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Bis(3-hydroxypyridine-κN)(nitrato-$\kappa^2 O,O'$)silver(I)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.026
wR factor = 0.078
Data-to-parameter ratio = 15.6

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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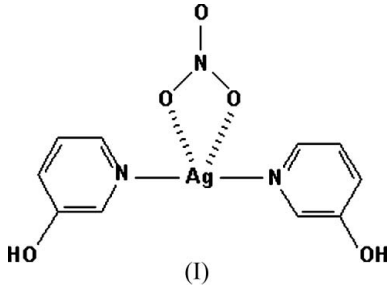
In the mononuclear title complex, $[Ag(NO_3)(3\text{-PyOH})_2]$ (3-PyOH = 3-hydroxypyridine, C_5H_5NO), the Ag^I atom shows a linear geometry defined by two N atoms of the 3-PyOH ligands, and the NO_3^- anion interacts with the Ag^I atom in a chelating mode through very weak Ag···O bonds. A three-dimensional supramolecular framework is formed by both hydrogen bonds and π–π interactions.

Comment

3-Hydroxypyridine (3-PyOH), when deprotonated, is a good building block in directing polymeric coordination architectures with interesting properties, such as magnetic (Castillo *et al.*, 2000; Kawata *et al.*, 1997) and fluorescent (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 centers but can also form regular hydrogen bonds by functioning as both a hydrogen-bond donor and acceptor (Breeze & Wang, 1993). However, structural reports of hydrogen-bonded supramolecular complexes based on 3-PyOH are relatively rare. Recently, we have reported the chain and layer hydrogen-bonding architectures of two copper(II) complexes with 3-PyOH ligands (Gao, Zhang *et al.*, 2004; Gao, Lu *et al.*, 2004). In this paper, a novel three-dimensional supramolecular complex, *viz*. $[Ag(NO_3)(3\text{-PyOH})_2]$, (I), is presented.



(I)

The Ag^I atom in (I) is coordinated by two neutral 3-PyOH molecules through the N atoms [Ag—N = 2.156 (3) and 2.166 (3) Å], and shows a linear geometry with an N—Ag—N angle of 162.54 (9)°. The deviation from perfect linearity may be caused by the interaction of the NO_3^- ion, which interacts with the Ag^I atom in a chelating mode through very weak Ag···O interactions [Ag···O = 2.760 (3) and 2.801 (3) Å]. The dihedral angle between the two pyridine rings is 44.9 (1)° (Fig. 1). The mononuclear units are linked by O—H···O hydrogen bonds between the hydroxyl groups and the O atoms of the NO_3^- anion into a hydrogen-bonded layer structure (Fig. 2). The O···O distances and O—H···O angles

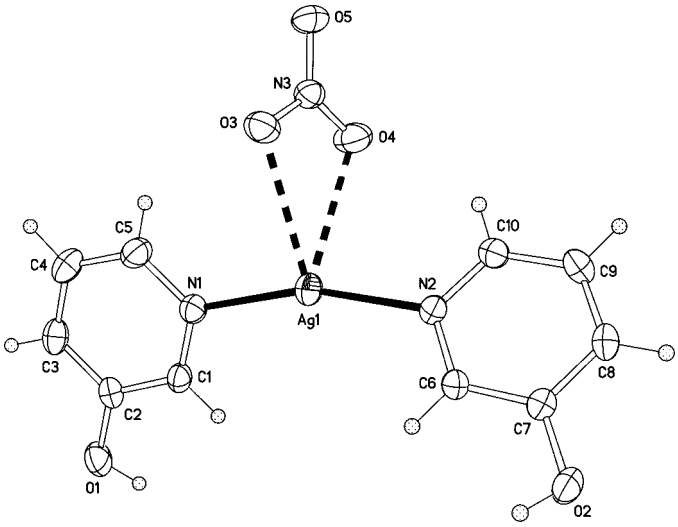


Figure 1
The coordination environment of the Ag^{I} atom in (I), with displacement ellipsoids drawn at the 30% probability level.

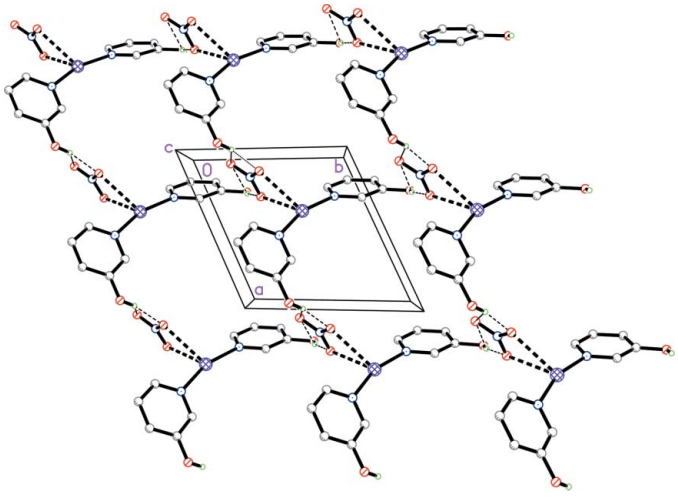


Figure 2
Perspective view of the hydrogen-bonded layer structure of (I). Weak Ag···O contacts and the hydrogen bonds are denoted by bold and narrow dashed lines, respectively. The H atoms of the aromatic rings have been omitted for clarity.

are in the ranges 2.713 (4)–3.233 (4) Å and 128 (4)–169 (5)°, respectively (Table 1). Aryl–aryl π–π interactions, formed between pyridine rings from adjacent layers [centroid-to-centroid distance = 3.740 (4) Å], connect the hydrogen-bonded layers into a three-dimensional supramolecular framework, as shown in Fig. 3.

Experimental

The title complex, (I), was synthesized by the addition of $AgNO_3$ (2 mmol) to an ethanol solution of 3-hydroxypyridine (6 mmol). The reaction mixture was protected from light and allowed to evaporate slowly at room temperature, whereupon colorless prismatic crystals of (I) were isolated after about 7 d. Analysis calculated for $C_{10}H_{10}AgN_3O_5$: C 33.36, H 2.80, N 11.67%; found: C 33.25,H 2.83, N 11.66%.

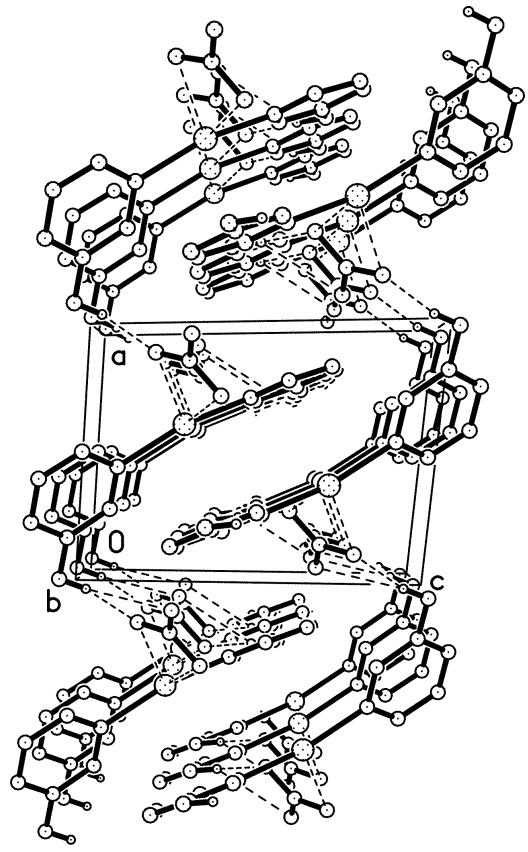


Figure 3
The three-dimensional supramolecular framework, showing the π–π interactions (dashed lines) between the hydrogen-bonded layers. The H atoms of the aromatic rings have been omitted for clarity.

Crystal data

$[Ag(NO_3)(C_5H_5NO)_2]$
M_r = 360.08
Triclinic, $P\overline{1}$
a = 8.2474 (16) Å
b = 8.4577 (17) Å
c = 10.488 (2) Å
α = 70.05 (3)°
β = 76.83 (3)°
γ = 62.73 (3)°
V = 609.0 (3) Å^3
Z = 2
D_x = 1.964 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5573 reflections
θ = 3.0–27.5°
μ = 1.68 mm^{-1}
T = 296 (2) K
Plate, colorless
0.37 × 0.28 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.576, T_{max} = 0.824
6026 measured reflections
2770 independent reflections
2502 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 27.5°
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.078
S = 1.06
2770 reflections
178 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0402P)^2 + 0.4922P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.60 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N2	2.156 (3)	Ag1—O3	2.760 (3)
Ag1—N1	2.166 (3)	Ag1—O4	2.801 (3)
O3—Ag1—N1	90.14 (9)	O4—Ag1—N2	91.22 (9)
O3—Ag1—N2	106.93 (9)	O4—Ag1—O3	45.71 (9)
O4—Ag1—N1	103.92 (9)	N2—Ag1—N1	162.54 (9)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H11···O3^{i}	0.85 (4)	1.87 (4)	2.713 (4)	169 (5)
O1—H11···O5^{i}	0.85 (4)	2.64 (4)	3.233 (4)	128 (4)
O2—H12···O4^{ii}	0.85 (4)	1.91 (2)	2.727 (4)	160 (5)
O2—H12···O5^{ii}	0.85 (4)	2.54 (4)	3.194 (4)	135 (4)

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

H atoms bound to carbon were placed in calculated positions [C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C)] using the riding-model approximation. The H atoms of the hydroxyl groups were located in a difference map and refined with O—H distance restraints of 0.85 (1) Å and with U_{iso}(H) = 1.5U_{eq}(O).

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

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