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Poly[[silver(I)-μ-4,4′-bipyridine-μ-formato] monohydrate formic acid solvate]

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Key indicators

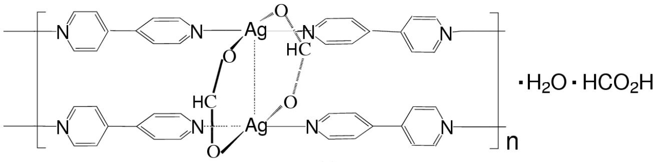
Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.010 Å
H-atom completeness 93%
Disorder in solvent or counterion
R factor = 0.070
wR factor = 0.136
Data-to-parameter ratio = 11.3

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

The reaction of silver formate with HCO_2H and 4,4′-bipyridine in CH_3CN produced the title compound, $[Ag(CHO_2)(C_{10}H_8N_2)]\cdot H_2O\cdot CH_2O_2$. In the structure, each 4,4′-bipyridine moiety acts as a bidentate ligand that binds two Ag atoms, thus forming a linear chain. The formate ions bridge the adjacent chains through Ag—O bonds [Ag—O = 2.709 (6)–3.089 (5) Å] to form molecular ladders. The molecular ladders are stacked into layers and are interconnected by O—H···O hydrogen bonds.

Comment

A large number of silver salts furnish polydimensional supramolecular compounds by the direct reaction of these salts with symmetrically bridging ligands (Batten & Robson, 1998; Hagrman *et al.*, 1999; Tong, Zheng & Chen, 2000), and some of the anionic groups themselves are also able to function as a bridge (Bertelli *et al.*, 1997; Tong *et al.*, 1999; Tong, Chen & Ng, 2000; Robinson & Zaworotko, 1995; Sharma *et al.*, 1998; Yaghi & Li, 1996). The carboxylate system has also been well explored, except for the formate homolog. However, only a few complexes containing metal/formate/4,4′-bipyridine have been reported so far. We report here the structure of the title silver–4,4′-bipyridine–formate complex, (I).



(I)

In (I), each Ag atom adopts a distorted square-planar coordination, a geometry that is relatively uncommon (Lippert & Neuggebauer, 1982; Villanneau *et al.*, 1998; Tong, Chen & Ng, 2000). Each Ag atom is bonded to two symmetry-related 4,4′-bipyridine units [Ag—N = 2.167 (5) Å], with the donor ends of the ligand occupying *trans* positions of the square [N—Ag—N = 168.1 (2)°], thus generating linear chains. In adjacent chains, two neighboring Ag atoms are bridged by two formate ions through Ag—O coordination, resulting in the formation of a molecular ladder. The Ag—O distances lie in the range 2.709 (6)–3.089 (5) Å (Table 1) and are much longer than those of dinuclear Ag–carboxylate complexes (Bowmaker *et al.*, 2000; Chen & Mak, 1991; Huang *et al.*, 1991). The Ag atoms are also linked by formate-supported Ag—Ag interactions with a separation of 3.1748 (14) Å, which is similar to those found in dinuclear Ag^I–carboxylate complexes (Chen & Mak, 1991; Huang *et al.*, 1991). The

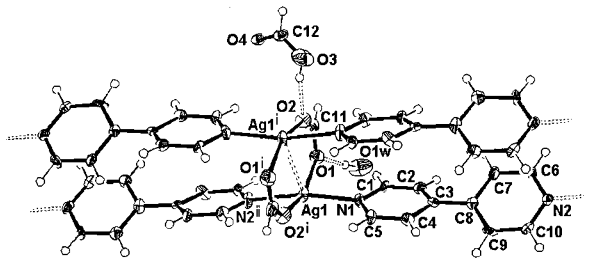


Figure 1
A part of the polymeric chain, illustrating the coordination environment of the Ag atom in (I). Displacement ellipsoids are shown at the 50% probability level. Only one component of the disordered formic acid molecule is shown. H atoms are drawn as small spheres of arbitrary radii. [Symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}-y, 1-z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, z-\frac{1}{2}$.]

geometry of the HCO_2^- and bipyridine ligands agrees with those observed in other systems (Manson *et al.*, 2001; Han *et al.*, 2000).

The molecular ladders are stacked into layers, which are further interconnected by hydrogen-bonding networks formed by formic acid and water molecules, resulting in a three-dimensional network (Table 2).

Experimental

To a suspension of silver formate (0.046 g, 0.2 mmol) in acetonitrile (2 ml) was added formic acid (0.042 g, 0.8 mmol) to furnish a clear solution. To this solution was added 4,4′-bipyridine (0.063 g, 0.4 mmol) in the same solvent (2 ml). The precipitate that formed was removed by filtration; the filtrate, when set aside at room temperature, afforded colorless prism-shaped crystals, which were collected by filtration, washed with methanol and diethyl ether, and dried in a vacuum. Yield 0.050 g, 64.2%.

Crystal data

$[Ag(CHO_2)(C_{10}H_8N_2)]\cdot H_2O\cdot CH_2O_2$
$M_r = 373.11$
Monoclinic, $C2/c$
$a = 17.848\ (4)$ Å
$b = 16.863\ (3)$ Å
$c = 9.485\ (3)$ Å
$\beta = 108.79\ (1)°$
$V = 2702.6\ (12)$ Å^3
$Z = 8$
$D_x = 1.834$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3186 reflections
$\theta = 3.1$–$27.5°$
$\mu = 1.51$ mm^{-1}
$T = 193\ (2)$ K
Prism, colorless
0.35 × 0.18 × 0.06 mm

Data collection

Rigaku Mercury area-detector diffractometer
ω scans
Absorption correction: multi-scan (Blessing, 1995; Jacobson, 1998)
$T_{min} = 0.784$, $T_{max} = 0.915$
8855 measured reflections
2365 independent reflections
2176 reflections with $I > 2\sigma(I)$
$R_{int} = 0.054$
$\theta_{max} = 25.0°$
$h = -21 \rightarrow 21$
$k = -16 \rightarrow 20$
$l = -11 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.070$
$wR(F^2) = 0.136$
$S = 1.37$
2365 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 20.891P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.53$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.167 (5)	Ag1—O2^i	3.089 (5)
Ag1—O1	2.709 (6)	Ag1—Ag1^i	3.1748 (14)
Ag1—O2	2.809 (5)		
N2^{ii}—Ag1—N1	168.1 (2)	N2^{ii}—Ag1—O2^i	88.47 (18)
N2^{ii}—Ag1—O1	91.2 (2)	N1—Ag1—O2^i	87.80 (18)
N1—Ag1—O1	95.83 (19)	O1—Ag1—O2^i	162.27 (16)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3O···O2	0.84	1.75	2.57 (2)	167
O3′—H3O′···O2	0.84	1.70	2.52 (3)	163
O1W—H1W1···O1	0.83	1.93	2.74 (1)	166

The formic acid molecule is disordered over two positions with populations of 50% each. The disordered atoms were anisotropically refined with their U_{ij} components approximated to isotropic behavior and with suitable restraints for C—O distances. Only one of the H atoms of the water molecule was located in a difference map, and this atom was allowed to ride on the parent atom with the O—H distance fixed at 0.83 Å. All other H atoms were placed at calculated positions (O—H = 0.84 Å and C—H = 0.95 Å) and were included in the refinement in the riding-model approximation with $U_{iso}(H) = 1.2U_{eq}(C,O)$. The final difference Fourier map had a peak larger than 1 e Å^{-3} at about 1 Å from atom Ag1.

Data collection: *CrystalClear* (Rigaku/MSC, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2003); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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