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catena-Poly[[silver(I)-μ-*N*-(3-pyridylmethyl)pyridine-4-carboxamide] nitrate monohydrate]

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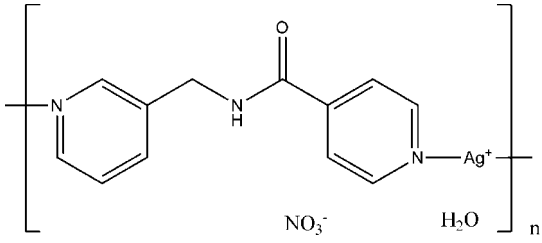
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.042; wR factor = 0.101; data-to-parameter ratio = 16.2.

In the title compound, $\{[Ag(C_{12}H_{11}N_3O)]NO_3\cdot H_2O\}_n$, the Ag atom is coordinated by two N atoms from the heterocyclic ligand, giving a linear polycationic chain. Two long $Ag\cdots O_{nitrate}$ interactions [2.667 (3) and 2.840 (3) Å] result in a three-dimensional network. The water molecule consolidates the network structure by forming hydrogen bonds, one to the polycationic chain and one to the nitrate anion.

Related literature

For related literature, see: Cordes & Hanton (2007); Kumar *et al.* (2006); Tong *et al.* (2002).



Experimental

Crystal data

$[Ag(C_{12}H_{11}N_3O)]NO_3\cdot H_2O$
M_r = 401.13
Monoclinic, $P2_1/c$
a = 12.177 (2) Å
b = 13.022 (3) Å
c = 8.9109 (18) Å
β = 94.21 (3)°
V = 1409.2 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.46 mm^{-1}
T = 293 (2) K
0.6 × 0.4 × 0.2 mm

Data collection

Rigaku Mercury CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2003)
T_{min} = 0.503, T_{max} = 0.742
14304 measured reflections
3230 independent reflections
2399 reflections with $I > 2\sigma(I)$
R_{int} = 0.065

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.101
S = 1.06
3230 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4A···O1W^{i}	0.86	2.04	2.837 (4)	154
O1W—H1WA···O1	0.85	1.94	2.790 (4)	174
O1W—H1WB···O3^{ii}	0.85	2.04	2.886 (4)	171

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z-\frac{1}{2}$; (ii) $x+1, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MSC, 2003); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 1999); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PK2069).

References

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supporting information

Acta Cryst. (2008). E**64**, m110 [https://doi.org/10.1107/S1600536807064744]

catena-Poly[[silver(I)-μ-*N*-(3-pyridylmethyl)pyridine-4-carboxamide] nitrate monohydrate]

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S1. Comment

The reactions of silver(I) salts with flexible pyridyl type ligands have received considerable attention (Cordes *et al.*, 2007; Kumar *et al.*, 2006; Tong *et al.*, 2002). Here, we report a new silver(I) complex (Fig. 1), which was prepared by the reaction of *N*-(3-pyridinylmethyl)-4-pyridine-carboxamide acting as a bidentate bridge ligand with $AgNO_3$. In the cation, the Ag(I) atom is in a linear coordination environment and the Ag1—N1A and Ag1—N3 bond length are 2.152 (3) and 2.157 (3) Å, respectively. The N3—Ag1—N1^{i} (i = -1 + *x*, 0.5 - *y*, 1/2 + *z*) bond angle is 172.55 (15) °, indicating that the N–Ag–N skeleton that gives rise to a chain structure is distorted by the presence of two Ag···$O_{nitrate}$ interactions. If these are regarded as formal bonds, the compound may be described as a three dimensional network structure (Fig. 2).

S2. Experimental

An aqueous solution (5 ml) of silver nitrate (1.0 mmol) was layered carefully over a methanol (5 ml) solution of *N*-(4-pyridylmethyl)-4-pyridinecarboxamide (1.0 mmol) in a tube, which was covered and kept away from light. Colorless crystals were obtained after two weeks. These were washed with methanol and collected in 50% yield. CHN elemental analysis: found C 35.86, H 3.55, N 13.79%; calc. for $C_{12}H_{13}AgN_4O_5$: C 35.93, H 3.27, N 13.96%.

S3. Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å, N—H distances of 0.86 Å and OW1—H distances of 0.85 Å, and with U_{iso}(H) = 1.2U_{eq}(C, N or O).

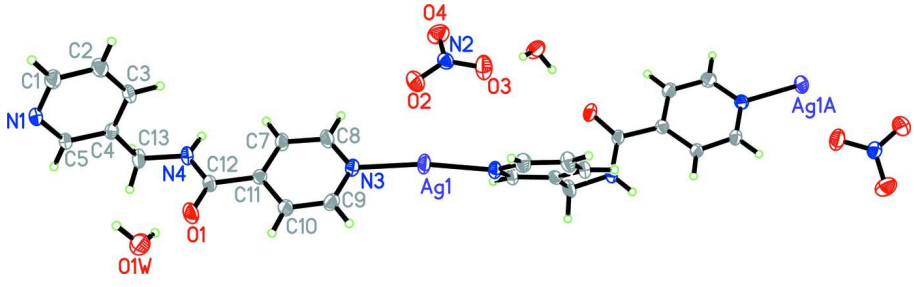

Figure 1

The structure of the title complex, showing 30% probability displacement ellipsoids and the atom-numbering scheme. Symmetry-generated atoms in the plot are related by (-1 + *x*, 0.5 - *y*, 1/2 + *z*).

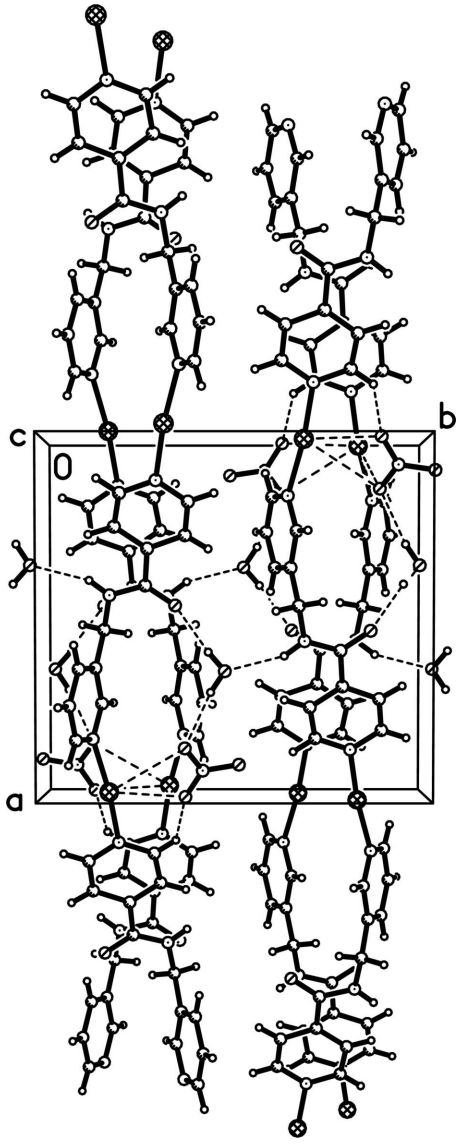

Figure 2

Crystal packing viewed down the *c* axis.

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Crystal data

$[Ag(C_{12}H_{11}N_3O)]NO_3{\cdot}H_2O$
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Hall symbol: -P 2ybc
$a = 12.177\ (2)$ Å
$b = 13.022\ (3)$ Å
$c = 8.9109\ (18)$ Å
$\beta = 94.21\ (3)°$
$V = 1409.2\ (5)$ Å^3
$Z = 4$
$F(000) = 800$
$D_x = 1.891$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5866 reflections
$\theta = 3.2–27.5°$
$\mu = 1.46$ mm^{-1}
$T = 293$ K
Block, colorless
0.6 × 0.4 × 0.2 mm

Data collection

Rigaku Mercury CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2003)
T_{min} = 0.503, T_{max} = 0.742
14304 measured reflections
3230 independent reflections
2399 reflections with $I > 2\sigma(I)$
R_{int} = 0.065
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −15→15
k = −16→16
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.101
S = 1.06
3230 reflections
199 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
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 0.2355P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

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

	x	y	z	U_{iso}*/U_{eq}
Ag1	−0.01568 (2)	0.32484 (2)	0.11987 (4)	0.04917 (14)
N3	0.1306 (2)	0.3030 (2)	0.0011 (3)	0.0377 (7)
C9	0.1867 (3)	0.3832 (3)	−0.0444 (4)	0.0453 (9)
H9A	0.1644	0.4486	−0.0176	0.054*
C7	0.2524 (3)	0.1954 (3)	−0.1219 (4)	0.0426 (9)
H7A	0.2731	0.1291	−0.1467	0.051*
C8	0.1637 (3)	0.2107 (3)	−0.0387 (4)	0.0448 (9)
H8A	0.1249	0.1537	−0.0087	0.054*
C11	0.3109 (3)	0.2785 (3)	−0.1690 (4)	0.0321 (7)
C10	0.2755 (3)	0.3746 (3)	−0.1283 (4)	0.0418 (9)
H10A	0.3120	0.4331	−0.1580	0.050*
C12	0.4107 (3)	0.2716 (3)	−0.2571 (4)	0.0348 (8)
N4	0.4370 (2)	0.1789 (2)	−0.3061 (3)	0.0396 (7)
H4A	0.3962	0.1273	−0.2872	0.047*
C13	0.5327 (3)	0.1630 (3)	−0.3904 (4)	0.0444 (9)
H13A	0.5431	0.2231	−0.4520	0.053*

H13B	0.5188	0.1051	−0.4576	0.053*
C4	0.6375 (3)	0.1431 (3)	−0.2938 (4)	0.0335 (8)
C5	0.7368 (3)	0.1578 (3)	−0.3533 (4)	0.0358 (8)
H5A	0.7365	0.1849	−0.4499	0.043*
N1	0.8337 (2)	0.1358 (2)	−0.2817 (3)	0.0387 (7)
C1	0.8340 (3)	0.0972 (3)	−0.1428 (4)	0.0472 (9)
H1B	0.9007	0.0798	−0.0917	0.057*
C2	0.7385 (3)	0.0825 (3)	−0.0737 (4)	0.0485 (10)
H2A	0.7410	0.0577	0.0243	0.058*
C3	0.6391 (3)	0.1044 (3)	−0.1492 (4)	0.0413 (9)
H3A	0.5738	0.0933	−0.1038	0.050*
O1	0.4653 (2)	0.3480 (2)	−0.2803 (3)	0.0550 (8)
O2	−0.0055 (2)	0.1263 (3)	0.1929 (4)	0.0669 (8)
N2	−0.0802 (3)	0.0813 (3)	0.2490 (3)	0.0427 (7)
O3	−0.1439 (3)	0.1264 (3)	0.3279 (4)	0.0735 (9)
O1W	0.6452 (2)	0.4755 (2)	−0.2057 (4)	0.0624 (8)
H1WA	0.5932	0.4332	−0.2267	0.075*
H1WB	0.7033	0.4393	−0.1928	0.075*
O4	−0.0959 (3)	−0.0117 (2)	0.2228 (4)	0.0702 (9)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.03123 (18)	0.0563 (2)	0.0621 (2)	0.00455 (13)	0.01775 (14)	−0.00438 (15)
N3	0.0300 (16)	0.0400 (18)	0.0435 (18)	0.0011 (13)	0.0066 (13)	−0.0052 (13)
C9	0.042 (2)	0.034 (2)	0.061 (3)	0.0054 (17)	0.0109 (19)	−0.0029 (18)
C7	0.041 (2)	0.033 (2)	0.057 (2)	−0.0023 (16)	0.0209 (18)	−0.0077 (16)
C8	0.039 (2)	0.043 (2)	0.055 (2)	−0.0071 (17)	0.0197 (18)	−0.0027 (18)
C11	0.0277 (17)	0.0366 (19)	0.0319 (18)	0.0012 (15)	0.0013 (14)	0.0008 (14)
C10	0.039 (2)	0.035 (2)	0.053 (2)	−0.0021 (17)	0.0105 (17)	0.0004 (17)
C12	0.0267 (18)	0.042 (2)	0.0363 (19)	−0.0045 (16)	0.0048 (14)	−0.0007 (16)
N4	0.0270 (15)	0.0483 (19)	0.0448 (18)	−0.0020 (13)	0.0127 (13)	−0.0045 (14)
C13	0.032 (2)	0.062 (3)	0.041 (2)	0.0028 (18)	0.0105 (16)	−0.0027 (17)
C4	0.0324 (19)	0.0360 (18)	0.0324 (18)	0.0020 (15)	0.0060 (15)	−0.0046 (14)
C5	0.0305 (18)	0.041 (2)	0.0373 (19)	0.0019 (15)	0.0103 (15)	0.0014 (15)
N1	0.0285 (16)	0.0443 (17)	0.0447 (18)	−0.0018 (14)	0.0108 (13)	0.0025 (14)
C1	0.036 (2)	0.056 (3)	0.050 (2)	0.0012 (18)	0.0028 (17)	0.0017 (19)
C2	0.045 (2)	0.066 (3)	0.036 (2)	0.002 (2)	0.0075 (17)	0.0058 (18)
C3	0.037 (2)	0.048 (2)	0.041 (2)	−0.0032 (17)	0.0150 (16)	−0.0004 (17)
O1	0.0404 (16)	0.0537 (17)	0.073 (2)	−0.0142 (13)	0.0212 (14)	−0.0028 (14)
O2	0.055 (2)	0.068 (2)	0.080 (2)	−0.0126 (16)	0.0235 (16)	0.0100 (18)
N2	0.0371 (18)	0.050 (2)	0.0413 (18)	−0.0045 (15)	0.0028 (14)	0.0039 (15)
O3	0.066 (2)	0.076 (2)	0.082 (2)	−0.0028 (18)	0.0310 (18)	−0.0178 (18)
O1W	0.0471 (17)	0.0461 (17)	0.094 (2)	−0.0057 (14)	0.0067 (15)	−0.0046 (15)
O4	0.068 (2)	0.0443 (18)	0.098 (3)	−0.0020 (16)	0.0053 (18)	0.0006 (16)

Geometric parameters (Å, º)

Ag1—N1^{i}	2.152 (3)	C13—H13A	0.9700
Ag1—N3	2.157 (3)	C13—H13B	0.9700
N3—C8	1.324 (5)	C4—C5	1.369 (5)
N3—C9	1.328 (5)	C4—C3	1.382 (5)
C9—C10	1.363 (5)	C5—N1	1.331 (4)
C9—H9A	0.9300	C5—H5A	0.9300
C7—C8	1.369 (5)	N1—C1	1.336 (5)
C7—C11	1.378 (5)	N1—Ag1^{ii}	2.152 (3)
C7—H7A	0.9300	C1—C2	1.368 (5)
C8—H8A	0.9300	C1—H1B	0.9300
C11—C10	1.381 (5)	C2—C3	1.370 (5)
C11—C12	1.497 (5)	C2—H2A	0.9300
C10—H10A	0.9300	C3—H3A	0.9300
C12—O1	1.222 (4)	O2—N2	1.220 (4)
C12—N4	1.331 (4)	N2—O3	1.234 (4)
N4—C13	1.447 (5)	N2—O4	1.245 (4)
N4—H4A	0.8600	O1W—H1WA	0.8499
C13—C4	1.508 (5)	O1W—H1WB	0.8500
N1^{i}—Ag1—N3	172.19 (11)	C4—C13—H13A	108.7
C8—N3—C9	117.3 (3)	N4—C13—H13B	108.7
C8—N3—Ag1	122.0 (2)	C4—C13—H13B	108.7
C9—N3—Ag1	120.5 (2)	H13A—C13—H13B	107.6
N3—C9—C10	123.3 (3)	C5—C4—C3	117.3 (3)
N3—C9—H9A	118.3	C5—C4—C13	119.3 (3)
C10—C9—H9A	118.3	C3—C4—C13	123.3 (3)
C8—C7—C11	119.8 (3)	N1—C5—C4	124.2 (3)
C8—C7—H7A	120.1	N1—C5—H5A	117.9
C11—C7—H7A	120.1	C4—C5—H5A	117.9
N3—C8—C7	123.0 (3)	C5—N1—C1	117.8 (3)
N3—C8—H8A	118.5	C5—N1—Ag1^{ii}	120.4 (2)
C7—C8—H8A	118.5	C1—N1—Ag1^{ii}	121.6 (2)
C7—C11—C10	117.0 (3)	N1—C1—C2	121.7 (4)
C7—C11—C12	124.8 (3)	N1—C1—H1B	119.2
C10—C11—C12	118.3 (3)	C2—C1—H1B	119.2
C9—C10—C11	119.6 (4)	C1—C2—C3	120.0 (4)
C9—C10—H10A	120.2	C1—C2—H2A	120.0
C11—C10—H10A	120.2	C3—C2—H2A	120.0
O1—C12—N4	122.4 (3)	C2—C3—C4	119.0 (3)
O1—C12—C11	120.8 (3)	C2—C3—H3A	120.5
N4—C12—C11	116.8 (3)	C4—C3—H3A	120.5
C12—N4—C13	121.5 (3)	O2—N2—O3	121.6 (4)
C12—N4—H4A	119.2	O2—N2—O4	119.9 (4)
C13—N4—H4A	119.2	O3—N2—O4	118.4 (3)
N4—C13—C4	114.1 (3)	H1WA—O1W—H1WB	105.6
N4—C13—H13A	108.7		

C8—N3—C9—C10	−0.2 (6)	C11—C12—N4—C13	−179.1 (3)
Ag1—N3—C9—C10	−175.6 (3)	C12—N4—C13—C4	87.7 (4)
C9—N3—C8—C7	0.6 (6)	N4—C13—C4—C5	−160.2 (3)
Ag1—N3—C8—C7	175.9 (3)	N4—C13—C4—C3	23.9 (5)
C11—C7—C8—N3	−0.5 (7)	C3—C4—C5—N1	1.0 (5)
C8—C7—C11—C10	−0.1 (6)	C13—C4—C5—N1	−175.1 (3)
C8—C7—C11—C12	178.4 (4)	C4—C5—N1—C1	−0.2 (5)
N3—C9—C10—C11	−0.3 (6)	C4—C5—N1—Ag1^{ii}	−174.5 (3)
C7—C11—C10—C9	0.4 (6)	C5—N1—C1—C2	−1.5 (6)
C12—C11—C10—C9	−178.1 (3)	Ag1^{ii}—N1—C1—C2	172.8 (3)
C7—C11—C12—O1	−171.7 (4)	N1—C1—C2—C3	2.2 (6)
C10—C11—C12—O1	6.7 (5)	C1—C2—C3—C4	−1.3 (6)
C7—C11—C12—N4	7.3 (6)	C5—C4—C3—C2	−0.3 (5)
C10—C11—C12—N4	−174.2 (3)	C13—C4—C3—C2	175.7 (4)
O1—C12—N4—C13	0.0 (6)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4*A*···O1*W*^{iii}	0.86	2.04	2.837 (4)	154
O1*W*—H1*WA*···O1	0.85	1.94	2.790 (4)	174
O1*W*—H1*WB*···O3^{ii}	0.85	2.04	2.886 (4)	171

Symmetry codes: (ii) *x*+1, −*y*+1/2, *z*−1/2; (iii) −*x*+1, *y*−1/2, −*z*−1/2.