Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

catena-Poly[[silver(I)-μ-2-[(pyrazin-2-yl-κ^2N^1:N^4)aminomethyl]phenol] nitrate]

Zhao-Peng Deng,[a] Shan Gao[a] and Seik Weng Ng[b,c]*

[a]Key Laboratory of Functional Inorganic Material Chemistry, Ministry of Education, Heilongjiang University, Harbin 150080, People's Republic of China, [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia, and [c]Chemistry Department, Faculty of Science, King Abdulaziz University, PO Box 80203 Jeddah, Saudi Arabia
Correspondence e-mail: seikweng@um.edu.my

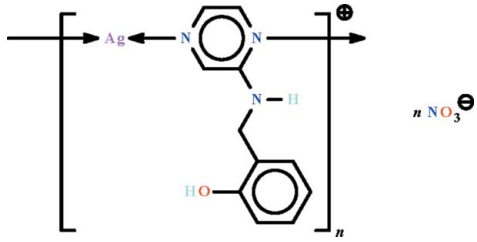
Received 31 July 2012; accepted 6 August 2012

Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; R factor = 0.075; wR factor = 0.224; data-to-parameter ratio = 16.1.

The Ag^I atom in the polycationic salt, $\{[Ag(C_{11}H_{11}N_3O)]NO_3\}_n$, shows a linear coordination [N—Ag—N = 175.0 (2)°]; the polymeric nature arises from bridging by the pyrazine portion of the ligand, resulting in chains extending parallel to [100]. The NO_3^- counter-ions surround the polymeric chain and interact only weakly with it [Ag···O = 2.701 (4) and 2.810 (5) Å]. Adjacent chains are linked into a three-dimensional network by O—H···O and N—H···O hydrogen bonds.

Related literature

For the structure of 2-{[(pyrazin-2-yl)amino]methyl}phenol, see: Gao & Ng (2012).



Experimental

Crystal data

$[Ag(C_{11}H_{11}N_3O)]NO_3$
M_r = 371.11
Monoclinic, $P2_1/c$
a = 7.1265 (9) Å
b = 9.5249 (14) Å
c = 18.654 (2) Å
β = 97.240 (4)°
V = 1256.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.63 mm^{-1}
T = 293 K
0.27 × 0.18 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.668, T_{max} = 0.817
11969 measured reflections
2864 independent reflections
2038 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.125
S = 1.02
2864 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.77 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—N1	2.172 (4)	Ag1—N2^{i}	2.195 (4)

Symmetry code: (i) $x-1, y, z$.

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O3^{ii}	0.84	1.96	2.795 (6)	171
N3—H3···O4^{iii}	0.88	2.22	2.982 (6)	145

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

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).

We thank the Key Project of the Natural Science Foundation of Heilongjiang Province (No. ZD200903), the Key Project of the Education Bureau of Heilongjiang Province (No. 12511z023, No. 2011CJHB006), the Innovation Team of the Education Bureau of Heilongjiang Province (No. 2010 t d03), Heilongjiang University (Hdtd2010–04) and the Ministry of Higher Education of Malaysia (grant No. UM.C/HIR/MOHE/SC/12) for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5602).

References

Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Gao, S. & Ng, S. W. (2012). *Acta Cryst.* E**68**, o2472.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalClear*. Rigaku/MSC Inc., The Woodlands, Texas, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2010). *J. Appl. Cryst.* **43**, 920–925.

supporting information

Acta Cryst. (2012). E**68**, m1171 [doi:10.1107/S1600536812034769]

catena-Poly[[silver(I)-μ-2-[(pyrazin-2-yl-κ^2N^1:N^4)aminomethyl]phenol] nitrate]

Zhao-Peng Deng, Shan Gao and Seik Weng Ng

S1. Comment

A recent study reports 2-[(pyrazin-2-ylamino)methyl]phenol, a reduced Schiff-base that possesses an acidic phenolic group (Gao & Ng, 2012). The reaction with silver nitrate yields polycationic $[Ag(C_{11}H_{11}N_3O)]_n nNO_3$ (Scheme I). The polymeric nature arises from bridging by the pyrazine portion of the ligand. The counterions surround the chain and interact only weakly with it [Ag···O 2.701 (4), 2.810 (5) Å] (Fig. 1). Adjacent chains are linked into a three-dimensional network by O–H···O and N–H···O hydrogen bonds (Table 1).

S2. Experimental

An acetonitrile solution (10 ml) of silver nitrate (1 mmol) was added to a methanol solution (5 ml) of 2-[(pyrazin-2-yl-amino)methyl]phenol (1 mmol). The solution was filtered and then side aside, away from light, for the growth of crystals. Colorless crystals were obtained after several days.

S3. Refinement

Hydrogen atoms were placed in calculated positions (C–H 0.93–0.97, N–H 0.88, O–H 0.84 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2–1.5U(C,*N*,*O*).

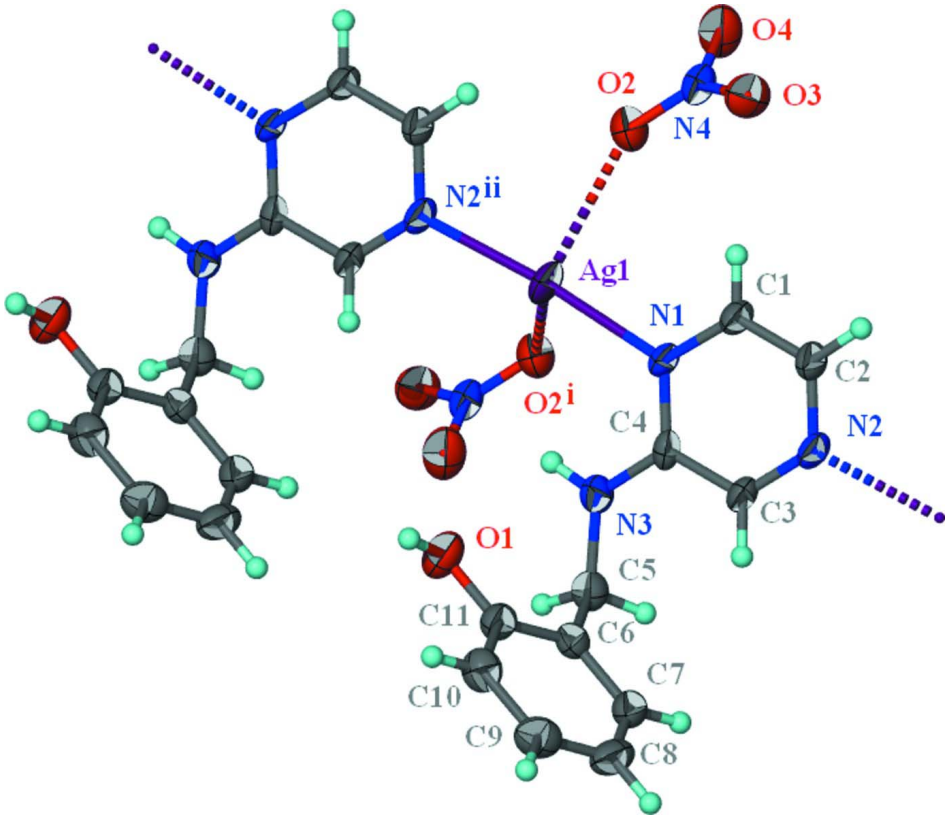


Figure 1

Thermal ellipsoid plot (Barbour, 2001) of the polymeric chain structure of $[Ag(C_{11}H_{11}N_3O)]_nNO_3$ at the 50% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

catena-Poly[[silver(I)-μ-2-[(pyrazin-2-yl- κ^2N^1:N^4)aminomethyl]phenol] nitrate]

Crystal data

$[Ag(C_{11}H_{11}N_3O)]NO_3$
M_r = 371.11
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 7.1265 (9) Å
b = 9.5249 (14) Å
c = 18.654 (2) Å
β = 97.240 (4)°
V = 1256.1 (3) Å^3
Z = 4
$F(000)$ = 736
D_x = 1.962 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 5867 reflections
θ = 3.1–27.5°
μ = 1.63 mm^{-1}
T = 293 K
Prism, colorless
0.27 × 0.18 × 0.13 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} = 0.668, T_{max} = 0.817
11969 measured reflections
2864 independent reflections
2038 reflections with $I > 2\sigma(I)$
R_{int} = 0.042
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −9→8
k = −12→12
l = −24→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.125$
$S = 1.02$
2864 reflections
182 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
$w = 1/[\sigma^2(F_o^2) + (0.0508P)^2 + 4.1394P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.64$ e Å^{-3}
$\Delta\rho_{min} = -0.77$ e Å^{-3}

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Ag1	0.06666 (5)	0.59659 (5)	0.58246 (2)	0.05110 (18)
O1	0.3023 (5)	0.4649 (5)	0.8136 (2)	0.0571 (10)
H1	0.2582	0.5291	0.8375	0.086*
O2	−0.0170 (6)	0.6917 (5)	0.4458 (2)	0.0575 (11)
O3	0.1837 (5)	0.8322 (5)	0.4064 (2)	0.0574 (11)
O4	−0.0257 (6)	0.7272 (6)	0.3321 (2)	0.0658 (12)
N1	0.3716 (5)	0.5848 (4)	0.5842 (2)	0.0316 (8)
N2	0.7616 (5)	0.5983 (4)	0.5896 (2)	0.0361 (9)
N3	0.4029 (6)	0.4097 (5)	0.6707 (2)	0.0434 (10)
H3	0.2785	0.4081	0.6661	0.052*
N4	0.0450 (6)	0.7509 (5)	0.3943 (2)	0.0414 (10)
C1	0.4556 (6)	0.6685 (5)	0.5406 (3)	0.0352 (10)
H1A	0.3804	0.7245	0.5078	0.042*
C2	0.6473 (7)	0.6755 (5)	0.5421 (3)	0.0397 (11)
H2	0.6993	0.7341	0.5100	0.048*
C3	0.6828 (6)	0.5159 (6)	0.6338 (3)	0.0368 (11)
H3A	0.7599	0.4648	0.6683	0.044*
C4	0.4845 (6)	0.5027 (5)	0.6304 (2)	0.0328 (10)
C5	0.5036 (8)	0.3108 (6)	0.7217 (3)	0.0442 (12)
H5A	0.6001	0.2642	0.6980	0.053*
H5B	0.4151	0.2395	0.7333	0.053*
C6	0.5967 (7)	0.3745 (5)	0.7914 (3)	0.0371 (11)
C7	0.7896 (7)	0.3554 (6)	0.8134 (3)	0.0451 (12)
H7	0.8625	0.3062	0.7839	0.054*
C8	0.8733 (8)	0.4086 (6)	0.8783 (3)	0.0510 (14)
H8	1.0016	0.3941	0.8926	0.061*
C9	0.7677 (8)	0.4832 (7)	0.9221 (3)	0.0529 (14)
H9	0.8247	0.5192	0.9658	0.063*
C10	0.5791 (8)	0.5042 (6)	0.9013 (3)	0.0472 (13)
H10	0.5082	0.5552	0.9308	0.057*
C11	0.4926 (7)	0.4498 (6)	0.8363 (3)	0.0404 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0201 (2)	0.0684 (3)	0.0657 (3)	0.00250 (18)	0.00874 (18)	0.0059 (2)
O1	0.039 (2)	0.071 (3)	0.062 (3)	0.008 (2)	0.0080 (19)	−0.008 (2)
O2	0.050 (2)	0.066 (3)	0.059 (2)	0.000 (2)	0.018 (2)	0.015 (2)
O3	0.039 (2)	0.064 (3)	0.067 (3)	−0.0142 (19)	−0.0030 (19)	0.011 (2)
O4	0.048 (2)	0.102 (4)	0.047 (2)	−0.010 (2)	0.0027 (19)	−0.012 (2)
N1	0.0186 (16)	0.038 (2)	0.038 (2)	0.0005 (15)	0.0023 (15)	0.0005 (17)
N2	0.0183 (16)	0.044 (2)	0.046 (2)	−0.0003 (16)	0.0028 (16)	0.0007 (19)
N3	0.028 (2)	0.059 (3)	0.043 (2)	−0.006 (2)	0.0052 (18)	0.010 (2)
N4	0.028 (2)	0.046 (3)	0.050 (3)	−0.0013 (18)	0.0086 (19)	−0.002 (2)
C1	0.024 (2)	0.035 (3)	0.047 (3)	0.0019 (19)	0.005 (2)	0.004 (2)
C2	0.029 (2)	0.041 (3)	0.050 (3)	−0.002 (2)	0.012 (2)	0.008 (2)
C3	0.022 (2)	0.048 (3)	0.041 (3)	0.005 (2)	0.0058 (19)	0.002 (2)
C4	0.025 (2)	0.041 (3)	0.034 (2)	−0.0041 (19)	0.0101 (18)	−0.007 (2)
C5	0.042 (3)	0.046 (3)	0.045 (3)	0.002 (2)	0.010 (2)	0.003 (2)
C6	0.038 (2)	0.036 (3)	0.039 (3)	−0.001 (2)	0.009 (2)	0.007 (2)
C7	0.038 (3)	0.047 (3)	0.051 (3)	0.005 (2)	0.013 (2)	0.014 (3)
C8	0.035 (3)	0.049 (3)	0.067 (4)	0.002 (2)	−0.002 (3)	0.014 (3)
C9	0.052 (3)	0.053 (4)	0.051 (3)	−0.008 (3)	−0.005 (3)	0.003 (3)
C10	0.052 (3)	0.046 (3)	0.044 (3)	−0.002 (3)	0.010 (3)	−0.006 (2)
C11	0.035 (2)	0.040 (3)	0.047 (3)	0.001 (2)	0.007 (2)	0.005 (2)

Geometric parameters (Å, º)

Ag1—N1	2.172 (4)	C1—H1A	0.9300
Ag1—N2^{i}	2.195 (4)	C2—H2	0.9300
Ag1—O2	2.701 (4)	C3—C4	1.412 (6)
Ag1—O2^{ii}	2.810 (5)	C3—H3A	0.9300
O1—C11	1.376 (6)	C5—C6	1.511 (7)
O1—H1	0.8400	C5—H5A	0.9700
O2—N4	1.242 (6)	C5—H5B	0.9700
O3—N4	1.254 (6)	C6—C7	1.396 (7)
O4—N4	1.225 (6)	C6—C11	1.386 (7)
N1—C1	1.333 (6)	C7—C8	1.377 (8)
N1—C4	1.352 (6)	C7—H7	0.9300
N2—C3	1.314 (6)	C8—C9	1.376 (9)
N2—C2	1.344 (6)	C8—H8	0.9300
N2—Ag1^{iii}	2.195 (4)	C9—C10	1.366 (8)
N3—C4	1.342 (6)	C9—H9	0.9300
N3—C5	1.461 (7)	C10—C11	1.390 (8)
N3—H3	0.8800	C10—H10	0.9300
C1—C2	1.364 (6)		
N1—Ag1—N2^{i}	175.01 (15)	C4—C3—H3A	119.0
N1—Ag1—O2	97.63 (13)	N1—C4—N3	118.3 (4)
N2^{i}—Ag1—O2	87.27 (14)	N1—C4—C3	119.3 (4)

N1—Ag1—O2^{ii}	93.12 (13)	N3—C4—C3	122.4 (5)
N2^{i}—Ag1—O2^{ii}	85.21 (14)	N3—C5—C6	115.3 (4)
O2—Ag1—O2^{ii}	98.24 (12)	N3—C5—H5A	108.5
C11—O1—H1	109.5	C6—C5—H5A	108.5
N4—O2—Ag1	145.6 (3)	N3—C5—H5B	108.5
C1—N1—C4	117.2 (4)	C6—C5—H5B	108.5
C1—N1—Ag1	119.1 (3)	H5A—C5—H5B	107.5
C4—N1—Ag1	123.6 (3)	C7—C6—C11	118.1 (5)
C3—N2—C2	117.9 (4)	C7—C6—C5	120.7 (5)
C3—N2—Ag1^{iii}	122.6 (3)	C11—C6—C5	121.2 (5)
C2—N2—Ag1^{iii}	119.1 (3)	C6—C7—C8	120.8 (5)
C4—N3—C5	125.3 (4)	C6—C7—H7	119.6
C4—N3—H3	117.3	C8—C7—H7	119.6
C5—N3—H3	117.3	C9—C8—C7	120.2 (5)
O4—N4—O2	120.3 (5)	C9—C8—H8	119.9
O4—N4—O3	120.3 (5)	C7—C8—H8	119.9
O2—N4—O3	119.4 (5)	C8—C9—C10	120.0 (5)
N1—C1—C2	122.9 (5)	C8—C9—H9	120.0
N1—C1—H1A	118.6	C10—C9—H9	120.0
C2—C1—H1A	118.6	C9—C10—C11	120.3 (5)
C1—C2—N2	120.6 (4)	C9—C10—H10	119.8
C1—C2—H2	119.7	C11—C10—H10	119.8
N2—C2—H2	119.7	C6—C11—C10	120.5 (5)
N2—C3—C4	121.9 (4)	C6—C11—O1	116.7 (5)
N2—C3—H3A	119.0	C10—C11—O1	122.7 (5)

N1—Ag1—O2—N4	−19.9 (6)	C5—N3—C4—N1	178.2 (5)
N2^{i}—Ag1—O2—N4	161.0 (6)	C5—N3—C4—C3	−0.7 (8)
O2^{ii}—Ag1—O2—N4	−114.2 (6)	N2—C3—C4—N1	−5.1 (7)
O2—Ag1—N1—C1	26.1 (4)	N2—C3—C4—N3	173.8 (5)
O2^{ii}—Ag1—N1—C1	124.9 (4)	C4—N3—C5—C6	73.9 (6)
O2^{ii}—Ag1—N1—C4	−59.3 (4)	N3—C5—C6—C7	−124.6 (5)
Ag1—O2—N4—O4	152.0 (5)	N3—C5—C6—C11	57.3 (6)
Ag1—O2—N4—O3	−26.1 (9)	C11—C6—C7—C8	0.7 (8)
C4—N1—C1—C2	−1.2 (7)	C5—C6—C7—C8	−177.4 (5)
Ag1—N1—C1—C2	174.9 (4)	C6—C7—C8—C9	−0.8 (8)
N1—C1—C2—N2	−1.3 (8)	C7—C8—C9—C10	0.2 (9)
C3—N2—C2—C1	0.5 (7)	C8—C9—C10—C11	0.5 (9)
Ag1^{iii}—N2—C2—C1	173.7 (4)	C7—C6—C11—C10	−0.1 (8)
C2—N2—C3—C4	2.6 (7)	C5—C6—C11—C10	178.1 (5)
Ag1^{iii}—N2—C3—C4	−170.3 (4)	C7—C6—C11—O1	−179.0 (5)
C1—N1—C4—N3	−174.8 (4)	C5—C6—C11—O1	−0.9 (7)
Ag1—N1—C4—N3	9.2 (6)	C9—C10—C11—C6	−0.6 (8)
C1—N1—C4—C3	4.2 (7)	C9—C10—C11—O1	178.4 (5)
Ag1—N1—C4—C3	−171.8 (3)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O3^{iv}	0.84	1.96	2.795 (6)	171
N3—H3···O4^{ii}	0.88	2.22	2.982 (6)	145

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