

Bis(pyridine-3-carboxylic acid- κ N)-silver(I) perchlorate

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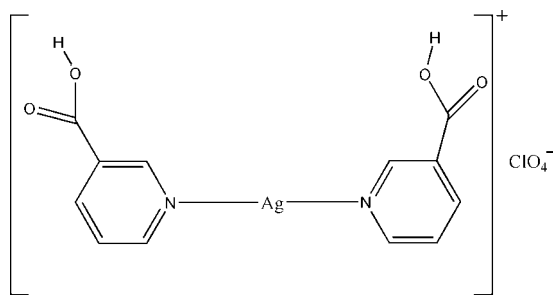
Received 18 December 2008; accepted 30 December 2008

Key indicators: single-crystal X-ray study; $T = 273$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å;
R factor = 0.043; wR factor = 0.123; data-to-parameter ratio = 12.5.

In the title compound, $[\text{Ag}(\text{C}_6\text{H}_5\text{NO}_2)_2]\text{ClO}_4$, the Ag^{I} atom shows an almost linear coordination geometry, defined by two N atoms from two pyridine-3-carboxylic acid ligands. The complex cations are linked by hydrogen bonds between the carboxyl groups into a chain. The chains are further connected through $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds and a weak $\text{Ag}\cdots\text{O}$ interaction [$2.757(8)$ Å] into a layer. Another $\text{Ag}\cdots\text{O}$ interaction [$2.899(2)$ Å] and a $\text{C}-\text{H}\cdots\text{O}$ hydrogen bond connect the layers into a three-dimensional network.

Related literature

For general background on coordination polymers and open-framework materials, see: James (2003); Serre *et al.* (2004); Yaghi *et al.* (1998, 2003). For related structures, see: Evans & Lin (2001); Luo *et al.* (2004).



Experimental

Crystal data

$[\text{Ag}(\text{C}_6\text{H}_5\text{NO}_2)_2]\text{ClO}_4$
 $M_r = 453.54$
Monoclinic, $P2_1/c$
 $a = 8.0139(4)$ Å
 $b = 26.3288(15)$ Å
 $c = 7.6891(4)$ Å
 $\beta = 110.728(1)^\circ$

$V = 1517.36(14)$ Å³
 $Z = 4$
Mo $K\alpha$ radiation
 $\mu = 1.55$ mm⁻¹
 $T = 273(2)$ K
 $0.29 \times 0.25 \times 0.21$ mm

Data collection

Bruker APEXII CCD
diffractometer
Absorption correction: multi-scan
(SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.649$, $T_{\text{max}} = 0.731$

7763 measured reflections
2729 independent reflections
2150 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.123$
 $S = 0.87$
2729 reflections

219 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.26$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.57$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ag1—N1	2.178 (4)	Ag1—N2	2.185 (4)
N1—Ag1—N2	165.65 (15)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1 \cdots O5 ⁱ	0.93	2.51	3.244 (8)	136
C4—H4 \cdots O7 ⁱⁱ	0.93	2.52	3.266 (8)	139
C6—H6 \cdots O7	0.93	2.52	3.248 (8)	136
C7—H7 \cdots O8 ⁱ	0.93	2.49	3.287 (9)	144
C12—H12 \cdots O7	0.93	2.38	3.228 (9)	152
O2—H2 \cdots O4 ⁱⁱⁱ	0.82	1.84	2.649 (5)	169
O3—H3 \cdots O1 ^{iv}	0.82	1.87	2.689 (5)	175

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The authors kindly acknowledge Bijie University for supporting this work.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2176).

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supplementary materials

Acta Cryst. (2009). E65, m148 [doi:10.1107/S1600536808044206]

Bis(pyridine-3-carboxylic acid- κ N)silver(I) perchlorate

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Comment

The use of multifunctional organic linker molecules in the preparation of coordination polymers and open-framework materials has led to the development of a rich field of chemistry owing to the potential applications of these materials in catalysis, separation, gas storage and molecular recognition (James, 2003; Serre *et al.*, 2004; Yaghi *et al.*, 1998, 2003). In our investigations we used nicotinic acid ligands for the preparation of new coordination polymers, because it can act as a multidentate ligand with versatile binding and coordination modes (Evans & Lin, 2001; Luo *et al.*, 2004). In this paper, we report the crystal structure of the title compound, a new Ag^{I} complex obtained by the reaction of nicotinic acid, AgNO_3 and perchloric acid in water.

As shown in Fig. 1, the title compound consists of a $[\text{Ag}(\text{C}_6\text{H}_5\text{NO}_2)_2]^+$ cation and a perchlorate anion. The Ag^{I} atom exhibits a linear coordination geometry, defined by two N atoms from two pyridine-3-carboxylic acid ligands (Table 1). The complex cations are linked by hydrogen bonds between the carboxyl groups into a chain (Table 2). The chains are further connected by $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds involving C1, C6, C7 and C12 atoms and the perchlorate anions, and by a weak $\text{Ag}1\cdots\text{O}5(x-1, y, z)$ interaction [2.757 (8) Å] into a layer (Fig. 2). Another $\text{Ag}1\cdots\text{O}1(x, 3/2-y, z-1/2)$ interaction [2.899 (2) Å] and a $\text{C}4-\text{H}4\cdots\text{O}7(x, 3/2-y, 1/2+z)$ hydrogen bond connect the layers into a three-dimensional network.

Experimental

A mixture of AgNO_3 (0.169 g, 1 mmol), perchloric acid (0.12 ml), nicotinic acid (0.123 g, 1 mmol) and H_2O (10 ml) was placed in a 23 ml Teflon-lined reactor, which was heated to 433 K for 3 d and then cooled to room temperature at a rate of 10 K h^{-1} . The crystals obtained were washed with water and dried in air.

Refinement

H atoms on C atoms were positioned geometrically and refined as riding atoms, with $\text{C}-\text{H} = 0.93 \text{ Å}$ and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms on O atoms were located in difference Fourier maps and were fixed with $\text{O}-\text{H} = 0.82 \text{ Å}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The highest residual electron density was found 1.31 Å from atom O7 and the deepest hole 0.46 Å from atom O7.

Figures

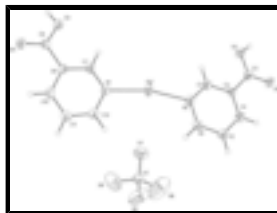


Fig. 1. The structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level.

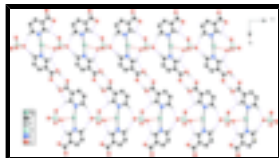


Fig. 2. The layer in the title compound. Hydrogen bonds and weak Ag...O interactions are shown as dashed lines.

Bis(pyridine-3-carboxylic acid- κ N)silver(I) perchlorate

Crystal data

$[\text{Ag}(\text{C}_6\text{H}_5\text{NO}_2)_2]\text{ClO}_4$	$F_{000} = 896$
$M_r = 453.54$	$D_x = 1.985 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
Hall symbol: -P 2ybc	$\lambda = 0.71073 \text{ \AA}$
$a = 8.0139 (4) \text{ \AA}$	Cell parameters from 5837 reflections
$b = 26.3288 (15) \text{ \AA}$	$\theta = 2.8\text{--}27.9^\circ$
$c = 7.6891 (4) \text{ \AA}$	$\mu = 1.55 \text{ mm}^{-1}$
$\beta = 110.728 (1)^\circ$	$T = 273 (2) \text{ K}$
$V = 1517.36 (14) \text{ \AA}^3$	Block, colourless
$Z = 4$	$0.29 \times 0.25 \times 0.21 \text{ mm}$

Data collection

Bruker APEXII CCD diffractometer	2729 independent reflections
Radiation source: fine-focus sealed tube	2150 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.029$
$T = 273(2) \text{ K}$	$\theta_{\text{max}} = 25.2^\circ$
φ and ω scans	$\theta_{\text{min}} = 1.6^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8 \rightarrow 9$
$T_{\text{min}} = 0.649$, $T_{\text{max}} = 0.731$	$k = -29 \rightarrow 31$
7763 measured reflections	$l = -9 \rightarrow 8$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.043$	H-atom parameters constrained
$wR(F^2) = 0.123$	$w = 1/[\sigma^2(F_o^2) + (0.0736P)^2 + 4.5241P]$
$S = 0.87$	where $P = (F_o^2 + 2F_c^2)/3$
2729 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
219 parameters	$\Delta\rho_{\text{max}} = 1.26 \text{ e \AA}^{-3}$
	$\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$

Primary atom site location: structure-invariant direct methods Extinction correction: none

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ag1	0.40344 (6)	0.612387 (13)	0.34075 (6)	0.05534 (19)
C1	0.3293 (6)	0.72596 (17)	0.4083 (7)	0.0438 (11)
H1	0.2115	0.7150	0.3691	0.053*
Cl1	0.97387 (18)	0.61558 (5)	0.3633 (2)	0.0544 (3)
N1	0.4208 (5)	0.53278 (14)	0.2719 (6)	0.0457 (9)
O1	0.2535 (4)	0.86018 (12)	0.4508 (5)	0.0488 (8)
C2	0.3650 (6)	0.77700 (16)	0.4460 (6)	0.0367 (10)
N2	0.4580 (5)	0.69166 (14)	0.4261 (6)	0.0437 (9)
O2	0.0616 (5)	0.79535 (13)	0.3776 (6)	0.0596 (10)
H2	-0.0120	0.8184	0.3499	0.089*
C3	0.2204 (6)	0.81428 (17)	0.4237 (7)	0.0425 (11)
O3	0.0023 (4)	0.43163 (13)	0.1274 (6)	0.0541 (9)
H3	-0.0738	0.4093	0.0982	0.081*
C4	0.5421 (6)	0.79317 (18)	0.5073 (7)	0.0466 (11)
H4	0.5706	0.8271	0.5356	0.056*
O4	0.1889 (5)	0.36546 (12)	0.1767 (5)	0.0519 (9)
C5	0.6742 (6)	0.75790 (19)	0.5251 (7)	0.0488 (12)
H5	0.7932	0.7678	0.5642	0.059*
O5	1.0454 (10)	0.6352 (3)	0.2338 (8)	0.147 (3)
C6	0.6276 (6)	0.70794 (18)	0.4842 (7)	0.0455 (11)
H6	0.7176	0.6843	0.4974	0.055*
O6	1.0605 (13)	0.6412 (4)	0.5267 (9)	0.174 (4)
C7	0.2868 (6)	0.49924 (17)	0.2338 (7)	0.0409 (10)
H7	0.1745	0.5107	0.2256	0.049*
O7	0.7884 (7)	0.6209 (2)	0.2885 (11)	0.117 (2)
C8	0.3093 (6)	0.44812 (16)	0.2063 (6)	0.0372 (10)
O8	1.0104 (10)	0.5643 (3)	0.3779 (16)	0.187 (4)
C9	0.1598 (6)	0.41126 (17)	0.1687 (7)	0.0409 (10)
C10	0.4758 (7)	0.43088 (19)	0.2185 (8)	0.0500 (12)
H10	0.4948	0.3966	0.2025	0.060*
C11	0.6130 (7)	0.4653 (2)	0.2546 (8)	0.0567 (14)
H11	0.7258	0.4547	0.2613	0.068*
C12	0.5813 (7)	0.5153 (2)	0.2807 (8)	0.0534 (13)
H12	0.6751	0.5383	0.3056	0.064*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag1	0.0591 (3)	0.0284 (2)	0.0765 (3)	0.00062 (16)	0.0214 (2)	-0.00512 (17)
C1	0.039 (2)	0.035 (2)	0.055 (3)	-0.0009 (19)	0.014 (2)	-0.005 (2)
Cl1	0.0416 (7)	0.0587 (8)	0.0659 (8)	0.0030 (6)	0.0228 (6)	0.0001 (6)
N1	0.044 (2)	0.033 (2)	0.060 (3)	-0.0025 (17)	0.0185 (19)	-0.0041 (18)
O1	0.0469 (19)	0.0275 (17)	0.067 (2)	-0.0023 (14)	0.0137 (17)	0.0003 (15)

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C2	0.041 (2)	0.030 (2)	0.040 (2)	-0.0015 (18)	0.0161 (19)	-0.0009 (18)
N2	0.044 (2)	0.032 (2)	0.054 (2)	0.0018 (17)	0.0163 (18)	-0.0036 (17)
O2	0.043 (2)	0.0321 (18)	0.100 (3)	0.0010 (15)	0.020 (2)	-0.0021 (18)
C3	0.044 (3)	0.034 (2)	0.050 (3)	-0.003 (2)	0.017 (2)	-0.002 (2)
O3	0.0402 (19)	0.0365 (18)	0.084 (3)	-0.0042 (15)	0.0195 (18)	-0.0055 (18)
C4	0.047 (3)	0.035 (2)	0.054 (3)	-0.005 (2)	0.014 (2)	0.000 (2)
O4	0.049 (2)	0.0302 (18)	0.074 (2)	0.0013 (15)	0.0181 (17)	0.0021 (16)
C5	0.038 (3)	0.042 (3)	0.065 (3)	-0.002 (2)	0.016 (2)	-0.002 (2)
O5	0.133 (5)	0.226 (9)	0.086 (4)	-0.095 (6)	0.043 (4)	-0.031 (5)
C6	0.042 (3)	0.043 (3)	0.051 (3)	0.006 (2)	0.016 (2)	0.000 (2)
O6	0.219 (9)	0.219 (9)	0.081 (4)	-0.109 (8)	0.050 (5)	-0.050 (5)
C7	0.036 (2)	0.033 (2)	0.051 (3)	0.0015 (18)	0.012 (2)	-0.0008 (19)
O7	0.061 (3)	0.086 (4)	0.210 (7)	0.007 (3)	0.055 (4)	0.005 (4)
C8	0.038 (2)	0.032 (2)	0.041 (2)	0.0006 (18)	0.0116 (19)	-0.0027 (18)
O8	0.118 (6)	0.104 (5)	0.323 (12)	0.054 (4)	0.057 (7)	-0.004 (7)
C9	0.042 (3)	0.031 (2)	0.047 (3)	0.0009 (19)	0.013 (2)	-0.0031 (19)
C10	0.052 (3)	0.034 (3)	0.064 (3)	0.004 (2)	0.021 (2)	-0.008 (2)
C11	0.044 (3)	0.051 (3)	0.079 (4)	0.001 (2)	0.027 (3)	-0.010 (3)
C12	0.043 (3)	0.045 (3)	0.075 (4)	-0.005 (2)	0.024 (3)	-0.004 (3)

Geometric parameters (Å, °)

Ag1—N1	2.178 (4)	O2—H2	0.8200
Ag1—N2	2.185 (4)	O3—C9	1.303 (6)
Ag1—O1 ⁱ	2.899 (2)	O3—H3	0.8200
Ag1—O5 ⁱⁱ	2.757 (8)	C4—C5	1.378 (7)
C1—N2	1.341 (6)	C4—H4	0.9300
C1—C2	1.383 (6)	O4—C9	1.226 (6)
C1—H1	0.9300	C5—C6	1.373 (7)
C11—O8	1.378 (7)	C5—H5	0.9300
C11—O6	1.378 (6)	C6—H6	0.9300
C11—O7	1.398 (6)	C7—C8	1.384 (6)
C11—O5	1.411 (6)	C7—H7	0.9300
N1—C7	1.341 (6)	C8—C10	1.381 (7)
N1—C12	1.345 (6)	C8—C9	1.489 (6)
O1—C3	1.239 (5)	C10—C11	1.375 (7)
C2—C4	1.394 (6)	C10—H10	0.9300
C2—C3	1.482 (6)	C11—C12	1.370 (7)
N2—C6	1.342 (6)	C11—H11	0.9300
O2—C3	1.294 (6)	C12—H12	0.9300
N1—Ag1—N2	165.65 (15)	C2—C4—H4	120.6
N2—C1—C2	122.6 (4)	C6—C5—C4	119.1 (5)
N2—C1—H1	118.7	C6—C5—H5	120.5
C2—C1—H1	118.7	C4—C5—H5	120.5
O8—C11—O6	112.4 (6)	N2—C6—C5	122.9 (4)
O8—C11—O7	107.2 (4)	N2—C6—H6	118.5
O6—C11—O7	116.4 (6)	C5—C6—H6	118.5
O8—C11—O5	106.8 (6)	N1—C7—C8	122.4 (4)

O6—C11—O5	105.3 (4)	N1—C7—H7	118.8
O7—C11—O5	108.1 (5)	C8—C7—H7	118.8
C7—N1—C12	117.6 (4)	C10—C8—C7	119.0 (4)
C7—N1—Ag1	124.9 (3)	C10—C8—C9	119.4 (4)
C12—N1—Ag1	117.3 (3)	C7—C8—C9	121.6 (4)
C1—C2—C4	118.5 (4)	O4—C9—O3	124.6 (4)
C1—C2—C3	121.6 (4)	O4—C9—C8	120.4 (4)
C4—C2—C3	119.9 (4)	O3—C9—C8	115.0 (4)
C1—N2—C6	118.1 (4)	C11—C10—C8	118.8 (5)
C1—N2—Ag1	123.2 (3)	C11—C10—H10	120.6
C6—N2—Ag1	118.5 (3)	C8—C10—H10	120.6
C3—O2—H2	109.5	C12—C11—C10	119.1 (5)
O1—C3—O2	123.6 (4)	C12—C11—H11	120.4
O1—C3—C2	120.9 (4)	C10—C11—H11	120.4
O2—C3—C2	115.4 (4)	N1—C12—C11	123.0 (5)
C9—O3—H3	109.5	N1—C12—H12	118.5
C5—C4—C2	118.8 (4)	C11—C12—H12	118.5
C5—C4—H4	120.6		

Symmetry codes: (i) $x, -y+3/2, z-1/2$; (ii) $x-1, y, z$.

Hydrogen-bond geometry (Å, °)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C1—H1 \cdots O5 ⁱⁱ	0.93	2.51	3.244 (8)	136
C4—H4 \cdots O7 ⁱⁱⁱ	0.93	2.52	3.266 (8)	139
C6—H6 \cdots O7	0.93	2.52	3.248 (8)	136
C7—H7 \cdots O8 ⁱⁱ	0.93	2.49	3.287 (9)	144
C12—H12 \cdots O7	0.93	2.38	3.228 (9)	152
O2—H2 \cdots O4 ^{iv}	0.82	1.84	2.649 (5)	169
O3—H3 \cdots O1 ^v	0.82	1.87	2.689 (5)	175

Symmetry codes: (ii) $x-1, y, z$; (iii) $x, -y+3/2, z+1/2$; (iv) $-x, y+1/2, -z+1/2$; (v) $-x, y-1/2, -z+1/2$.

Fig. 1

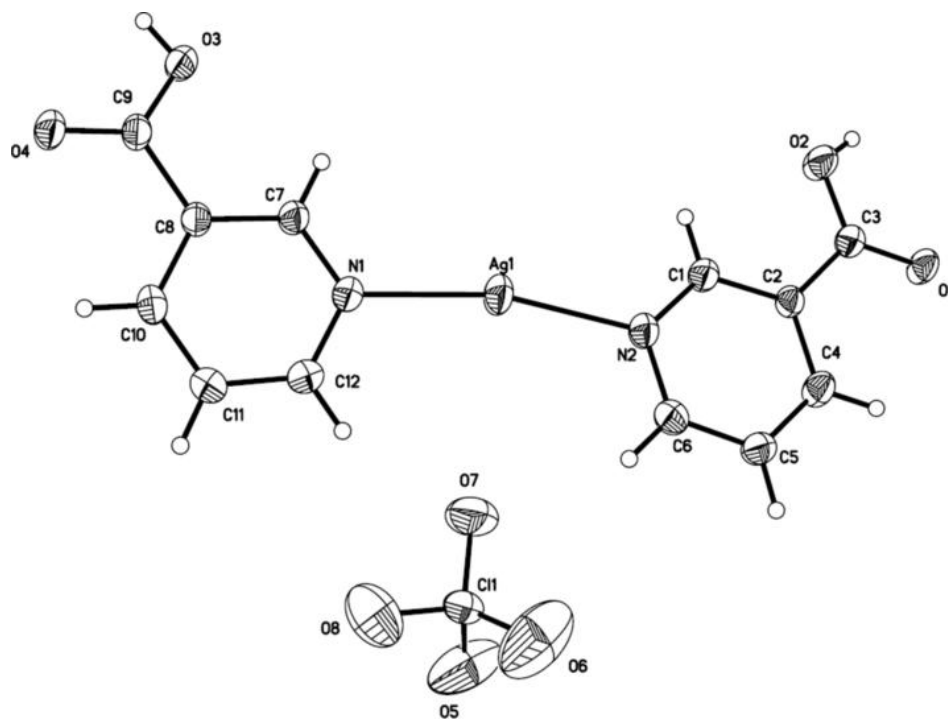


Fig. 2

