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μ-Ethylenediamine-κ^2N:N'-bis[(quinoline-2-carboxylato-κ^2N,O)silver(I)] tetrahydrate

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.075
Data-to-parameter ratio = 15.9

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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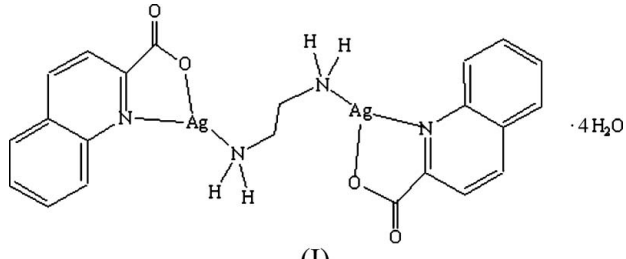
In the title compound, $[Ag_2(C_{10}H_6NO_2)_2(C_2H_8N_2)]\cdot 4H_2O$, each Ag^I atom is three-coordinated by one N atom and one O atom from one quinoline-2-carboxylate anion, and by one N atom from one ethylenediamine ligand. The dinuclear molecule is centrosymmetric. A three-dimensional supramolecular structure is formed through hydrogen-bonding and π–π interactions.

Comment

The construction of metal–organic supramolecular architectures based on hydrogen-bonding and/or π–π interactions is attractive due to their intriguing structural topologies and their special properties for potential practical application as functional materials (Meyer *et al.*, 2003; Hagrman *et al.*, 1999; Hartshorn & Steel, 1998). Many ligands containing N- or O-donors, such as 2,2′-bipyridyl-4,4′-dicarboxylic acid, 1,10-phenanthroline and 4,4-bipyridine, have been widely applied in the construction of supramolecular metal–organic compounds (Noro *et al.*, 2002; Liu *et al.*, 2002; Wan *et al.*, 2003). In these compounds, hydrogen-bonding interactions and aromatic π–π stacking interactions are frequently present and these are very important in forming multi-dimensional structures from low-dimensional ones. Quinoline-2-carboxylic acid, which consists of an N-containing aromatic ring and a carboxylate group, is also a good ligand to form hydrogen-bonding and π–π interactions (Dobrzyńska & Jerzykiewicz, 2004; Dobrzyńska *et al.*, 2005; Okabe & Muranishi, 2003). Here, we describe the supramolecular structure of the title silver(I) complex with this ligand, (I).



(I)

The structural unit of (I) contains a discrete centrosymmetric $[Ag_2(C_{10}H_6N_1O_2)_2(C_2H_8N_2)]$ unit and four uncoordinated water molecules (Fig. 1). In this unit, there are two crystallographically equivalent Ag^I atoms. Each Ag^I atom is three-coordinated with an N_2O donor set, in which one N atom (N1) and one O atom (O1) are from one quinoline-2-carboxylate anion, and the remaining N atom (N2) is from the ethylenediamine ligand. Two quinoline-2-carboxylate anions

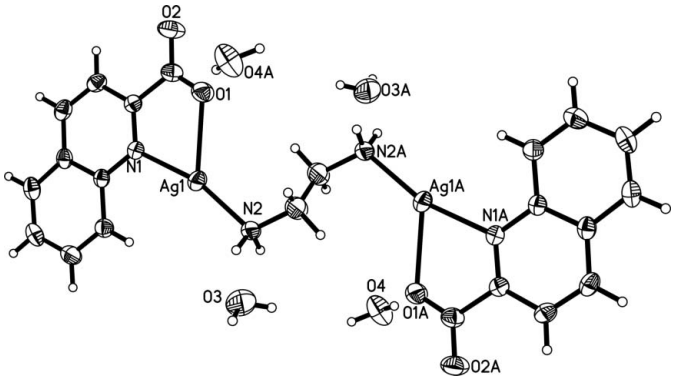


Figure 1
The structure of compound (I). Displacement ellipsoids are drawn at the 30% level. [Symmetry code: (A) $-x+1, -y+1, -z+1$.]

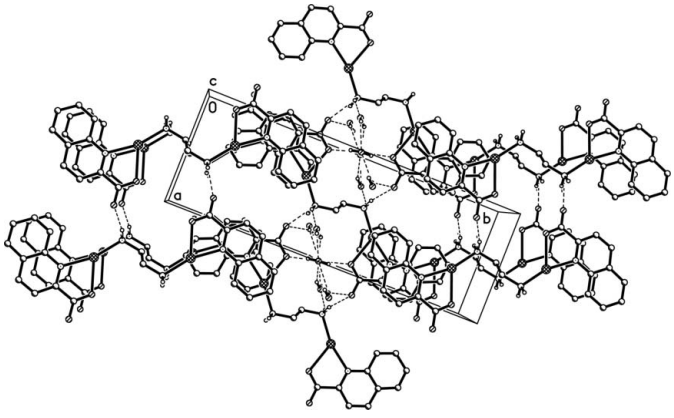


Figure 2
A packing diagram for (I), viewed down the *c* axis, showing the hydrogen-bonding interactions as dashed lines. H atoms not involved in hydrogen bonding have been omitted.

bind to two Ag atoms in a chelating mode and one ethylenediamine ligand bridges the two Ag atoms, forming the $[Ag_2(C_{10}H_6N_1O_2)_2(C_2H_8N_2)]$ unit. The ligand–Ag distances for the quinaldinate group are 2.439 (3) Å for Ag—O and 2.210 (2) Å for Ag—N. The Ag—N distance for the ethylenediamine ligand is 2.154 (3) Å, which is close to those reported for three-coordinate silver (Whitcomb & Rogers, 1997). The angles around the Ag atom are in the range 71.51 (9)–164.04 (10)°.

The molecules of compound (I) are interconnected by extensive hydrogen-bonding interactions (Fig. 2). Adjacent quinoline-2-carboxylate ligands are connected through hydrogen-bonding interactions with water molecules (Table 1), and neighbouring molecules of the complex interact with each other *via* the uncoordinated O atoms of the carboxyl group and the N atoms of the ethylenediamine ligand. There are also π–π stacking interactions between the aromatic rings. The distances between neighbouring parallel quinolinyl rings are 3.3883 and 3.3792 Å, respectively, which indicate a strong edge-to-face offset π–π stacking interaction (Janiak, 2000). These hydrogen-bonding and π–π stacking interactions play important roles in the formation of a multi-dimensional framework, and in compound (I), it is the existence of hydrogen-bonding and π–π stacking interactions that leads to the formation of a three-dimensional supramolecular architecture.

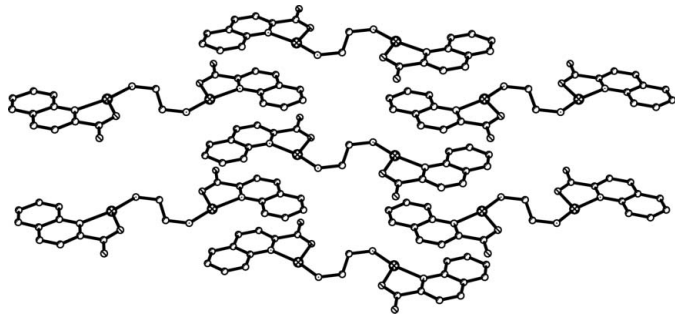


Figure 3
A packing diagram for (I), showing π–π stacking interactions. H atoms have been omitted.

Experimental

Quinoline-2-carboxylic acid was used as received from a commercial source (Aldrich) without further purification. Quinoline-2-carboxylic acid (0.173 g, 1 mmol) was added to water (10 ml) and the resulting solution was adjusted to pH 7.0 using aqueous ethylenediamine solution. $Ag(NO_3)$ (0.170 g, 1 mmol) was then added to this solution and the mixture was stirred for 10 min and then filtered. After two days, colourless single crystals of (I) suitable for X-ray analysis were obtained. Analysis, calculated for $C_{22}H_{28}Ag_2N_4O_8$: C 38.14, H 4.04, N 8.09%; found: C 38.07, H 3.99, N 8.14%.

Crystal data

$[Ag_2(C_{10}H_6NO_2)_2(C_2H_8N_2)]\cdot 4H_2O$
$M_r = 692.22$
Monoclinic, $P2_1/c$
$a = 7.9238$ (8) Å
$b = 22.405$ (2) Å
$c = 6.9939$ (7) Å
$\beta = 91.1690$ (10)°
$V = 1241.4$ (2) Å^3
$Z = 2$
$D_x = 1.852$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 1.63$ mm^{-1}
$T = 291$ (2) K
Block, colourless
0.31 × 0.13 × 0.11 mm

Data collection

Bruker APEX-2 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.633$, $T_{max} = 0.842$
10824 measured reflections
2847 independent reflections
2295 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.076$
$S = 1.04$
2847 reflections
179 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0219P)^2 + 1.8051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.98$ e Å^{-3}
$\Delta\rho_{min} = -0.71$ e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O3	0.90	2.25	3.063 (5)	150
N2—H2B···O2^{i}	0.90	2.08	2.957 (4)	165
O3—H2W···O4^{ii}	0.853 (10)	2.02 (2)	2.811 (6)	154 (4)
O4—H3W···O1^{i}	0.854 (10)	1.969 (19)	2.808 (5)	167 (7)
O4—H3W···O2^{i}	0.854 (10)	2.72 (4)	3.416 (5)	139 (6)
O4—H4W···O1^{iii}	0.853 (10)	1.999 (19)	2.840 (5)	169 (6)
O3—H1W···O2^{iv}	0.851 (10)	2.51 (5)	3.141 (6)	132 (6)
O3—H1W···O4^{v}	0.851 (10)	2.40 (4)	3.043 (6)	133 (4)

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

The H atoms of the water molecules were located in a difference Fourier map and refined freely. The other H atoms were included in calculated positions using the riding method, with N—H = 0.90 Å and C—H = 0.93–0.97 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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