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Bis(pyridine-4-carboxylic acid-κN)silver(I) nitrate dihydrate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.040
wR factor = 0.092
Data-to-parameter ratio = 15.8

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

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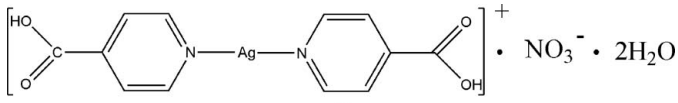
In the title compound, $[Ag(C_6H_5NO_2)_2]NO_3{\cdot}2H_2O$, the Ag atom is coordinated by two N atoms from pyridine-4-carboxylic acid ligands. An infinite hydrogen-bonding structure between cation, anion and water molecules results in the formation of a double chain parallel to the b axis. These double chains are interconnected by weak O···Ag interactions involving one O atom of a neighbouring nitrate.

Comment

It is known that pyridine-4-carboxylic acid and its anion are important ligands for building supramolecular networks with metals (Carlucci *et al.*, 2000; Li *et al.*, 2006; MacGillivray *et al.*, 1998). Coordination compounds of pyridine-4-carboxylic acid and silver have been reported previously (Jaber *et al.*, 1994; Liu & Yuan, 2005; Yang *et al.*, 2004).



(I)

In the title compound, (I), the Ag^I atom is coordinated by two N atoms from pyridine-4-carboxylic acid ligands. The asymmetric unit also contains a nitrate anion and two solvent water molecules (Fig. 1).

One interesting feature of the crystal structure of (I) is the occurrence of hydrogen-bonding interactions between the nitrate anion, the solvent water molecules and the cation to form a double chain (Table 1, Fig. 2). These double chains are

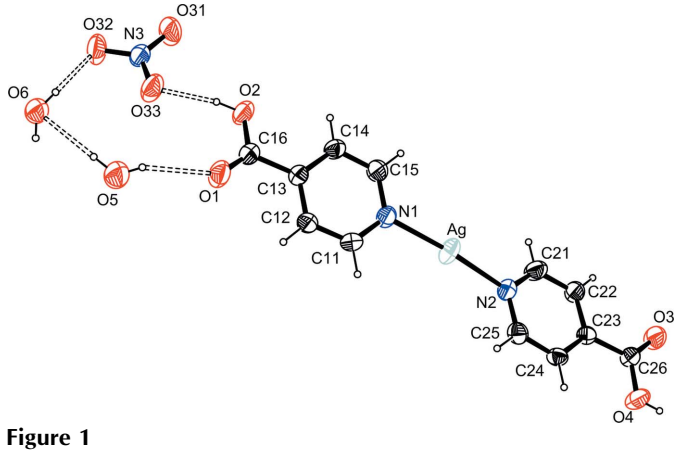


Figure 1
The asymmetric unit of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as small spheres of arbitrary radii. Hydrogen bonds are shown as dashed lines.

connected to each other by Ag···O interactions involving one O atom of the nitrate anion [Ag···O31^{i} = 3.006 (3) Å; symmetry code: (i) $\frac{3}{2} - x, \frac{1}{2} + x, \frac{3}{2} - z$], leading to a supramolecular three-dimensional structure.

Experimental

Pyridine-4-carboxyllic acid and $AgNO_3$ were of analytical grade and were used without further purification. Pyridine-4-carboxylic acid (1.24 g, 10 mmol) and $AgNO_3$ (0.85 g, 5 mmol) were dissolved in water (15 ml). The mixture was stirred for 3 h. The resultant solution was filtered, and the filtrate was allowed to stand at room temperature for one week to give colourless block crystals of (I).

Crystal data

$[Ag(C_6H_5NO_2)_2]NO_3·2H_2O$
M_r = 452.13
Monoclinic, $P2_1/n$
a = 6.954 (4) Å
b = 21.605 (9) Å
c = 10.849 (7) Å
β = 103.93 (2)°
V = 1582.0 (14) Å^3
Z = 4
D_x = 1.898 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 1.33 mm^{-1}
T = 295 (2) K
Block, colourless
0.30 × 0.29 × 0.26 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.690, T_{max} = 0.721
15087 measured reflections
3598 independent reflections
2607 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.092
S = 1.05
3598 reflections
228 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0446P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.70 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O33	0.82	1.81	2.618 (3)	167
O2—H2···N3	0.82	2.59	3.340 (3)	152
O4—H4···O6^{i}	0.82	1.80	2.606 (3)	167
O5—H5*A*···O1	0.73	2.16	2.846 (3)	158
O5—H5*B*···O6	0.87	2.20	3.069 (3)	180
O6—H6*A*···O5^{ii}	0.85	1.92	2.775 (4)	179
O6—H6*B*···O32	0.84	1.94	2.783 (4)	179

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

H atoms attached to carbon were treated as riding on their parent atoms, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). The hydroxy H atoms were treated as riding on their parent atoms, with O—H = 0.82 Å and U_{iso}(H) = 1.5U_{eq}(C). The water H atoms were located in a difference Fourier map and treated as riding on their parent O atoms, with U_{iso}(H) = 1.5U_{eq}(O).

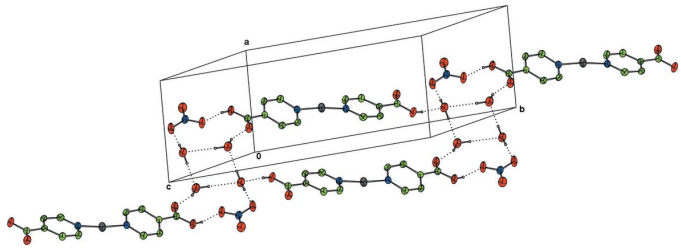


Figure 2
The hydrogen-bonded (dotted lines) chain in compound (I).

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* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996), *ORTEP-3 for Windows* (Farrugia, 1997) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *SHELXL97*.

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