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catena-Poly[[silver(I)-μ-[*N*-(4-pyridylmethyl)pyridine-4-carboxamide-κ^2N:*N*′]] nitrate monohydrate]

Yu-Tao Ma,[a] Bai-Wang Sun[a]* and Seik Weng Ng[b]

[a]Ordered Matter Science Research Center, Department of Chemistry and Chemical Engineering, Southeast University, Nanjing 210096, People's Republic of China, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia
Correspondence e-mail: chmsunbw@seu.edu.cn

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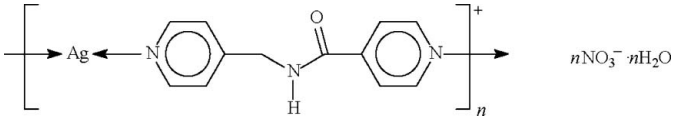
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.006 Å; R factor = 0.053; wR factor = 0.141; data-to-parameter ratio = 15.4.

The title coordination polymer, $\{[Ag(C_{12}H_{11}N_3O)]NO_3\cdot H_2O\}_n$, has a polycationic chain motif in which the Ag atom is bridged by the heterocyclic ligand; the Ag atom shows linear coordination. If the two long Ag$\cdots$O$_{nitrate}$ interactions [2.794 (6) and 2.867 (5) Å] are regarded as bonds, the compound adopts a three-dimensional network structure. 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 the structure of the hydrated disilver oxalate adduct of the heterocyclic ligand, see Tong *et al.* (2002).



Experimental

Crystal data

$[Ag(C_{12}H_{11}N_3O)]NO_3\cdot H_2O$
M_r = 401.13
Orthorhombic, *Pbca*
a = 12.912 (7) Å
b = 9.021 (5) Å
c = 24.52 (1) Å
V = 2856 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 1.45 mm^{-1}
T = 295 (2) K
0.6 × 0.4 × 0.2 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.50, T_{max} = 0.75
25888 measured reflections
3249 independent reflections
2433 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.141
S = 1.06
3249 reflections
211 parameters
3 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.91 e Å^{-3}
$\Delta\rho_{min}$ = −0.75 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—N3^{i}	2.162 (4)	Ag1—O2	2.803 (6)
Ag1—N1	2.170 (4)	Ag1—O3^{ii}	2.874 (6)

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

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
N2—H2N$\cdots$O1W	0.86 (4)	2.04 (2)	2.827 (6)	154 (5)
O1W—H1W1$\cdots$O1^{iii}	0.85 (4)	2.05 (3)	2.831 (5)	154 (7)
O1W—H1W2$\cdots$O4^{iv}	0.85 (4)	2.09 (4)	2.888 (7)	157 (9)

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); 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: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2109).

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supplementary materials

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catena-Poly[[silver(I)--[*N*-(4-pyridylmethyl)pyridine-4-carboxamide-^{2}*N*:*N*']] nitrate monohydrate]

Y.-T. Ma, B.-W. Sun and S. W. Ng

Comment

The 4-C_5H_4N–CH_2–NH–C(O)–4-C_5H_4N ligand is a spacer heterocycle that should function like 4,4'-bipyridine, which forms numerous coordination polymers, but should be flexible. There is, however, only one crystal structure report of an adduct, a hydrated disilver oxalate adduct (Tong *et al.*, 2002). The title silver nitrate adduct has the metal in a linear enviroment, but 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 adopts a three-dimensional network structure.

Experimental

An aqueous solution (5 ml) of silver nitrate (1.0 mmol) was layed over a methanol (5 ml) solution of *N*-(4-pyridylmethyl)-4-pyridinecarboxamide (1.0 mmol) in a thin tube. The tube was placed vertically and kept away from light. Colorless crystals were obtained after two weeks. These were washed with methanol and collected in 50% yield. CH&N elemental analysis. Found: C 35.88, H 3.53, N 13.76%; calc. for $C_{12}H_{13}AgN_4O_5$: C 35.93, H 3.27, N 13.96%.

Refinement

Carbon-bound H-atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.97 Å and U(H) set to 1.2U_{eq}(C). The amino and water H-atoms were located in a difference Fourier map, and were refined with a distance restraint of N—H = O—H = 0.85 (1) Å.

Figures

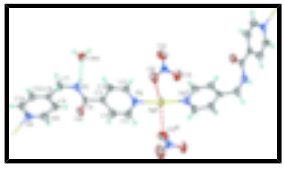


Fig. 1. A portion of the chain structure. Ellipsoids are drawn at the 50% probability level, and H atoms of spheres of arbitry radius. The red dashed lines denote the long Ag···O bonds and the dashed cyan line denotes the hydrogen bond. Symmetry codes (i) = 1/2 − x, 1 − y, z − 1/2; (ii) x − 1/2, 3/2 − y, −z.

catena-Poly[[silver(I)-μ-[*N*-(4-pyridylmethyl)pyridine-4- carboxamide-κ^2*N*:*N*']] nitrate monohydrate]

Crystal data

$[Ag(C_{12}H_{11}N_3O)]NO_3·H_2O$	F_{000} = 1600
M_r = 401.13	D_x = 1.879 Mg m^{-3}
Orthorhombic, *Pbca*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -P 2ac 2ab	Cell parameters from 5655 reflections

a = 12.912 (7) Å	θ = 3.2–27.5º
b = 9.021 (5) Å	μ = 1.45 mm^{-1}
c = 24.52 (1) Å	T = 295 (2) K
V = 2856 (3) Å^3	Column, colourless
Z = 8	0.6 × 0.4 × 0.2 mm

Data collection

Rigaku Mercury diffractometer	3249 independent reflections
Radiation source: medium-focus sealed tube	2433 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 295(2) K	θ_{max} = 27.5º
ω scans	θ_{min} = 3.2º
Absorption correction: multi-scan (Jacobson, 1998)	h = −16→16
T_{min} = 0.50, T_{max} = 0.75	k = −11→11
25888 measured reflections	l = −30→31

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.053	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2)$ = 0.141	$w = 1/[\sigma^2(F_o^2) + (0.0589P)^2 + 5.5451P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.06	$(\Delta/\sigma)_{max}$ = 0.001
3249 reflections	$\Delta\rho_{max}$ = 0.91 e Å^{-3}
211 parameters	$\Delta\rho_{min}$ = −0.75 e Å^{-3}
3 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
Ag1	0.16581 (3)	0.61149 (5)	0.002207 (15)	0.05996 (18)
O1	0.1859 (3)	0.1438 (4)	0.23653 (13)	0.0598 (9)
O2	0.3756 (4)	0.6914 (6)	0.00374 (16)	0.0905 (14)
O3	0.5035 (4)	0.7095 (7)	−0.0481 (2)	0.1077 (17)
O4	0.3682 (5)	0.8329 (7)	−0.0644 (2)	0.118 (2)
O1W	0.5539 (3)	0.2042 (5)	0.17401 (17)	0.0660 (10)
H1W1	0.608 (3)	0.189 (8)	0.193 (2)	0.10 (2)*
H1W2	0.562 (8)	0.176 (10)	0.1412 (13)	0.15 (4)*
N1	0.1990 (3)	0.4795 (4)	0.07408 (14)	0.0448 (8)
N2	0.3572 (3)	0.1578 (4)	0.22161 (14)	0.0458 (9)

H2N	0.408 (3)	0.198 (5)	0.2048 (19)	0.061 (16)*
N3	0.3656 (3)	0.2837 (4)	0.42466 (15)	0.0470 (9)
N4	0.4163 (3)	0.7500 (4)	−0.03557 (16)	0.0469 (9)
C1	0.1231 (4)	0.4240 (6)	0.1046 (2)	0.0567 (12)
H1	0.0551	0.4506	0.0967	0.068*
C2	0.1412 (4)	0.3281 (6)	0.14763 (19)	0.0528 (12)
H2	0.0859	0.2895	0.1674	0.063*
C3	0.2413 (3)	0.2900 (4)	0.16112 (14)	0.0377 (9)
C4	0.3201 (4)	0.3498 (6)	0.1298 (2)	0.0524 (12)
H4	0.3890	0.3279	0.1376	0.063*
C5	0.2952 (4)	0.4425 (6)	0.08692 (19)	0.0513 (11)
H5	0.3489	0.4809	0.0659	0.062*
C6	0.2592 (4)	0.1894 (5)	0.20953 (15)	0.0417 (9)
C7	0.3844 (4)	0.0665 (5)	0.26853 (17)	0.0487 (11)
H7A	0.4547	0.0307	0.2639	0.058*
H7B	0.3390	−0.0191	0.2694	0.058*
C8	0.3770 (3)	0.1465 (4)	0.32274 (16)	0.0379 (9)
C9	0.3479 (4)	0.2929 (5)	0.32757 (19)	0.0474 (11)
H9A	0.3325	0.3486	0.2967	0.057*
C10	0.3418 (4)	0.3559 (5)	0.3786 (2)	0.0515 (12)
H10	0.3201	0.4540	0.3812	0.062*
C11	0.3960 (4)	0.1419 (5)	0.41994 (18)	0.0514 (11)
H11	0.4134	0.0895	0.4513	0.062*
C12	0.4021 (4)	0.0715 (5)	0.37027 (17)	0.0482 (11)
H12	0.4233	−0.0270	0.3686	0.058*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0659 (3)	0.0671 (3)	0.0469 (3)	0.00106 (19)	−0.01097 (16)	0.01944 (19)
O1	0.065 (2)	0.074 (2)	0.0410 (18)	−0.0126 (18)	0.0093 (16)	0.0097 (17)
O2	0.111 (4)	0.103 (4)	0.058 (3)	−0.013 (3)	0.013 (2)	0.026 (2)
O3	0.076 (3)	0.171 (5)	0.076 (3)	0.009 (3)	0.003 (2)	−0.016 (3)
O4	0.130 (4)	0.135 (5)	0.089 (4)	0.049 (4)	0.001 (3)	0.050 (3)
O1W	0.056 (2)	0.087 (3)	0.055 (2)	0.005 (2)	−0.0059 (19)	0.011 (2)
N1	0.052 (2)	0.048 (2)	0.0343 (18)	0.0005 (18)	−0.0060 (16)	0.0031 (16)
N2	0.058 (2)	0.047 (2)	0.0318 (18)	0.0024 (19)	0.0050 (17)	0.0092 (16)
N3	0.053 (2)	0.049 (2)	0.0394 (19)	−0.0026 (18)	−0.0003 (17)	−0.0094 (17)
N4	0.053 (2)	0.048 (2)	0.041 (2)	−0.0017 (19)	0.0040 (18)	0.0014 (17)
C1	0.047 (3)	0.071 (3)	0.052 (3)	0.001 (2)	−0.008 (2)	0.014 (2)
C2	0.046 (2)	0.071 (3)	0.041 (2)	−0.011 (2)	−0.0001 (19)	0.006 (2)
C3	0.049 (2)	0.037 (2)	0.0265 (17)	−0.0034 (19)	0.0008 (17)	−0.0015 (15)
C4	0.043 (2)	0.063 (3)	0.051 (3)	0.007 (2)	0.005 (2)	0.018 (2)
C5	0.045 (2)	0.059 (3)	0.049 (3)	0.005 (2)	0.007 (2)	0.022 (2)
C6	0.056 (3)	0.043 (2)	0.0255 (18)	−0.004 (2)	0.0057 (18)	−0.0009 (16)
C7	0.071 (3)	0.043 (2)	0.032 (2)	0.008 (2)	−0.001 (2)	0.0033 (18)
C8	0.043 (2)	0.037 (2)	0.0333 (19)	−0.0026 (18)	−0.0003 (17)	−0.0010 (16)
C9	0.057 (3)	0.041 (2)	0.044 (2)	0.005 (2)	−0.009 (2)	−0.0001 (19)

C10	0.057 (3)	0.043 (2)	0.054 (3)	0.006 (2)	−0.006 (2)	−0.009 (2)
C11	0.073 (3)	0.046 (3)	0.035 (2)	0.001 (2)	−0.005 (2)	−0.0004 (19)
C12	0.069 (3)	0.037 (2)	0.039 (2)	0.004 (2)	0.002 (2)	0.0023 (18)

Geometric parameters (Å, °)

Ag1—N3^{i}	2.162 (4)	C2—C3	1.377 (6)
Ag1—N1	2.170 (4)	C2—H2	0.9300
Ag1—O2	2.803 (6)	C3—C4	1.385 (6)
Ag1—O3^{ii}	2.874 (6)	C3—C6	1.512 (5)
O1—C6	1.226 (5)	C4—C5	1.381 (6)
O2—N4	1.219 (5)	C4—H4	0.9300
O3—N4	1.223 (6)	C5—H5	0.9300
O4—N4	1.202 (6)	C7—C8	1.516 (6)
O1W—H1W1	0.85 (4)	C7—H7A	0.9700
O1W—H1W2	0.85 (4)	C7—H7B	0.9700
N1—C5	1.325 (6)	C8—C9	1.378 (6)
N1—C1	1.331 (6)	C8—C12	1.386 (6)
N2—C6	1.330 (6)	C9—C10	1.377 (6)
N2—C7	1.458 (5)	C9—H9A	0.9300
N2—H2N	0.86 (4)	C10—H10	0.9300
N3—C10	1.340 (6)	C11—C12	1.376 (6)
N3—C11	1.343 (6)	C11—H11	0.9300
C1—C2	1.385 (7)	C12—H12	0.9300
C1—H1	0.9300		
N3^{i}—Ag1—N1	172.52 (14)	C5—C4—H4	120.4
N3^{i}—Ag1—O2	94.61 (13)	C3—C4—H4	120.4
N1—Ag1—O2	86.53 (14)	N1—C5—C4	123.5 (4)
N3^{i}—Ag1—O3^{ii}	87.80 (15)	N1—C5—H5	118.3
N1—Ag1—O3^{ii}	97.73 (15)	C4—C5—H5	118.3
O2—Ag1—O3^{ii}	123.69 (16)	O1—C6—N2	122.8 (4)
N4—O2—Ag1	121.2 (4)	O1—C6—C3	120.5 (4)
H1W1—O1W—H1W2	111 (8)	N2—C6—C3	116.7 (4)
C5—N1—C1	117.5 (4)	N2—C7—C8	114.0 (4)
C5—N1—Ag1	121.1 (3)	N2—C7—H7A	108.7
C1—N1—Ag1	121.2 (3)	C8—C7—H7A	108.7
C6—N2—C7	121.8 (4)	N2—C7—H7B	108.7
C6—N2—H2N	122 (4)	C8—C7—H7B	108.7
C7—N2—H2N	116 (4)	H7A—C7—H7B	107.6
C10—N3—C11	117.2 (4)	C9—C8—C12	117.4 (4)
C10—N3—Ag1^{iii}	119.1 (3)	C9—C8—C7	123.3 (4)
C11—N3—Ag1^{iii}	123.2 (3)	C12—C8—C7	119.3 (4)
O4—N4—O2	120.8 (5)	C10—C9—C8	119.3 (4)
O4—N4—O3	120.9 (5)	C10—C9—H9A	120.4
O2—N4—O3	117.8 (5)	C8—C9—H9A	120.4
N1—C1—C2	122.6 (5)	N3—C10—C9	123.5 (4)
N1—C1—H1	118.7	N3—C10—H10	118.2

C2—C1—H1	118.7	C9—C10—H10	118.2
C3—C2—C1	119.8 (4)	N3—C11—C12	122.2 (4)
C3—C2—H2	120.1	N3—C11—H11	118.9
C1—C2—H2	120.1	C12—C11—H11	118.9
C2—C3—C4	117.4 (4)	C11—C12—C8	120.3 (4)
C2—C3—C6	118.8 (4)	C11—C12—H12	119.8
C4—C3—C6	123.8 (4)	C8—C12—H12	119.8
C5—C4—C3	119.1 (4)		
N3^{i}—Ag1—O2—N4	−7.1 (5)	C7—N2—C6—O1	−0.4 (7)
N1—Ag1—O2—N4	165.5 (5)	C7—N2—C6—C3	177.7 (4)
O3^{ii}—Ag1—O2—N4	−97.5 (4)	C2—C3—C6—O1	−0.7 (6)
O2—Ag1—N1—C5	−17.8 (4)	C4—C3—C6—O1	177.8 (4)
O3^{ii}—Ag1—N1—C5	−141.4 (4)	C2—C3—C6—N2	−178.8 (4)
O2—Ag1—N1—C1	167.1 (4)	C4—C3—C6—N2	−0.3 (6)
O3^{ii}—Ag1—N1—C1	43.5 (4)	C6—N2—C7—C8	−76.5 (6)
Ag1—O2—N4—O4	33.5 (7)	N2—C7—C8—C9	−0.5 (7)
Ag1—O2—N4—O3	−138.7 (4)	N2—C7—C8—C12	−179.3 (4)
C5—N1—C1—C2	−1.5 (8)	C12—C8—C9—C10	−2.1 (7)
Ag1—N1—C1—C2	173.8 (4)	C7—C8—C9—C10	179.1 (4)
N1—C1—C2—C3	1.7 (8)	C11—N3—C10—C9	−0.6 (7)
C1—C2—C3—C4	−0.7 (7)	Ag1^{iii}—N3—C10—C9	−172.5 (4)
C1—C2—C3—C6	177.9 (4)	C8—C9—C10—N3	1.9 (7)
C2—C3—C4—C5	−0.5 (7)	C10—N3—C11—C12	−0.5 (7)
C6—C3—C4—C5	−179.0 (4)	Ag1^{iii}—N3—C11—C12	171.1 (4)
C1—N1—C5—C4	0.2 (8)	N3—C11—C12—C8	0.2 (8)
Ag1—N1—C5—C4	−175.1 (4)	C9—C8—C12—C11	1.1 (7)
C3—C4—C5—N1	0.8 (8)	C7—C8—C12—C11	180.0 (5)

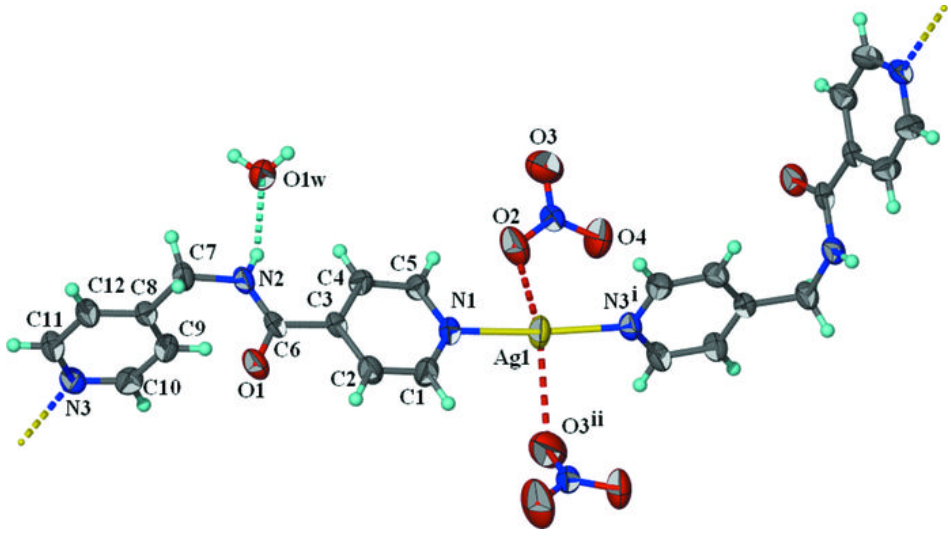
Symmetry codes: (i) −*x*+1/2, −*y*+1, *z*−1/2; (ii) *x*−1/2, −*y*+3/2, −*z*; (iii) −*x*+1/2, −*y*+1, *z*+1/2.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2N···O1W	0.86 (4)	2.04 (2)	2.827 (6)	154 (5)
O1W—H1W1···O1^{iv}	0.85 (4)	2.05 (3)	2.831 (5)	154 (7)
O1W—H1W2···O4^{v}	0.85 (4)	2.09 (4)	2.888 (7)	157 (9)

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

Fig. 1


O1w
O3
O2
O4
C7
N2
C4
C5
C12
C8
C3
N1
N3i
C11
C9
C6
Ag1
C10
O1
C2
C1
N3
O3ii