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catena-Poly[bis[silver(I)-μ_2-4,4′-bipyridine-κ^2N:N'] naphthalene-2,6-dicarboxylate tetrahydrate]: self-assembly of a supramolecular framework *via* coordination bonds and supramolecular interactions

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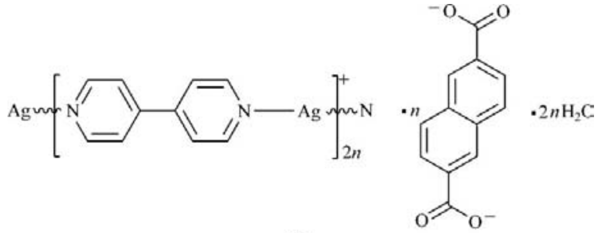
The ultrasonic reaction of $AgNO_3$, 4,4′-bipyridine (bipy) and naphthalene-2,6-dicarboxylic acid (H_2NDC) gives rise to the title compound, $\{[Ag_2(C_{10}H_8N_2)_2](C_{12}H_6O_4)\cdot 4H_2O\}_n$. The NDC dianion is located on an inversion centre. The Ag^I centre is coordinated in a linear manner by two N atoms from two bipy ligands. The crystal structure consists of one-dimensional Ag^I–bipy cationic chains and two-dimensional NDC–H_2O anionic sheets, constructed by coordination bonds and supramolecular interactions, respectively.

Comment

Interest in crystal engineering and supramolecular chemistry is rapidly increasing due to the diverse and aesthetic structural topologies of the resulting compounds and their potential use in optical, electrical, catalytic and adsorptive applications as functional solid materials (Blake, Brooks *et al.*, 1999; Blake, Champness *et al.*, 1999; Blake *et al.*, 1997; Evans & Lin, 2002; Kitagawa *et al.*, 2004; Yaghi *et al.*, 2003; Applegarth *et al.*, 2005). In the past few years, the development of supramolecular self-assembly has allowed the possibility of the rational design and preparation of supramolecular architectures through noncovalent interactions, in which it is crucial to meet both geometric and energetic considerations (Pedireddi *et al.*, 1996). Doubtless, the hydrogen bond is the most familiar secondary force in supramolecular assembly, since it is a moderately directional intermolecular interaction that may control molecular packing (Kolotuchin *et al.*, 1995; Zartilas *et al.*, 2007), and many reports have focused on studies of the hydrogen bond (Li *et al.*, 2006; Sun *et al.*, 2003; Lough *et al.*, 2000; Massoud & Langer, 2009). Compared with the hydrogen bond, C—H$\cdots\pi$ and π–π interactions have been somewhat less well covered (Blake *et al.*, 2000; Goodgame *et al.*, 2002). 4,4′-Bipyridine (bipy) and its analogues are neutral linear ligands widely used as spacers in the construction of novel supramolecular compounds incorporating diverse supramolecular interactions (Wang & Englert, 2007; Withersby *et al.*, 1997). Recently, we have undertaken a series of investigations into the assembly of Ag^I cations with different angular and linear bipodal N-donor ligands, such as aminopyrimidine and aminopyrazine (Luo, Huang, Chen *et al.*, 2008; Luo, Huang, Zhang *et al.*, 2008; Luo *et al.*, 2009; Sun, Luo, Huang *et al.*, 2009; Sun, Luo, Xu *et al.*, 2009; Sun, Luo, Zhang *et al.*, 2009), with the principal aim of obtaining supramolecular compounds or multifunctional coordination polymers. In an attempt to exploit Ag–bipy/dicarboxylates under ammoniacal conditions, we successfully synthesized the title supramolecular coordination polymer, (I).



(I)

The asymmetric unit of (I) contains one Ag^I cation, one-half of a naphthalene-2,6-dicarboxylate (NDC) dianion located on an inversion centre, one bipy ligand and two water molecules. The coordination geometry of the Ag^I cation is nearly linear

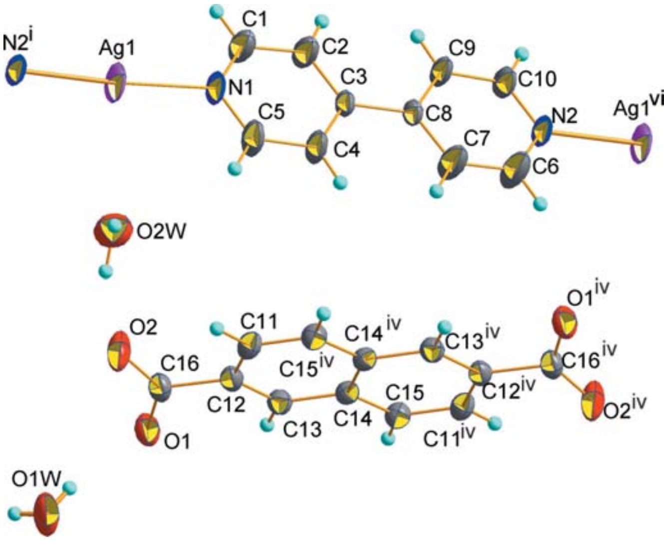


Figure 1
The structure of (I), showing the atom-numbering scheme and the coordination environment around the Ag^I centre. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. [Symmetry codes: (i) $x, y, z-1$; (iv) $-x+1, -y, -z+2$; (vi) $x, y, z+1$.]

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[N—Ag—N = 176.00 (7)°] and each Ag$^{\rm I}$ cation is coordinated by N atoms from two different bipy ligands (Fig. 1). The Ag—N bond lengths (Table 1) are comparable with those in related compounds (Turner *et al.*, 2005; Oxtoby *et al.*, 2002; Fan *et al.*, 2007). There are also weak Ag$\cdots$O$_{\rm water}$ interactions, with Ag$\cdots$O distances in the range 2.797 (2)–3.173 (3) Å, which are a little longer but still fall in the secondary bonding range (the sum of the van der Waals radii of Ag and O is 3.24 Å; Pan *et al.*, 2003). The bipy ligands have a nontwisted nearly planar conformation, with a dihedral angle between the two pyridyl rings of 3.45 (16)°, and act as *N,N′*-bidentate ligands linking Ag$^{\rm I}$ cations into one-dimensional cationic chains. Between neighboring cationic chains, the shortest Ag$\cdots$Ag separations are 3.5592 (5) and 3.8982 (5) Å, which are longer than twice the van der Waals radius of Ag$^{\rm I}$ (3.44 Å), indicating no direct metal–metal interaction (Bondi, 1964). Weak aromatic π–π stacking interactions [$Cg1\cdots Cg2^{\rm vii}$ = 3.6808 (18) Å and $Cg1\cdots Cg2^{\rm viii}$ = 3.7586 (19) Å; *Cg*1 and *Cg*2 are the centroids of the N1/C1–C5 and N2/C6–C10 rings, respectively; symmetry codes: (vii) $-x + 1, -y + 1, -z + 2$; (viii) $-x, -y + 1, -z + 2$] also exist between the pyridyl rings of neighbouring bipy ligands (Fig. 2).

In addition, the ancillary H$_2$NDC ligand deprotonates to balance the charge and does not participate in coordinating to the Ag$^{\rm I}$ centres. Each O1*W* atom acts as a donor to two O atoms (Table 2) from two different carboxylate groups, forming centrosymmetric $R_4^4(12)$ (Bernstein *et al.*, 1995) water-bridged carboxylate rings. The NDC anions thus form a supramolecular one-dimensional anionic chain. Neighbouring anionic chains are interlinked to form a two-dimensional anionic sheet (Fig. 3) through C—H$\cdots$O and O—H$\cdots$O hydrogen bonds (Table 2).

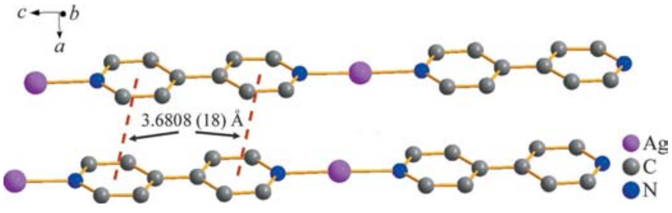

Figure 2
A ball-and-stick perspective view of the weak π–π stacking (dashed lines) between the pyridyl rings of neighbouring bipy ligands.

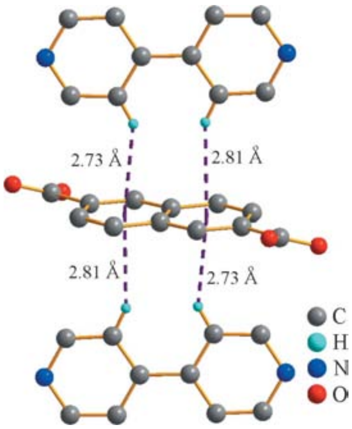

Figure 4
A ball-and-stick perspective view of the C—H$\cdots\pi$ interactions (dashed lines) between the bipy and NDC ligands.

The crystal structure features one-dimensional Ag$^{\rm I}$–bipy cationic chains and two-dimensional NDC–H$_2$O anionic sheets, constructed by coordination bonds and supramolecular interactions, respectively. To the best of our knowledge, most of the reported Ag$^{\rm I}$-containing complexes exhibiting one-dimensional chains only have one type of charge-neutral chain; however, the chains are usually not independent and are interconnected by coordination bonds (Shi *et al.*, 2000). In (I), C—H$\cdots$O intermolecular hydrogen bonds (Table 2) and C—H$\cdots\pi$ interactions are observed [C2—H2$\cdots Cg3^{\rm ix}$ = 154°, H2$\cdots Cg3^{\rm ix}$ = 2.81 Å and C2$\cdots Cg3^{\rm ix}$ = 3.671 (3) Å; C9—H9$\cdots Cg4^{\rm ix}$ = 143°, H9$\cdots Cg4^{\rm ix}$ = 2.73 Å and C9$\cdots Cg4^{\rm ix}$ = 3.521 (2) Å; *Cg*3 and *Cg*4 are the centroids of C11–C14/C14$^{\rm iv}$/C15$^{\rm iv}$ and C14/C15/C11$^{\rm iv}$/C12$^{\rm iv}$/C13$^{\rm iv}$/C14$^{\rm iv}$ rings, respectively; symmetry codes: (iv) $-x + 1, -y, -z + 2$; (ix) $x, y + 1, z$; Fig. 4], which link the one-dimensional cationic chains and two-dimensional anionic sheets into a three-dimensional supramolecular framework.

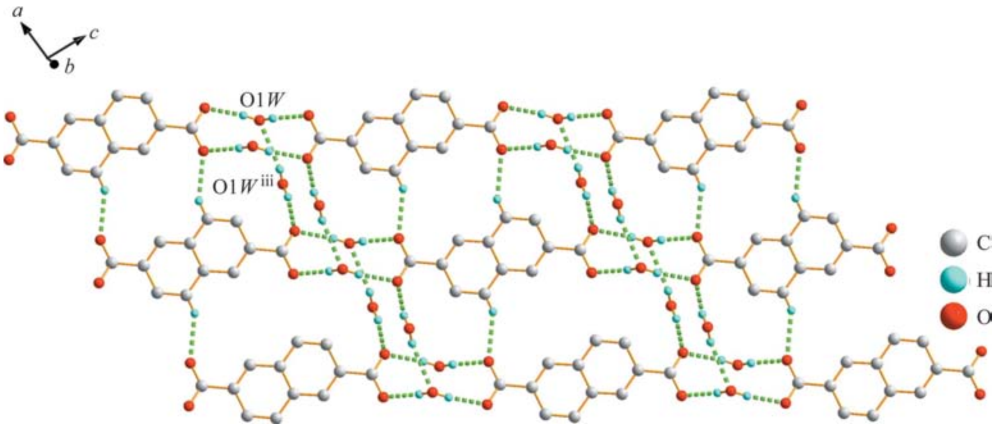

Figure 3
A ball-and-stick perspective view of the two-dimensional anionic sheet incorporating hydrogen bonds (dashed lines). [Symmetry code: (iii) $-x + 1, -y, -z + 1$.]

Experimental

All reagents and solvents were used as obtained commercially without further purification. A mixture of $AgNO_3$ (170 mg, 1 mmol), 4,4′-bipyridine (156 mg, 1 mmol) and H_2NDC (216 mg, 1mmol) were added to a methanol–water solvent mixture (12 ml, 1:2 *v*/*v*) under ultrasonic conditions, which helped to dissolve the white precipitate. An aqueous NH_3 solution (25%) was added dropwise to the mixture to give a clear solution. The formation of the products is not affected by changing the reaction mole ratio of organic ligands to metal ions. The resulting solution was left to evaporate slowly in the dark at room temperature for several weeks to give colourless block-shaped crystals of (I). The crystals were isolated using deionized water and dried in air (yield *ca* 56%, based on Ag). Analysis calculated for $C_{16}H_{15}AgN_2O_4$: C 64.21, H 5.05, N 9.36%; found: C 64.18, H. 5.09, N 9.29%.

Crystal data

$[Ag_2(C_{10}H_8N_2)_2](C_{12}H_6O_4)\cdot 4H_2O$
$M_r = 814.34$
Triclinic, $P\overline{1}$
$a = 7.1444$ (3) Å
$b = 9.6123$ (5) Å
$c = 11.4228$ (5) Å
$\alpha = 90.460$ (1)°
$\beta = 94.924$ (1)°
$\gamma = 108.783$ (2)°
$V = 739.40$ (6) Å^3
$Z = 1$
Mo *Kα* radiation
$\mu = 1.39$ mm^{-1}
$T = 298$ K
0.20 × 0.15 × 0.15 mm

Data collection

Oxford Gemini S Ultra diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2008)
$T_{min} = 0.769$, $T_{max} = 0.819$
6452 measured reflections
2894 independent reflections
2689 reflections with $I > 2\sigma(I)$
$R_{int} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.029$
$wR(F^2) = 0.078$
$S = 1.01$
2894 reflections
220 parameters
4 restraints
H-atom parameters constrained
$\Delta\rho_{max} = 0.68$ e Å^{-3}
$\Delta\rho_{min} = -0.80$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.1579 (19)	Ag1—N2^i	2.1620 (19)
N1—Ag1—N2^i	176.00 (7)		

Symmetry code: (i) *x*, *y*, *z* − 1.

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
O1*W*—H1*WA*⋯O1	0.840 (10)	1.919 (14)	2.744 (3)	167 (4)
O1*W*—H1*WB*⋯O2^{ii}	0.841 (10)	1.966 (11)	2.803 (3)	174 (4)
O2*W*—H2*WA*⋯O2	0.848 (10)	1.979 (13)	2.819 (3)	170 (4)
O2*W*—H2*WB*⋯O1*W*^{iii}	0.840 (10)	2.49 (2)	3.193 (3)	142 (3)
C5—H5⋯O1*W*^{iii}	0.93	2.56	3.312 (3)	139
C6—H6⋯O1^{iv}	0.93	2.51	3.381 (3)	155
C15—H15⋯O1^{v}	0.93	2.36	3.197 (3)	150

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

The aromatic H atoms were generated geometrically (C—H = 0.93 Å) and were allowed to ride on their parent atoms in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The positions of the water H atoms were refined with the O—H distances restrained to 0.85 (1) Å, and with $U_{iso}(H) = 1.2U_{eq}(O)$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2008); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2008); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2008); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2009).

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Supplementary data for this paper are available from the IUCr electronic archives (Reference: LG3022). Services for accessing these data are described at the back of the journal.

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