1W—H1WB	0.8500
N2—Ag1—N1	169.90 (19)	O4—C8—C3	117.8 (4)
N3—Ag2—N4	174.05 (16)	Ag1—N1—H1A	109.5
N2—Ag1—O1W ⁱ	91.79 (15)	Ag1—N1—H1B	109.5
N1—Ag1—O1W ⁱ	98.31 (16)	H1A—N1—H1B	109.5
N3—Ag2—O1W ⁱⁱ	74.69 (14)	Ag1—N1—H1C	109.5
N4—Ag2—O1W ⁱⁱ	110.21 (14)	H1A—N1—H1C	109.5
C6—C1—C2	119.3 (4)	H1B—N1—H1C	109.5
C6—C1—C7	120.7 (4)	Ag1—N2—H2A	109.5
C2—C1—C7	119.9 (4)	Ag1—N2—H2B	109.5
C1—C2—C3	121.6 (4)	H2A—N2—H2B	109.5
C1—C2—H2	119.2	Ag1—N2—H2C	109.5
C3—C2—H2	119.2	H2A—N2—H2C	109.5
C4—C3—C2	118.7 (4)	H2B—N2—H2C	109.5
C4—C3—C8	120.4 (4)	Ag2—N3—H3A	109.5
C2—C3—C8	120.9 (4)	Ag2—N3—H3B	109.5
C5—C4—C3	119.1 (4)	H3A—N3—H3B	109.5
C5—C4—H4	120.4	Ag2—N3—H3C	109.5
C3—C4—H4	120.4	H3A—N3—H3C	109.5
C4—C5—C6	122.4 (4)	H3B—N3—H3C	109.5
C4—C5—N5	118.5 (4)	Ag2—N4—H4A	109.5
C6—C5—N5	119.0 (4)	Ag2—N4—H4B	109.5
C1—C6—C5	118.8 (4)	H4A—N4—H4B	109.5
C1—C6—H6	120.6	Ag2—N4—H4C	109.5
C5—C6—H6	120.6	H4A—N4—H4C	109.5
O2—C7—O1	125.1 (4)	H4B—N4—H4C	109.5
O2—C7—C1	118.0 (4)	O6—N5—O5	124.1 (4)
O1—C7—C1	116.8 (4)	O6—N5—C5	118.1 (4)
O3—C8—O4	124.7 (4)	O5—N5—C5	117.8 (4)
O3—C8—C3	117.5 (4)	H1WA—O1W—H1WB	99.3

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O1W-H1WA\cdots O1^{iii}$	0.85	1.96	2.807 (5)	177
$O1W-H1WB\cdots O3$	0.85	1.88	2.684 (5)	156
$N1-H1B\cdots O4^{iv}$	0.89	2.35	3.082 (6)	140
$N1-H1C\cdots O1$	0.89	2.10	2.905 (6)	149
$N2-H2A\cdots O3^i$	0.89	2.09	2.954 (6)	164
$N2-H2B\cdots O4^v$	0.89	2.36	3.218 (6)	163
$N2-H2C\cdots O1W^{iv}$	0.89	2.28	3.059 (6)	147
$N2-H2C\cdots O6$	0.89	2.57	2.990 (6)	110
$N3-H3A\cdots O2^{ii}$	0.89	2.08	2.937 (6)	163
$N3-H3B\cdots O1^v$	0.89	2.06	2.930 (6)	167
$N3-H3C\cdots O4$	0.89	2.02	2.901 (5)	173
$N4-H4A\cdots O4^{vi}$	0.89	2.23	3.088 (6)	163
$N4-H4B\cdots O3^{vii}$	0.89	2.14	3.024 (6)	176
$N4-H4C\cdots O2^{iv}$	0.89	2.15	3.036 (5)	175

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