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Tris(2-aminopyridine-κN^1)(nitrato-κO)silver(I)

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Key indicators

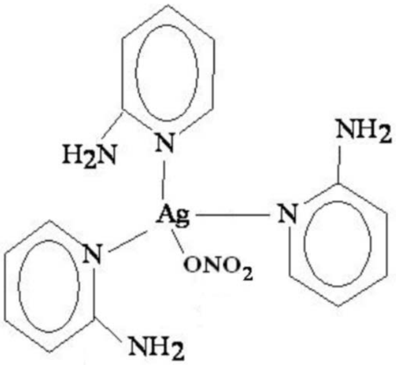
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.008 Å
R factor = 0.028
wR factor = 0.067
Data-to-parameter ratio = 12.6

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

In the title compound, $[Ag(NO_3)(C_{15}H_{18}N_6)]$, the Ag^I atom is four-coordinated by the three N atoms of the 2-aminopyridine ligands and by an O atom of the nitro group. The structure is stabilized by an extensive network of N—H—O and N—H—N hydrogen bonds.

Comment

2-Aminopyridine is used in the manufacture of pharmaceuticals, especially antihistaminic drugs (Windholz, 1976). The silver(I) ion exhibits a large flexibility in its coordination with nitrogen-containing aromatic ligands, with coordination numbers ranging from two to eight (Kristiansson, 2000). As a part of our investigation of the reactions of 2-aminopyridine with metals, we report here the crystal structure of the title compound, (I).



(I)

In (I), the Ag^+ ion is four-coordinated by three 2-aminopyridine ligands and one of the O atoms of the nitrate group, with Ag—N distances of 2.141 (4), 2.179 (4), and 2.392 (5) Å and an Ag1—O21 distance of 2.649 (4) Å, with highly distorted tetrahedral geometry. These values are comparable to those reported in the literature (Aakeroy *et al.*, 1998; Kristiansson, 2000; Liu & Zhu, 2004; Ni *et al.*, 2003). The N13—Ag1—N1, N13—Ag1—N7 and N1—Ag1—N7 bond angles are 141.02 (16), 111.83 (16) and 106.44 (16)°, respectively, which are comparable to the values reported in the literature (Sloufova & Slouf, 2000; Yoon *et al.*, 2002). The bond angles at the pyridine N atoms of two of the three 2-aminopyridine ligands [C2—N1—C6 = 118.9 (5)° and C14—N13—C18 = 119.3 (5)°] differ significantly from that of 2-aminopyridine in its uncomplexed form, which is 117.7 (1)° (Chao *et al.*, 1975). Interestingly there is a slight decrease in the bond angle at N7 for the third ligand [C8—N7—C12 =

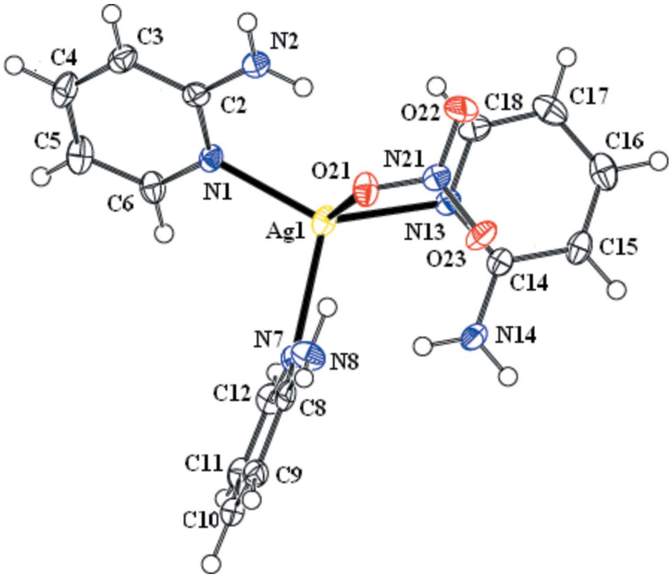


Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

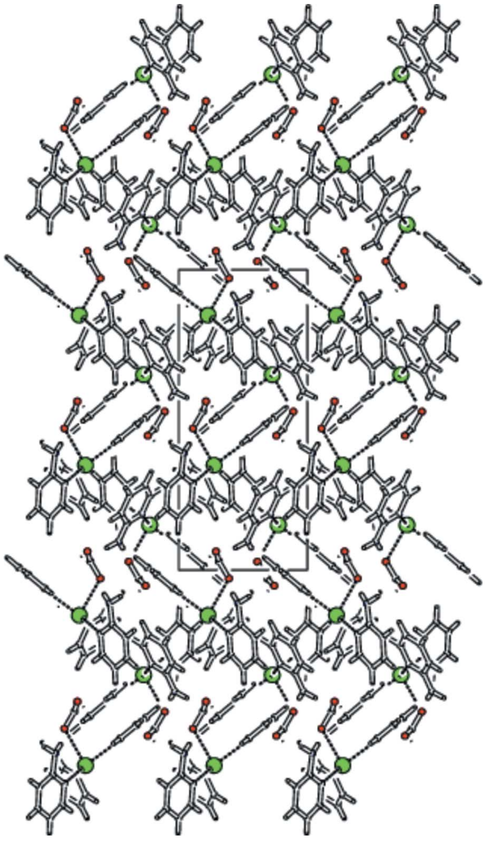


Figure 2
A packing diagram for (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.

116.7 (5)°]. This may be attributed to the flexibility of the coordination geometry of silver with the ligands. All the other bond lengths and bond angles of 2-aminopyridine are found to be normal.

The crystal structure is stabilized by an extensive network of hydrogen bonds of type N—H···O and N—H···N. There is a weak hydrogen bond between the amino group of 2-aminopyridine and the nitrate group.

Experimental

Silver nitrate (0.169 g) dissolved in 20 ml of ammonia solution and 2-aminopyridine (0.282 g) dissolved in ethanol were mixed in the molar ratio 3:1 and heated for 2 h. Pale-yellow needle-shaped crystals of (I) were obtained by slow evaporation over a period of two weeks.

Crystal data

$[Ag(NO_3)(C_{15}H_{18}N_6)]$
$M_r = 452.23$
Monoclinic, $P2_1/c$
$a = 10.932$ (3) Å
$b = 8.027$ (2) Å
$c = 18.948$ (6) Å
$\beta = 98.001$ (6)°
$V = 1646.4$ (8) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 1.26$ mm^{-1}
$T = 293$ (2) K
0.06 × 0.06 × 0.06 mm

Data collection

Rigaku CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.925$, $T_{max} = 0.927$
15950 measured reflections
2981 independent reflections
2755 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.067$
$S = 1.04$
2981 reflections
236 parameters
6 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

N1—Ag1	2.179 (4)	N13—Ag1	2.141 (4)
N7—Ag1	2.392 (5)	O21—Ag1	2.649 (4)
N21—O21—Ag1	120.0 (3)	N13—Ag1—O21	83.22 (14)
N13—Ag1—N1	141.02 (16)	N1—Ag1—O21	98.69 (14)
N13—Ag1—N7	111.83 (16)	N7—Ag1—O21	98.21 (14)
N1—Ag1—N7	106.44 (16)		

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O21	0.86	2.28	2.983 (6)	139
N2—H2*B*···O22^{i}	0.86	2.12	2.958 (6)	164
N8—H8*A*···O21	0.86	2.1	2.959 (6)	173
N8—H8*B*···O23^{ii}	0.86	2.07	2.904 (6)	164
N8—H8*B*···N21^{ii}	0.86	2.75	3.545 (6)	155
N14—H14*A*···N7	0.86	2.23	3.089 (6)	174
N14—H14*B*···O23^{iii}	0.86	2.12	2.934 (6)	158

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

After checking their presence in a difference map, H atoms were placed in calculated positions, with C—H = 0.93 Å and N—H = 0.86 Å, and refined using a riding model, with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *CrystalClear* (Rigaku, 2004); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve

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structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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