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Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(C-C) = 0.004$ Å
 R factor = 0.027
 wR factor = 0.068
Data-to-parameter ratio = 15.6For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Di- μ -nitrate- $\kappa^4 O:O'$ -bis[bis(3-hydroxypyridine- κN)-
silver(I)] dihydrate

The dinuclear title complex, $[Ag_2(NO_3)_2(3-PyOH)_4] \cdot 2H_2O$ (3-PyOH is 3-hydroxypyridine, C_5H_5NO), situated across a crystallographic inversion centre, can be described as a dimeric structure, in which two $[Ag(3-PyOH)_2]$ groups are held together by the $Ag \cdots Ag$ interaction [3.317 (1) Å]. Each Ag atom is two-coordinate and exists in an approximately linear geometry. The two NO_3^- ions interact with the Ag^I atoms in a bridging mode through very weak $Ag \cdots O$ interactions [$Ag \cdots O = 2.862$ (2) and 2.877 (2) Å]. A three-dimensional supramolecular framework is formed by $O-H \cdots O$ hydrogen bonds.

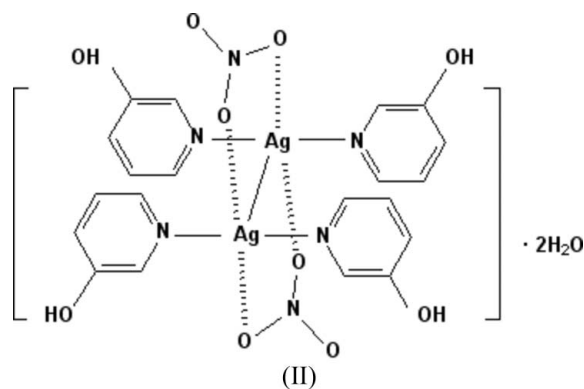
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Comment

3-Hydroxypyridine (3-PyOH), when deprotonated, is a good building block in directing polymeric coordination architectures with interesting properties, such as magnetism (Castillo *et al.*, 2000; Kawata *et al.*, 1997) and fluorescence (Gao *et al.*, 2005); in its neutral form, it is also useful in the synthesis of supramolecules and inorganic precursor compounds for solid-state materials, since it is not only capable of binding to metal centres but can also form regular hydrogen bonds by functioning as both a hydrogen-bond donor and an acceptor (Breeze & Wang, 1993). Recently, we have reported the chain and layer hydrogen-bonding architectures of two copper(II) complexes (Gao, Zhang *et al.*, 2004; Gao, Lu *et al.*, 2004), as well as the three-dimensional supramolecular framework structure of $[Ag(3-PyOH)_2]NO_3$, (I) (Lu *et al.*, 2005). In continuation of our research in the synthesis of supramolecular transition metal complexes with the 3-PyOH ligand, we have recently obtained the title compound, (II), from an aqueous solution of $AgNO_3$ and 3-PyOH. We report here the crystal structure of (II).



The asymmetric unit of (II) consists of one-half of $[Ag(3-PyOH)_2NO_3] \cdot 2H_2O$, situated across a crystallographic inver-

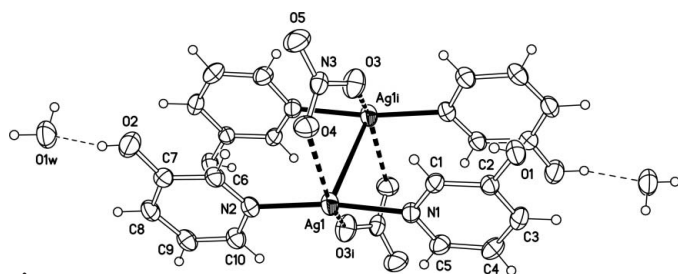


Figure 1
ORTEP (Johnson, 1976) plot of (II), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Unlabelled atoms are related to labelled atoms by $(1-x, 1-y, 1-z)$. Bold-dashed lines represent weak $\text{Ag}\cdots\text{O}$ contacts. Other dashed lines indicate hydrogen bonds.

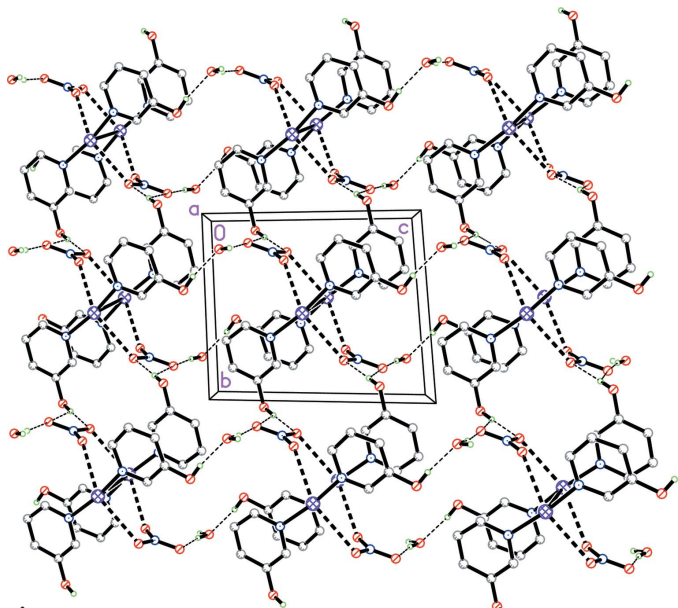


Figure 2
Perspective view of the hydrogen-bonded three-dimensional network of (II). Weak $\text{Ag}\cdots\text{O}$ contacts and hydrogen bonds are denoted by bold- and narrow-dashed lines, respectively. The H atoms of the aromatic rings have been omitted for clarity.

sion centre (Fig. 1). Each Ag^{I} atom is coordinated by two neutral 3-PyOH molecules through the N atoms [$\text{Ag}-\text{N} = 2.142(2)$ and $2.148(2)$ Å] and shows a linear geometry with an $\text{N}-\text{Ag}-\text{N}$ angle of $171.79(8)^\circ$. The two NO_3^- ions interact with the Ag^{I} atoms in a bridging mode through very weak $\text{Ag}\cdots\text{O}$ interactions [$\text{Ag}\cdots\text{O} = 2.862(2)$ and $2.877(2)$ Å]. The fact that the $\text{N}-\text{Ag}-\text{N}$ angle in (II) is wider than that in (I) [$162.54(9)^\circ$; Lu *et al.*, 2005] may be ascribed to the bridging mode of the two NO_3^- ions, rather than the chelating coordination of just one NO_3^- ion in (I). The $\text{Ag}\cdots\text{O}$ distances in (II) (Table 1) are longer than those in (I) [$2.760(3)$ and $2.801(3)$ Å; Lu *et al.*, 2005]. The $\text{Ag}\cdots\text{Ag}$ distance of $3.317(1)$ Å is within the sum of van der Waals radii for two Ag^{I} centres (3.44 Å; Bondi, 1964) and can be considered as an $\text{Ag}\cdots\text{Ag}$ interaction.

In the dinuclear unit, $\pi-\pi$ interactions are observed between adjacent pyridine rings, with a centroid-centroid distance of $3.579(2)$ Å. The dinuclear units are linked by $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds involving the water molecules, the

hydroxy groups in the 3-PyOH ligands and the NO_3^- ions, into a three-dimensional hydrogen-bonded framework (Fig. 2 and Table 2).

Experimental

The title complex, (II), was prepared by the addition of AgNO_3 (2 mmol) to an aqueous solution of 3-hydroxypyridine (6 mmol). The resulting solution was protected from light and allowed to evaporate slowly at room temperature, whereupon colourless prismatic crystals of (II) were isolated after 5 d. Analysis calculated for $\text{C}_{10}\text{H}_{12}\text{N}_3\text{O}_6\text{Ag}$: C 31.77, H 3.20, N 11.11%; found: C 31.71, H 3.21, N 11.12%.

Crystal data

$[\text{Ag}_2(\text{NO}_3)_2(\text{C}_5\text{H}_5\text{NO})_4]\cdot 2\text{H}_2\text{O}$
 $M_r = 756.19$
 Triclinic, $P\bar{1}$
 $a = 7.9912(16)$ Å
 $b = 8.8615(18)$ Å
 $c = 10.399(2)$ Å
 $\alpha = 81.37(3)^\circ$
 $\beta = 71.64(3)^\circ$
 $\gamma = 72.01(3)^\circ$
 $V = 663.6(3)$ Å³

$Z = 1$
 $D_x = 1.892$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 5742 reflections
 $\theta = 3.1-27.5^\circ$
 $\mu = 1.55$ mm⁻¹
 $T = 296(2)$ K
 Prism, colourless
 $0.36 \times 0.27 \times 0.19$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.610$, $T_{\text{max}} = 0.747$
 6582 measured reflections

3011 independent reflections
 2533 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.017$
 $\theta_{\text{max}} = 27.5^\circ$
 $h = -9 \rightarrow 10$
 $k = -11 \rightarrow 11$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.027$
 $wR(F^2) = 0.068$
 $S = 1.03$
 3011 reflections
 193 parameters

$w = 1/[\sigma^2(F_o^2) + (0.0416P)^2 + 0.0053P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.32$ e Å⁻³

H atoms treated by a mixture of independent and constrained refinement

Table 1

Selected geometric parameters (Å, °).

$\text{Ag1}-\text{N1}$	2.142 (2)	$\text{Ag1}-\text{O4}$	2.877 (2)
$\text{Ag1}-\text{N2}$	2.148 (2)	$\text{Ag1}-\text{Ag1}^{\text{i}}$	3.317 (1)
$\text{Ag1}-\text{O3}^{\text{i}}$	2.862 (2)		
$\text{O4}-\text{Ag1}-\text{N1}$	96.37 (7)	$\text{N1}-\text{Ag1}-\text{O3}^{\text{i}}$	91.78 (2)
$\text{O4}-\text{Ag1}-\text{N2}$	90.05 (8)	$\text{N2}-\text{Ag1}-\text{O3}^{\text{i}}$	84.98 (2)
$\text{N1}-\text{Ag1}-\text{N2}$	171.79 (8)	$\text{O4}-\text{Ag1}-\text{O3}^{\text{i}}$	151.50 (2)

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H11}\cdots\text{O4}^{\text{ii}}$	0.84 (4)	1.89 (4)	2.735 (3)	177 (3)
$\text{O1}-\text{H11}\cdots\text{O5}^{\text{ii}}$	0.84 (4)	2.58 (3)	3.163 (3)	128 (3)
$\text{O2}-\text{H12}\cdots\text{O1W}$	0.84 (4)	1.82 (4)	2.650 (3)	168 (4)
$\text{O1W}-\text{H1W1}\cdots\text{O1}^{\text{iii}}$	0.85 (4)	2.16 (2)	2.937 (3)	153 (4)
$\text{O1W}-\text{H1W2}\cdots\text{O5}^{\text{iv}}$	0.85 (3)	2.08 (3)	2.901 (3)	166 (4)

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

H atoms attached to O atoms were located in a difference Fourier map and refined with an O–H distance restraint of 0.85 (1) Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. Other H atoms were placed in calculated positions and were allowed to ride on their parent C atoms [C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$].

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK & Rigaku Corporation, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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