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(μ-5-Carboxy-1*H*-imidazole-4-carboxylato-κ⁴*N*¹,*O*⁵:*N*³,*O*⁴)bis[amminesilver(I)]

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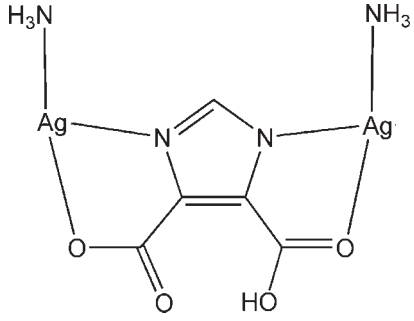
Key indicators: single-crystal X-ray study; T = 190 K; mean σ(C–C) = 0.004 Å; R factor = 0.018; wR factor = 0.044; data-to-parameter ratio = 11.4.

In the title compound, $[Ag_2(C_5H_2N_2O_4)(NH_3)_2]$, each of the two Ag^I atoms is coordinated by two N atoms from an ammonia molecule and a 5-carboxy-1*H*-imidazole-4-carboxylate ligand in an almost linear geometry, and by one carboxylate O atom with a weak interaction. The Ag atoms are assembled into a linear tetramer through Ag···Ag interactions. Each Ag tetramer is linked by four 5-carboxy-1*H*-imidazole-4-carboxylate ligands, forming a puckered chain. The complex involves a strong intramolecular O—H···O hydrogen bond.

Related literature

For general background to coordination polymers, see: Ferey (2008); Ma *et al.* (2009); Moulton & Zaworotko (2001); Tranchemontagne *et al.* (2009). For related structures with the 4,5-imidazoledicarboxylic acid ligand, see: Caudle *et al.* (1997); Fang & Zhang (2006); Han *et al.* (2005); Zhong *et al.* (2006).



Experimental

Crystal data

$[Ag_2(C_5H_2N_2O_4)(NH_3)_2]$
M_r = 403.89
Monoclinic, $C2/c$
a = 18.3800 (12) Å
b = 8.3243 (5) Å
c = 13.6696 (8) Å
β = 113.160 (1)°
V = 1922.9 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.07 mm^{-1}
T = 190 K
0.35 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
T_{min} = 0.330, T_{max} = 0.686
5211 measured reflections
1911 independent reflections
1721 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.044
S = 1.05
1911 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ag1—N1	2.134 (2)	Ag2—N3	2.133 (3)
Ag1—N4	2.123 (3)	Ag2—O1	2.607 (2)
Ag1—O4	2.628 (2)	Ag1···Ag1^{i}	2.9916 (5)
Ag2—N2	2.132 (2)	Ag1···Ag2^{ii}	3.0021 (4)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2···O3	1.19 (8)	1.26 (8)	2.448 (3)	172 (6)

Data collection: *SMART* (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: *DIAMOND* (Brandenburg, 1999); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2243).

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supporting information

Acta Cryst. (2009). E**65**, m1523 [doi:10.1107/S1600536809045747]

(*μ*-5-Carboxy-1*H*-imidazole-4-carboxylato-$\kappa^4N^1,O^5:N^3,O^4$)bis[amminesilver(I)]

Rui-Sha Zhou and Jiang-Feng Song

S1. Comment

Coordination polymers are rapidly increasing because of their intriguing structures and wide potential applications as functional materials (Ferey, 2008; Ma *et al.*, 2009; Moulton & Zaworotko, 2001; Tranchemontagne *et al.*, 2009). Complexes with 4,5-imidazoledicarboxylic acid ligand have been recently reported (Caudle *et al.*, 1997; Fang & Zhang, 2006; Zhong *et al.*, 2006). The title compound is a new Ag^I complex built with 4,5-imidazoledicarboxylic acid ligand.

The asymmetric unit consists of two crystallographically independent Ag^I atoms, one partly deprotonated 4,5-imidazoledicarboxylate ligand and two ammonia molecules (Fig. 1). Each Ag^I atom is bonded to an ammonia molecule and one N atom and one O atom from the 4,5-imidazoledicarboxylate ligand in a chelating coordination mode. The Ag—N distances range from 2.123 (3) to 2.134 (2) Å (Table 1), and the N—Ag—N bond angles range from 173.75 (11) to 177.4 (11)°. It is worth to note that the bond distances of Ag—O [2.628 (2) and 2.607 (2) Å] are much longer than that observed in the reported silver carboxylate complexes (Han *et al.*, 2005), indicating weak interaction between the Ag^I atom and the carboxylate O atom. Ag1 and Ag2 are assembled into an Ag2···Ag1···Ag1···Ag2 linear tetramer through the Ag···Ag interactions (Fig. 2) [$Ag1\cdots Ag1^{i}$ = 2.9916 (5) and $Ag1\cdots Ag2^{ii}$ = 3.0021 (4) Å; symmetry codes: (i) -*x*, *y*, 1/2 - *z*; (ii) *x*, 2 - *y*, -1/2 + *z*]. Moreover, there exists a strong hydrogen bond (O2—H2···O3) in the complex molecule (Table 2).

S2. Experimental

A solution of 4,5-imidazoledicarboxylic acid (6.5 mg, 0.05 mmol) in 2 ml water containing triethylamine (14 *μ*l, 1 mmol) was directly mixed with a solution of $AgNO_3$ in 2 ml of 25% aqueous ammonia. The resulting yellow solution was allowed to slowly crystalize at room temperature in dark. After one week, brown single crystals were collected by filtration, washed with small amounts of water and dried in air.

S3. Refinement

H atoms were located in a difference Fourier map and refined isotropically.

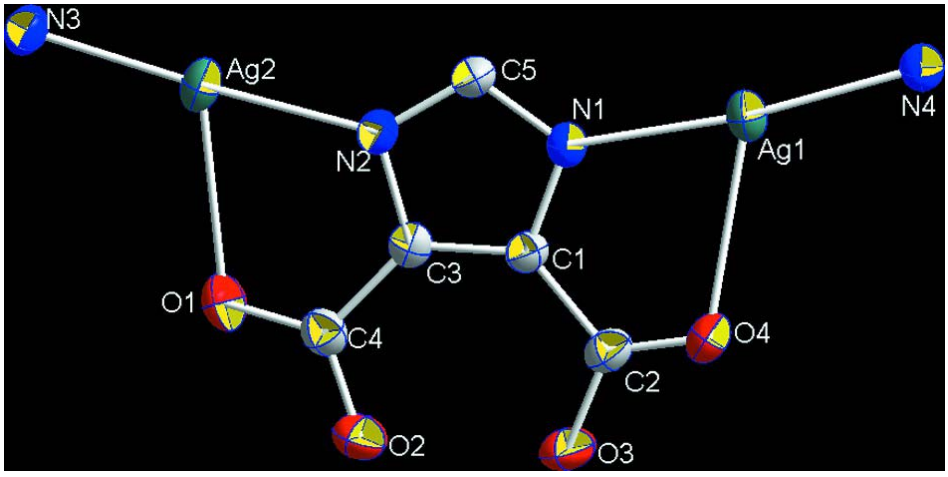

Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

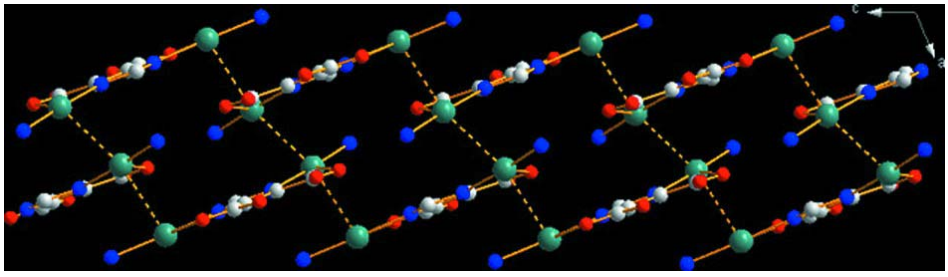

Figure 2

The one-dimensional puckered chain assembled by Ag tetramers and 4,5-imidazoledicarboxylate ligands. Dashed lines denote Ag···Ag interactions.

(*μ*-5-Carboxy-1*H*-imidazole-4-carboxylato- $\kappa^4N^1,O^5:N^3,O^4$)bis[amminesilver(I)]

Crystal data

$[Ag_2(C_5H_2N_2O_4)(NH_3)_2]$
$M_r = 403.89$
Monoclinic, *C*2/*c*
Hall symbol: -C 2yc
$a = 18.3800\ (12)$ Å
$b = 8.3243\ (5)$ Å
$c = 13.6696\ (8)$ Å
$\beta = 113.160\ (1)°$
$V = 1922.9\ (2)$ Å^3
$Z = 8$
$F(000) = 1536$
$D_x = 2.790$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1780 reflections
$\theta = 2.4–26.1°$
$\mu = 4.07$ mm^{-1}
$T = 190$ K
Block, brown
0.35 × 0.25 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.330$, $T_{max} = 0.686$
5211 measured reflections
1911 independent reflections
1721 reflections with $I > 2\sigma(I)$

R_{int} = 0.019
θ_{max} = 26.1°, θ_{min} = 2.4°
h = −22→18
k = −10→9
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.018
$wR(F^2)$ = 0.044
S = 1.05
1911 reflections
168 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.02P)^2 + 2.4121P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.50 e Å^{-3}

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

	x	y	z	U_{iso}*/U_{eq}
Ag2	0.206133 (14)	0.79951 (3)	0.660249 (17)	0.03620 (8)
O1	0.17397 (15)	0.5366 (3)	0.54751 (18)	0.0476 (6)
N2	0.15598 (14)	0.8616 (3)	0.49573 (18)	0.0306 (5)
Ag1	0.060181 (14)	1.13414 (3)	0.201582 (18)	0.03346 (8)
C1	0.11079 (17)	0.8155 (3)	0.3218 (2)	0.0269 (6)
C2	0.08372 (18)	0.7496 (4)	0.2126 (2)	0.0322 (7)
C3	0.13893 (16)	0.7428 (4)	0.4199 (2)	0.0275 (6)
C4	0.15067 (17)	0.5712 (4)	0.4527 (2)	0.0323 (7)
C5	0.13741 (19)	0.9977 (4)	0.4412 (2)	0.0332 (7)
N1	0.11022 (14)	0.9785 (3)	0.33560 (18)	0.0302 (5)
N3	0.25466 (19)	0.7478 (4)	0.8265 (2)	0.0366 (6)
N4	0.0094 (2)	1.3080 (4)	0.0800 (2)	0.0368 (6)
O2	0.13419 (14)	0.4656 (3)	0.37827 (19)	0.0436 (6)
O3	0.08142 (16)	0.5948 (3)	0.20328 (18)	0.0480 (6)
O4	0.06587 (15)	0.8395 (3)	0.13591 (16)	0.0441 (6)
H1	0.1399 (19)	1.094 (4)	0.467 (3)	0.040 (9)*
H2	0.112 (4)	0.523 (9)	0.291 (6)	0.17 (3)*
H3	0.275 (2)	0.836 (5)	0.869 (3)	0.062 (12)*
H4	0.300 (2)	0.686 (5)	0.843 (3)	0.058 (12)*
H5	0.218 (2)	0.696 (4)	0.844 (3)	0.042 (10)*
H6	0.041 (2)	1.385 (5)	0.078 (3)	0.060 (13)*
H7	−0.034 (3)	1.348 (5)	0.083 (3)	0.060 (13)*
H8	−0.004 (3)	1.271 (6)	0.024 (4)	0.073 (16)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ag2	0.03743 (15)	0.04560 (16)	0.02245 (12)	0.00084 (10)	0.00842 (10)	0.00281 (10)
O1	0.0657 (16)	0.0373 (12)	0.0384 (13)	0.0061 (11)	0.0189 (12)	0.0123 (10)
N2	0.0315 (13)	0.0331 (13)	0.0236 (12)	0.0025 (10)	0.0072 (11)	−0.0013 (10)

Ag1	0.03572 (14)	0.03391 (14)	0.02914 (13)	0.00315 (10)	0.01104 (10)	0.00742 (9)
C1	0.0292 (15)	0.0262 (14)	0.0257 (14)	−0.0018 (11)	0.0112 (12)	−0.0028 (11)
C2	0.0312 (16)	0.0350 (16)	0.0281 (15)	−0.0025 (13)	0.0091 (13)	−0.0058 (13)
C3	0.0238 (14)	0.0324 (15)	0.0271 (14)	0.0005 (11)	0.0110 (12)	0.0006 (12)
C4	0.0318 (16)	0.0319 (16)	0.0357 (16)	0.0040 (12)	0.0159 (13)	0.0032 (13)
C5	0.0407 (18)	0.0283 (16)	0.0256 (14)	0.0030 (13)	0.0076 (13)	−0.0036 (12)
N1	0.0348 (14)	0.0288 (12)	0.0236 (11)	0.0020 (10)	0.0078 (11)	0.0023 (10)
N3	0.0409 (17)	0.0394 (16)	0.0255 (13)	−0.0030 (13)	0.0087 (13)	−0.0003 (12)
N4	0.0449 (18)	0.0308 (15)	0.0293 (15)	0.0008 (13)	0.0089 (14)	0.0015 (12)
O2	0.0585 (15)	0.0284 (11)	0.0447 (13)	0.0004 (10)	0.0212 (12)	−0.0026 (10)
O3	0.0710 (17)	0.0340 (12)	0.0370 (12)	−0.0047 (12)	0.0189 (12)	−0.0112 (10)
O4	0.0606 (15)	0.0428 (13)	0.0230 (11)	0.0044 (11)	0.0100 (11)	−0.0014 (10)

Geometric parameters (Å, º)

Ag1—N1	2.134 (2)	C2—O4	1.223 (4)
Ag1—N4	2.123 (3)	C2—O3	1.294 (4)
Ag1—O4	2.628 (2)	C3—C4	1.487 (4)
Ag2—N2	2.132 (2)	C4—O2	1.287 (4)
Ag2—N3	2.133 (3)	C5—N1	1.338 (4)
Ag2—O1	2.607 (2)	C5—H1	0.87 (4)
Ag1—Ag1^{i}	2.9916 (5)	N3—H3	0.92 (4)
Ag1—Ag2^{ii}	3.0021 (4)	N3—H4	0.93 (4)
O1—C4	1.228 (4)	N3—H5	0.90 (4)
N2—C5	1.325 (4)	N4—H6	0.87 (4)
N2—C3	1.377 (4)	N4—H7	0.87 (4)
C1—N1	1.371 (4)	N4—H8	0.77 (5)
C1—C3	1.373 (4)	O2—H2	1.19 (8)
C1—C2	1.481 (4)	O3—H2	1.26 (8)
N2—Ag2—N3	177.40 (11)	C1—C3—C4	132.2 (3)
N2—Ag2—O1	71.12 (8)	N2—C3—C4	120.0 (2)
N3—Ag2—O1	111.27 (10)	O1—C4—O2	123.4 (3)
N2—Ag2—Ag1^{iii}	96.10 (7)	O1—C4—C3	119.5 (3)
N3—Ag2—Ag1^{iii}	82.35 (9)	O2—C4—C3	117.1 (3)
O1—Ag2—Ag1^{iii}	104.71 (6)	N2—C5—N1	114.1 (3)
C4—O1—Ag2	109.3 (2)	N2—C5—H1	127 (2)
C5—N2—C3	105.0 (2)	N1—C5—H1	119 (2)
C5—N2—Ag2	135.2 (2)	C5—N1—C1	104.3 (2)
C3—N2—Ag2	119.74 (19)	C5—N1—Ag1	134.8 (2)
N4—Ag1—N1	173.75 (11)	C1—N1—Ag1	120.49 (18)
N4—Ag1—O4	115.67 (10)	Ag2—N3—H3	114 (3)
N1—Ag1—O4	70.43 (8)	Ag2—N3—H4	109 (2)
N4—Ag1—Ag1^{i}	99.91 (10)	H3—N3—H4	101 (3)
N1—Ag1—Ag1^{i}	76.36 (7)	Ag2—N3—H5	109 (2)
O4—Ag1—Ag1^{i}	106.67 (5)	H3—N3—H5	112 (3)
N4—Ag1—Ag2^{ii}	82.99 (10)	H4—N3—H5	111 (3)
N1—Ag1—Ag2^{ii}	99.09 (7)	Ag1—N4—H6	115 (3)

O4—Ag1—Ag2^{ii}	87.07 (6)	Ag1—N4—H7	111 (3)
Ag1^{i}—Ag1—Ag2^{ii}	162.610 (12)	H6—N4—H7	111 (4)
N1—C1—C3	108.8 (2)	Ag1—N4—H8	112 (4)
N1—C1—C2	119.1 (2)	H6—N4—H8	103 (4)
C3—C1—C2	132.0 (3)	H7—N4—H8	104 (4)
O4—C2—O3	122.5 (3)	C4—O2—H2	113 (3)
O4—C2—C1	120.6 (3)	C2—O3—H2	113 (3)
O3—C2—C1	116.9 (3)	C2—O4—Ag1	108.15 (19)
C1—C3—N2	107.8 (2)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2···O3	1.19 (8)	1.26 (8)	2.448 (3)	172 (6)