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(Nitrato-κ^2O,O')bis[(*E*)-*N*-(pyridin-4-ylmethylidene-κN)hydroxyamine]silver(I)

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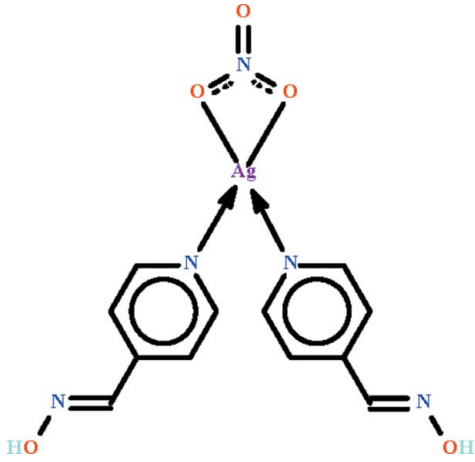
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.050; wR factor = 0.162; data-to-parameter ratio = 15.8.

In the mononuclear title compound, $[Ag(NO_3)(C_6H_6N_2O)_2]$, the Ag^I atom is located on a twofold rotation axis and the nitrate-chelated Ag^I atom is further coordinated by two aromatic N atoms of hydroxylamine ligands in a distorted tetrahedral geometry. In the crystal, the nitrate ion has 2 symmetry with the N atom and one O atom located on the twofold rotation axis, and is linked to hydroxy groups of the hydroxylamine ligands by O—H···O hydrogen bonds, generating a chain running along the *b* axis.

Related literature

For (nitrato)(picolinaldehyde oxime)silver(I), see: Abu-Youssef *et al.* (2010).



Experimental

Crystal data

$[Ag(NO_3)(C_6H_6N_2O)_2]$
M_r = 414.14
Orthorhombic, *Pccn*
a = 18.027 (3) Å
b = 4.6907 (6) Å
c = 17.7020 (19) Å
V = 1496.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.38 mm^{-1}
T = 293 K
0.20 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.770, T_{max} = 0.852
13223 measured reflections
1705 independent reflections
1038 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.162
S = 1.13
1705 reflections
108 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.92 e Å^{-3}
$\Delta\rho_{min}$ = −0.67 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2^{i}	0.84	1.90	2.740 (6)	173

Symmetry code: (i) $-x+1, y+\frac{3}{2}, -z+\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5647).

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S1. Comment

Picolinylaldehyde oxime reacts with silver nitrate to yield a monomeric adduct in which the metal atom is *N*,*N*′-chelated by the ligand. The nitrate ion is also involved in coordination (Abu-Youssef *et al.*, 2010). The corresponding reaction with isonicotinylaldehyde in place of picolinylaldehyde yields a bis adduct (Scheme I). The nitrate-chelated Ag^I atom in mononuclear $Ag(NO_3)(C_6H_6N_2O)_2$ is coordinated to the hydroxylamine through its aromatic N atom, and it exists in an approximate tetrahedral geometry (Fig. 1). The hydroxyl OH group forms a hydrogen bond with a nitrate O atom to generate a chain running along the longest axis of the orthorhombic unit cell (Table 1).

S2. Experimental

Isonicotinaldehyde oxime was synthesized from the reaction of isonicotinaldehyde and hydroxylamine. Silver nitrate (1 mmol) dissolved in water (5 ml) was added to picolinaldehyde oxime (1 mmol) dissolved in ethanol (5 ml). The solution was filtered and set aside, away from light, for the growth of colorless crystals.

S3. Refinement

Carbon- and oxygen-bound H-atoms were placed in calculated positions (C–H 0.93 Å, O–H 0.84 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2–1.5*U*(C,*O*).

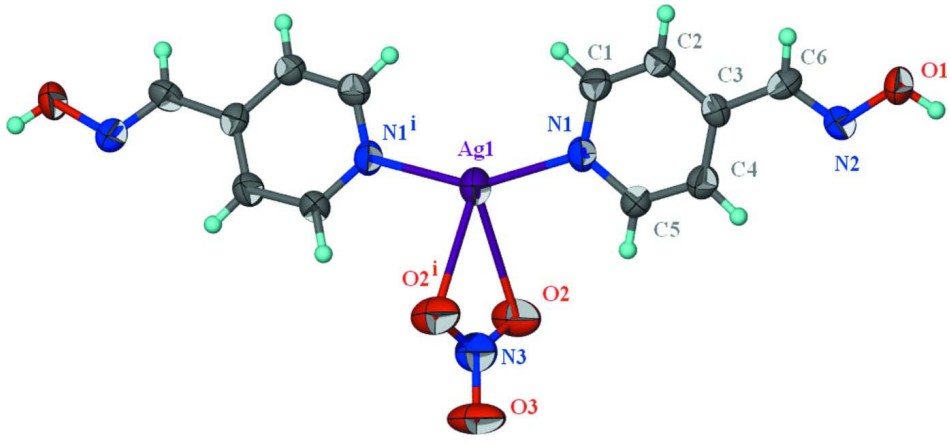

Figure 1

Thermal ellipsoid plot (Barbour, 2001) of $Ag(NO_3)(C_6H_6N_2O)_2$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

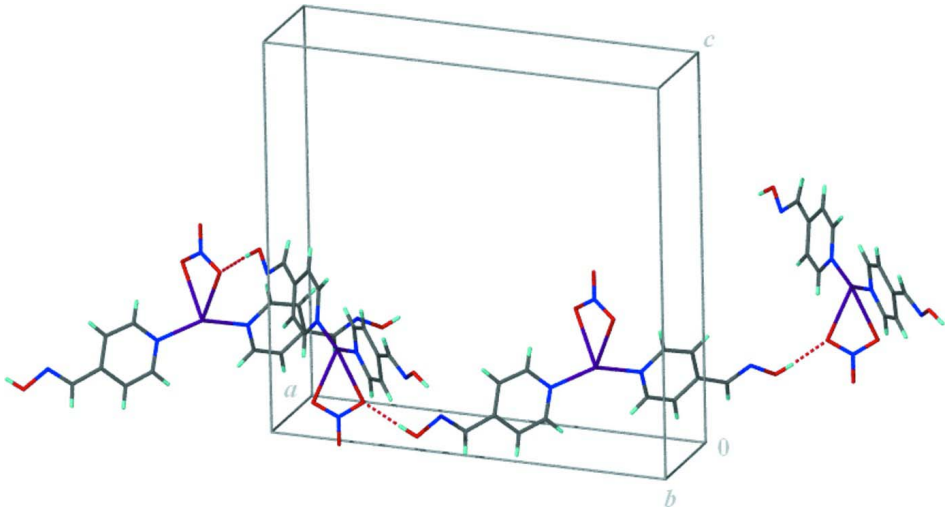

Figure 2

Hydrogen-bonded chain motif.

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Crystal data

$[Ag(NO_3)(C_6H_6N_2O)_2]$
$M_r = 414.14$
Orthorhombic, *Pccn*
Hall symbol: -P 2ab 2ac
$a = 18.027$ (3) Å
$b = 4.6907$ (6) Å
$c = 17.7020$ (19) Å
$V = 1496.9$ (3) Å^3
$Z = 4$
$F(000) = 824$
$D_x = 1.838$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4605 reflections
$\theta = 3.2$–$27.5°$
$\mu = 1.38$ mm^{-1}
$T = 293$ K
Prism, colorless
0.20 × 0.12 × 0.12 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.770$, $T_{max} = 0.852$
13223 measured reflections
1705 independent reflections
1038 reflections with $I > 2\sigma(I)$
$R_{int} = 0.082$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.2°$
$h = -23 \rightarrow 23$
$k = -5 \rightarrow 6$
$l = -21 \rightarrow 22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.050$
$wR(F^2) = 0.162$
$S = 1.13$
1705 reflections
108 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
$w = 1/[\sigma^2(F_o^2) + (0.073P)^2 + 1.2436P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.92$ e Å^{-3}
$\Delta\rho_{min} = -0.67$ e Å^{-3}

Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0096 (16)

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.2500	0.2500	0.18639 (3)	0.0532 (4)
O1	0.5757 (2)	1.5200 (8)	0.0886 (2)	0.0584 (11)
H1	0.6143	1.5575	0.1132	0.088*
O2	0.3058 (3)	0.1732 (13)	0.3234 (2)	0.0789 (15)
O3	0.2500	0.2500	0.4306 (3)	0.093 (3)
N1	0.3325 (2)	0.5683 (9)	0.1548 (2)	0.0454 (11)
N2	0.5350 (3)	1.3109 (9)	0.1264 (2)	0.0487 (11)
N3	0.2500	0.2500	0.3606 (4)	0.067 (2)
C1	0.3371 (3)	0.6602 (14)	0.0824 (3)	0.0487 (13)
H1A	0.3067	0.5752	0.0464	0.058*
C2	0.3841 (3)	0.8714 (12)	0.0598 (2)	0.0426 (12)
H2	0.3840	0.9318	0.0098	0.051*
C3	0.4321 (2)	0.9961 (10)	0.1113 (3)	0.0397 (11)
C4	0.4286 (3)	0.9016 (12)	0.1858 (3)	0.0466 (13)
H4	0.4601	0.9782	0.2222	0.056*
C5	0.3783 (3)	0.6940 (12)	0.2050 (3)	0.0454 (13)
H5	0.3756	0.6371	0.2552	0.055*
C6	0.4830 (3)	1.2177 (11)	0.0848 (3)	0.0459 (13)
H6	0.4771	1.2919	0.0365	0.055*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0461 (5)	0.0541 (5)	0.0594 (5)	−0.0093 (3)	0.000	0.000
O1	0.051 (2)	0.064 (3)	0.060 (2)	−0.022 (2)	−0.0052 (18)	0.007 (2)
O2	0.054 (3)	0.124 (4)	0.059 (3)	0.037 (3)	0.006 (2)	0.002 (2)
O3	0.084 (6)	0.155 (10)	0.040 (3)	0.050 (5)	0.000	0.000
N1	0.038 (2)	0.047 (3)	0.051 (2)	−0.007 (2)	0.0030 (19)	−0.003 (2)
N2	0.049 (3)	0.050 (3)	0.046 (2)	−0.009 (2)	0.003 (2)	0.0004 (19)
N3	0.057 (5)	0.084 (6)	0.061 (5)	0.020 (4)	0.000	0.000
C1	0.040 (3)	0.061 (3)	0.045 (3)	0.002 (3)	−0.002 (2)	−0.005 (3)
C2	0.039 (3)	0.050 (3)	0.039 (3)	0.000 (3)	0.000 (2)	0.003 (2)
C3	0.034 (2)	0.040 (3)	0.045 (3)	0.002 (2)	0.003 (2)	0.001 (2)
C4	0.047 (3)	0.045 (3)	0.047 (3)	−0.004 (3)	−0.004 (2)	0.000 (2)
C5	0.043 (3)	0.053 (3)	0.041 (3)	−0.009 (2)	−0.001 (2)	−0.002 (2)
C6	0.046 (3)	0.051 (3)	0.041 (2)	0.002 (2)	−0.005 (2)	0.000 (2)

Geometric parameters (Å, º)

Ag1—N1^{i}	2.180 (4)	N3—O2^{i}	1.256 (6)
Ag1—N1	2.180 (4)	C1—C2	1.364 (9)
Ag1—O2	2.651 (4)	C1—H1A	0.9300

Ag1—O2^{i}	2.651 (4)	C2—C3	1.386 (7)
O1—N2	1.396 (5)	C2—H2	0.9300
O1—H1	0.8400	C3—C4	1.393 (6)
O2—N3	1.256 (6)	C3—C6	1.463 (7)
O3—N3	1.239 (9)	C4—C5	1.374 (8)
N1—C5	1.349 (6)	C4—H4	0.9300
N1—C1	1.354 (6)	C5—H5	0.9300
N2—C6	1.270 (7)	C6—H6	0.9300

N1^{i}—Ag1—N1	150.3 (2)	C2—C1—H1A	118.4
N1^{i}—Ag1—O2	113.62 (18)	C1—C2—C3	120.1 (4)
N1—Ag1—O2	93.94 (18)	C1—C2—H2	119.9
N1^{i}—Ag1—O2^{i}	93.94 (18)	C3—C2—H2	119.9
N1—Ag1—O2^{i}	113.62 (18)	C2—C3—C4	117.4 (4)
O2—Ag1—O2^{i}	47.57 (19)	C2—C3—C6	118.7 (4)
N2—O1—H1	109.5	C4—C3—C6	123.9 (4)
N3—O2—Ag1	97.9 (4)	C5—C4—C3	119.3 (5)
C5—N1—C1	116.5 (5)	C5—C4—H4	120.3
C5—N1—Ag1	123.2 (3)	C3—C4—H4	120.3
C1—N1—Ag1	120.2 (3)	N1—C5—C4	123.5 (5)
C6—N2—O1	110.6 (4)	N1—C5—H5	118.3
O3—N3—O2^{i}	121.6 (4)	C4—C5—H5	118.3
O3—N3—O2	121.6 (4)	N2—C6—C3	121.4 (5)
O2^{i}—N3—O2	116.7 (7)	N2—C6—H6	119.3
N1—C1—C2	123.2 (5)	C3—C6—H6	119.3
N1—C1—H1A	118.4		

N1^{i}—Ag1—O2—N3	−72.7 (4)	Ag1—N1—C1—C2	175.7 (4)
N1—Ag1—O2—N3	118.8 (3)	N1—C1—C2—C3	2.3 (9)
O2^{i}—Ag1—O2—N3	0.000 (1)	C1—C2—C3—C4	−1.5 (8)
N1^{i}—Ag1—N1—C5	−171.4 (4)	C1—C2—C3—C6	178.7 (5)
O2—Ag1—N1—C5	−12.8 (4)	C2—C3—C4—C5	−0.5 (8)
O2^{i}—Ag1—N1—C5	32.1 (5)	C6—C3—C4—C5	179.4 (5)
N1^{i}—Ag1—N1—C1	12.1 (4)	C1—N1—C5—C4	−1.1 (8)
O2—Ag1—N1—C1	170.6 (4)	Ag1—N1—C5—C4	−177.7 (4)
O2^{i}—Ag1—N1—C1	−144.4 (4)	C3—C4—C5—N1	1.8 (9)
Ag1—O2—N3—O3	180.0	O1—N2—C6—C3	179.9 (4)
Ag1—O2—N3—O2^{i}	0.000 (1)	C2—C3—C6—N2	−170.0 (5)
C5—N1—C1—C2	−1.0 (8)	C4—C3—C6—N2	10.2 (8)

Symmetry code: (i) −*x*+1/2, −*y*+1/2, *z*.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2^{ii}	0.84	1.90	2.740 (6)	173

Symmetry code: (ii) −*x*+1, *y*+3/2, −*z*+1/2.