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catena-Poly[[silver(I)-μ-pyrazine-κ^2N:N'] perchlorate]

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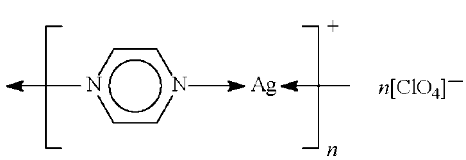
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(Cl–O) = 0.003 Å; disorder in main residue; R factor = 0.021; wR factor = 0.052; data-to-parameter ratio = 10.7.

In the title compound, $[Ag(C_4H_4N_2)]ClO_4$, pyrazine ligands bridge two symmetry-related Ag atoms [Ag—N = 2.222 (3) Å] to form linear polycationic chains which run along the c axis of the orthorhombic unit cell. The Ag^I ion has $m2m$ site symmetry. The N atoms of the pyrazine ligand lie on a crystallographic mirror plane and each C atom of this ligand possesses crystallographically imposed disorder with two components of equal occupancy. The Cl atom of the perchlorate anion has $m2m$ site symmetry and the two unique O atoms of this anion lie on a mirror plane. In addition, in the crystal structure, one-dimensional chains are linked through weak interactions involving perchlorate anions [Ag$\cdots$O = 2.726 (2) Å] into a motif that can be described as a 4(4).6(2) sheet.

Related literature

For details of the related silver nitrite–pyrazine adduct, see Blake *et al.* (1999); for the silver hexafluorophosphate–pyrazine adduct, see Carlucci *et al.* (1995*a*,*b*); for the silver tetrafluoroborate–pyrazine adduct, see Carlucci *et al.* (1995*c*); and for the silver nitrate–pyrazine adduct, see Vranka & Amma (1966).



Experimental

Crystal data

$[Ag(C_4H_4N_2)]ClO_4$
M_r = 287.41
Orthorhombic, $Cmcm$
a = 7.4838 (2) Å
b = 7.1954 (2) Å
c = 14.3623 (4) Å
V = 773.39 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.93 mm^{-1}
T = 295 (2) K
0.29 × 0.23 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.489, T_{max} = 0.621
2749 measured reflections
493 independent reflections
443 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.021
$wR(F^2)$ = 0.052
S = 1.08
493 reflections
46 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *publCIF* (Westrip, 2007).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2524).

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supplementary materials

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catena-Poly[[silver(I)-μ-pyrazine-κ^2N:N'] perchlorate]

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Comment

Silver salts react with the bidentate pyrazine *N*-heterocycles to furnish adducts that display a diverse range of architectures. The nitrate adduct consists of a polycationic $[Ag(C_4H_4N_2)]\infty$ chain that is surrounded by the nitrate anions, albeit at somewhat long distances (Vranka & Amma, 1966). In silver nitrite adduct, the anion is much closer to the metal atom, the anion chelating to it (Blake *et al.*, 1999) in the resulting pyrazine-bridged chain. With the hexafluorophosphate counterion, the adduct exists as a chain as the counterion is not Lewis-basic enough to have any coordinating ability. One adduct shows the chain motif in whcih the silver atom shows linear coordination; another is a cocrystal that has both $[Ag(C_4H_4N_2)]\infty$ and $[Ag_2(C_4H_4N_2)_5]\infty$ chains (Carlucci *et al.*, 1995*a*). Another adduct has the silver in a four-coordinate N_4Ag environment (Carlucci *et al.*, 1995*b*). The silver tetrafluoroborate adduct exists in two forms. One form has polycationic chains and non-interacting tetrafluoroborate anions; in other polymorphs, the silver atom shows three- and four-coordinate heterocycle-linked silver (Carlucci *et al.*, 1995*c*).

Experimental

Silver perchlorate (0.207 g, 1 mmol), pyrazine (0.08 g, 1 mmol) and water (10 ml) were sealed in a Teflon-lined stainless-steel autoclave (20 ml capacity). The autoclave was heated 433 K for 3 days. It was then cooled at 5 K h^{-1}. Colorless crystals were obtained in about 60% yield based on Ag.

Refinement

The pyrazine molecule is disordered with respect to the carbon atoms, which were refined as four atoms, each of half-site occupancy. The four carbon-bound H atoms were placed at calculated positions (C–H 0.93 Å) and were included in the refinement in the riding model approximation, with *U*(H) set to 1.2 times U_{eq}(C).

Figures

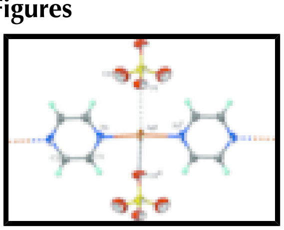

Fig. 1. Thermal ellipsoid plot of a portion of the chain structure; displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are drawn as spheres of arbitrary radii. The weak $Ag\cdots O_{perchlorate}$ interactions are depicted as dashed lines. [Symmetry code: *i* = *x*, *y*, 1/2 − *z*; *ii* = 1 − *x*, *y*, *z*.]

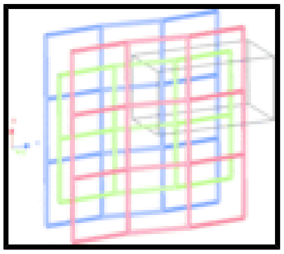

Fig. 2. Layer structure as illustrated by *OLEX* (Dolomanov *et al.*, 2003).

catena-Poly[[silver(I)-μ-pyrazine-κ^2*N*:*N*'] perchlorate]

Crystal data

$[Ag(C_4H_4N_2)]ClO_4$	$F_{000} = 552$
$M_r = 287.41$	$D_x = 2.468$ Mg m^{-3}
Orthorhombic, *Cmcm*	Mo *K*α radiation λ = 0.71073 Å
Hall symbol: -C 2c 2	Cell parameters from 1486 reflections
a = 7.4838 (2) Å	θ = 2.8–27.8°
b = 7.1954 (2) Å	μ = 2.93 mm^{-1}
c = 14.3623 (4) Å	*T* = 295 (2) K
V = 773.39 (4) Å^3	Block, colorless
Z = 4	0.29 × 0.23 × 0.18 mm

Data collection

Bruker APEXII area-detector diffractometer	493 independent reflections
Radiation source: fine-focus sealed tube	443 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
T = 295(2) K	$\theta_{max} = 27.5°$
φ and ω scans	$\theta_{min} = 2.8°$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 9$
$T_{min} = 0.489$, $T_{max} = 0.621$	$k = -9 \rightarrow 7$
2749 measured reflections	$l = -18 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.021$	$w = 1/[\sigma^2(F_o^2) + (0.0321P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.052$	$(\Delta/\sigma)_{max} = 0.001$
S = 1.08	$\Delta\rho_{max} = 0.46$ e Å^{-3}
493 reflections	$\Delta\rho_{min} = -0.36$ e Å^{-3}

46 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0057 (6)
Secondary atom site location: difference Fourier map	

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ag1	0.5000	0.05768 (4)	0.2500	0.0418 (2)	
Cl1	0.0000	0.0621 (1)	0.2500	0.0397 (3)	
O1	0.1546 (3)	0.1779 (3)	0.2500	0.0588 (7)	
O2	0.0000	−0.0517 (4)	0.3301 (3)	0.093 (1)	
N1	0.5000	0.0229 (4)	0.40375 (18)	0.0366 (6)	
C1	0.6234 (7)	−0.0790 (6)	0.4472 (3)	0.046 (1)	0.50
H1	0.7133	−0.1351	0.4125	0.055*	0.50
C2	0.6208 (7)	−0.1030 (7)	0.5424 (3)	0.046 (1)	0.50
H2	0.7071	−0.1783	0.5697	0.055*	0.50

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0551 (3)	0.0518 (3)	0.0186 (2)	0.000	0.000	0.000
Cl1	0.0362 (6)	0.0377 (6)	0.0452 (7)	0.000	0.000	0.000
O1	0.036 (2)	0.056 (2)	0.084 (2)	−0.007 (1)	0.000	0.000
O2	0.085 (2)	0.096 (3)	0.097 (3)	0.000	0.000	0.054 (2)
N1	0.043 (1)	0.044 (1)	0.023 (1)	0.000	0.000	0.003 (1)
C1	0.046 (3)	0.064 (3)	0.028 (2)	0.016 (2)	0.005 (2)	−0.002 (2)
C2	0.047 (3)	0.061 (3)	0.029 (2)	0.020 (2)	0.000 (2)	0.005 (2)

Geometric parameters (Å, °)

Ag1—N1	2.222 (3)	N1—C2^{iv}	1.322 (5)
Ag1—N1^{i}	2.222 (3)	N1—C2^{v}	1.322 (5)
Ag1—O1	2.726 (2)	N1—C1^{ii}	1.334 (5)
Ag1—O1^{ii}	2.726 (2)	N1—C1	1.334 (5)
Cl1—O2^{i}	1.412 (3)	C1—C2	1.377 (7)
Cl1—O2	1.412 (3)	C2—N1^{v}	1.322 (5)
Cl1—O1	1.426 (2)	C1—H1	0.9300
Cl1—O1^{iii}	1.426 (2)	C2—H2	0.9300
N1^{i}—Ag1—N1	167.1 (1)	C2^{v}—N1—C1^{ii}	59.5 (3)
N1—Ag1—O1	92.05 (2)	C2^{iv}—N1—C1	59.5 (3)
N1—Ag1—O1^{ii}	92.05 (2)	C2^{v}—N1—C1	116.0 (3)
N1^{i}—Ag1—O1	92.05 (2)	C1^{ii}—N1—C1	87.6 (4)
N1^{i}—Ag1—O1^{ii}	92.05 (2)	C2^{iv}—N1—Ag1	122.2 (2)
O1—Ag1—O1^{ii}	143.0 (1)	C2^{v}—N1—Ag1	122.2 (2)

O1—Cl1—O1^{iii}	108.5 (2)	C1^{ii}—N1—Ag1	121.8 (2)
O1—Cl1—O2	109.8 (1)	C1—N1—Ag1	121.8 (2)
O1—Cl1—O2^{i}	109.8 (1)	N1—C1—C2	121.6 (4)
O1^{iii}—Cl1—O2	109.8 (1)	N1^{v}—C2—C1	122.4 (4)
O1^{iii}—Cl1—O2^{i}	109.8 (1)	N1—C1—H1	119.2
O2—Cl1—O2^{i}	109.1 (3)	C2—C1—H1	119.2
Cl1—O1—Ag1	125.8 (1)	N1^{v}—C2—H2	118.8
C2^{iv}—N1—C2^{v}	86.3 (5)	C1—C2—H2	118.8
C2^{iv}—N1—C1^{ii}	116.0 (3)		

O2^{i}—Cl1—O1—Ag1	−60.0 (2)	N1^{i}—Ag1—N1—C1^{ii}	−54.5 (3)
O2—Cl1—O1—Ag1	60.0 (2)	O1^{ii}—Ag1—N1—C1^{ii}	−162.9 (3)
O1^{iii}—Cl1—O1—Ag1	180.0	O1—Ag1—N1—C1^{ii}	53.9 (3)
N1^{i}—Ag1—O1—Cl1	83.87 (6)	N1^{i}—Ag1—N1—C1	54.5 (3)
N1—Ag1—O1—Cl1	−83.87 (6)	O1^{ii}—Ag1—N1—C1	−53.9 (3)
O1^{ii}—Ag1—O1—Cl1	180.0	O1—Ag1—N1—C1	162.9 (3)
N1^{i}—Ag1—N1—C2^{iv}	126.1 (3)	C2^{iv}—N1—C1—C2	70.1 (4)
O1^{ii}—Ag1—N1—C2^{iv}	17.7 (3)	C2^{v}—N1—C1—C2	1.9 (7)
O1—Ag1—N1—C2^{iv}	−125.5 (3)	C1^{ii}—N1—C1—C2	−52.2 (6)
N1^{i}—Ag1—N1—C2^{v}	−126.1 (3)	Ag1—N1—C1—C2	−178.7 (3)
O1^{ii}—Ag1—N1—C2^{v}	125.5 (3)	N1—C1—C2—N1^{v}	−2.0 (8)
O1—Ag1—N1—C2^{v}	−17.7 (3)		

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

Fig. 1

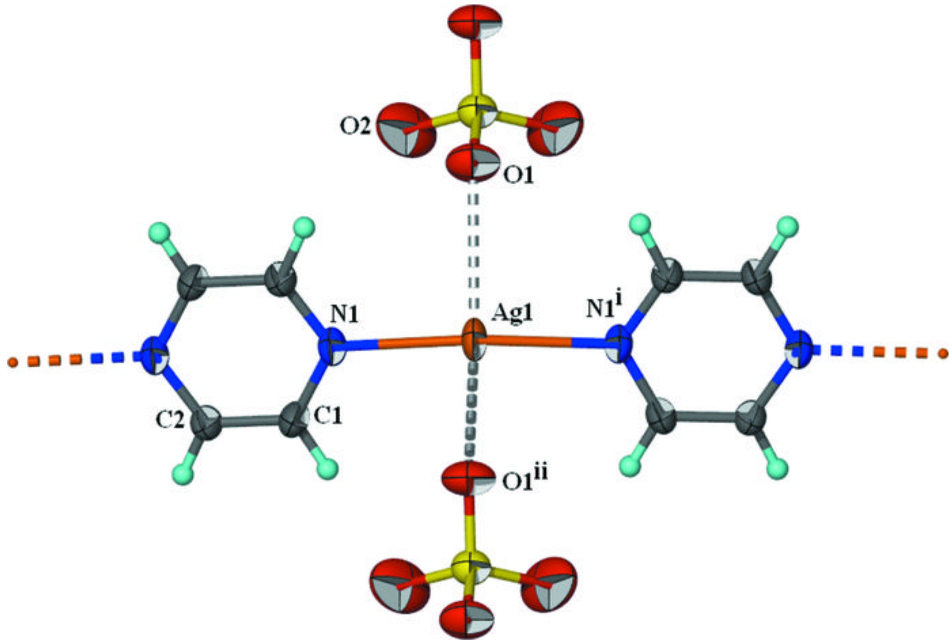

Fig. 2