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Key indicators

Single-crystal X-ray study
 $T = 294$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
 R factor = 0.037
 wR factor = 0.096
Data-to-parameter ratio = 14.8

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

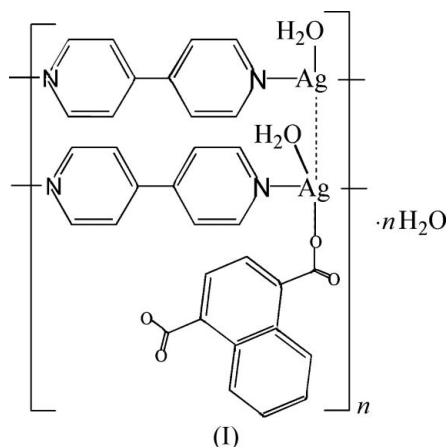
catena-Poly[aquasilver(I)- μ -4,4'-bipyridine] catena-poly[[aqua(naphthalene-1,4-dicarboxylato)- silver(I)]- μ -4,4'-bipyridine] polyhydrate

The title complex, $\{[\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})][\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_{12}\text{H}_6\text{O}_4)(\text{H}_2\text{O})]\cdot\text{H}_2\text{O}\}_n$, consists of cationic complex chains, anionic complex chains and solvent water molecules. In the cationic chain, the Ag atom adopts a trigonal coordination geometry, while the Ag atom in the anionic chain assumes a square-planar coordination geometry.

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Comment

The photoluminescent property of polynuclear d^{10} metal complexes has attracted extensive interest (Chen & Liu, 2002). Recently, a series of polynuclear d^{10} metal complexes with 1,4-benzenedicarboxylates has been investigated (Yaghi *et al.*, 2003). We present here the structure of a similar Ag^{I} complex, (I), incorporating the naphthalenedicarboxylate (NDC) ligand (Vodak *et al.*, 2001).



The structure of (I) consists of 4,4'-bipyridine-bridged cationic complex chains, anionic complex chains and solvent water molecules. A segment of the polymeric structure of (I) is shown in Fig. 1. Within the cationic chain, atom Ag1 adopts a distorted trigonal coordination geometry, defined by two N donors from two 4,4'-bipyridine ligands and one water molecule, while in the anionic chain, atom Ag2 has a distorted square-planar coordination geometry, formed by two N donors from two 4,4'-bipyridine ligands, one water molecule and one O atom of the NDC ligand.

The $\text{Ag1}-\text{O2W}$, $\text{Ag2}-\text{O3}$ and $\text{Ag2}-\text{O3W}$ distances (Table 1) are much shorter than the sum of the van der Waals radii and imply a bonding interaction between the Ag and O atoms, but these bonding interactions are weak, because the bond distances are much longer than the sum of the covalent radii (Ma *et al.*, 2005). The average $\text{Ag}-\text{N}$ bond distance of 2.164 (2) Å agrees with that found in a reported Ag^{I} complex with 4,4'-bipyridine (Sun *et al.*, 2003).

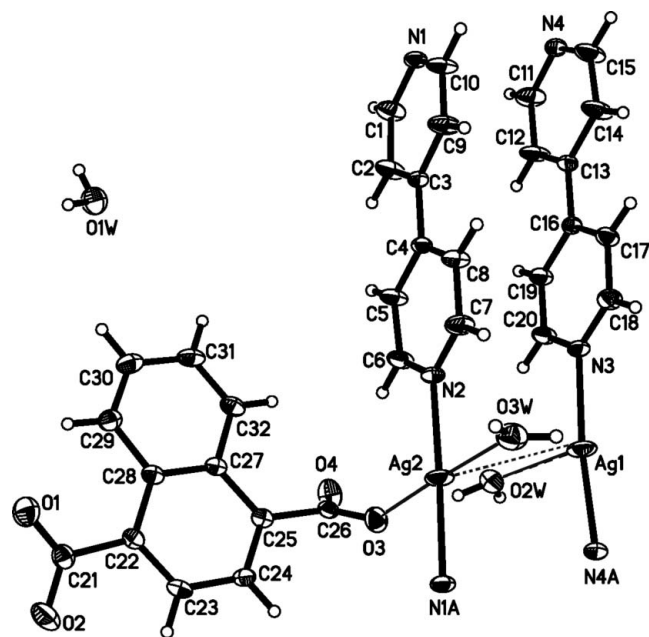


Figure 1

A segment of the polymeric Ag^{I} complex chains, with 50% probability displacement ellipsoids (arbitrary spheres for H atoms) [symmetry code: (A) $x, -1 + y, z$]. The dashed line indicates the weak van der Waals interaction between Ag atoms of neighbouring chains.

The nearest $\text{Ag}1 \cdots \text{Ag}2$ separation between neighbouring polymeric chains is 3.3978 (8) Å, which is identical to the sum of the van der Waals radii of Ag atoms and implies a weak interaction between the Ag atoms of neighbouring chains. The centroid-to-centroid separations of 3.548 (2) Å between parallel N2-pyridine and N2($-x, 1 - y, 1 - z$)-pyridine rings, and 3.559 (2) Å between nearly parallel N2-pyridine and N3-pyridine rings, suggest the existence of π - π stacking. Extensive hydrogen bonding occurs in the crystal structure of (I) (Table 2).

Experimental

A mixture of AgNO_3 (0.170 g, 1 mmol), H_2NDC (0.108 g, 0.5 mmol) and NaOH (0.04 g, 1 mmol) in water (10 ml) was stirred for 10 min at room temperature. 4,4'-Bipyridine (0.090 g, 0.5 mmol) was then added to the mixture. After stirring for a further 10 min, a white precipitate was collected and dissolved in 14 M ammonia (10 ml). Single crystals of (I) were obtained by slow evaporation at room temperature (yield 55%, based on Ag). Analysis, calculated for $\text{C}_{32}\text{H}_{28}\text{Ag}_2\text{N}_4\text{O}_7$: C 48.22, H 3.52, N 7.03%; found: C 48.35, H 3.44, N 7.18%.

Crystal data

$[\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{H}_2\text{O})][\text{Ag}(\text{C}_{10}\text{H}_8\text{N}_2)(\text{C}_{12}\text{H}_6\text{O}_4)(\text{H}_2\text{O})] \cdot \text{H}_2\text{O}$
 $M_r = 796.32$
 Triclinic, $P\bar{1}$
 $a = 9.5977$ (19) Å
 $b = 11.444$ (2) Å
 $c = 14.018$ (3) Å
 $\alpha = 78.50$ (3)°
 $\beta = 71.77$ (3)°
 $\gamma = 86.82$ (3)°
 $V = 1433.0$ (6) Å³

$Z = 2$
 $D_x = 1.846$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 10623 reflections
 $\theta = 3.1$ – 27.4 °
 $\mu = 1.43$ mm⁻¹
 $T = 294$ (2) K
 Block, colourless
 $0.50 \times 0.33 \times 0.24$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.506$, $T_{\text{max}} = 0.710$
 13653 measured reflections

6361 independent reflections
 4888 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$
 $\theta_{\text{max}} = 27.4$ °
 $h = -12 \rightarrow 11$
 $k = -14 \rightarrow 14$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.096$
 $S = 1.10$
 6361 reflections
 430 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0401P)^2 + 0.6543P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 1.19$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.97$ e Å⁻³

Table 1

Selected geometric parameters (Å).

Ag1–N3	2.165 (2)	Ag2–N2	2.166 (2)
Ag1–N4 ⁱ	2.163 (2)	Ag2–O3	2.826 (3)
Ag1–O2W	2.696 (3)	Ag2–O3W	2.831 (3)
Ag2–N1 ⁱ	2.163 (2)		

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W–HW11 \cdots O1 ⁱⁱ	0.86 (5)	2.14 (5)	2.904 (4)	148 (4)
O1W–HW12 \cdots O2 ⁱⁱⁱ	0.79 (4)	2.03 (4)	2.790 (5)	162 (4)
O2W–HW21 \cdots O3	0.82 (4)	2.02 (5)	2.825 (4)	170 (4)
O2W–HW22 \cdots O1W ^{iv}	0.82 (4)	2.09 (4)	2.900 (5)	171 (4)
O3W–HW31 \cdots O4 ^v	0.84 (6)	1.99 (6)	2.812 (4)	163 (6)
O3W–HW32 \cdots O1W ^{vi}	0.82 (4)	2.03 (4)	2.831 (5)	166 (4)

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

H atoms on C atoms were positioned geometrically and refined as riding atoms, with $C-H = 0.93$ Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Water H atoms were located in a difference Fourier map and refined isotropically. The highest peak in the difference map is 0.89 Å away from atom Ag1.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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