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catena-Poly[bis[silver(I)-μ-4,4′-bipyridine-κ^2N:N'] hexafluorosilicate dihydrate ethylene glycol disolvate]

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Key indicators

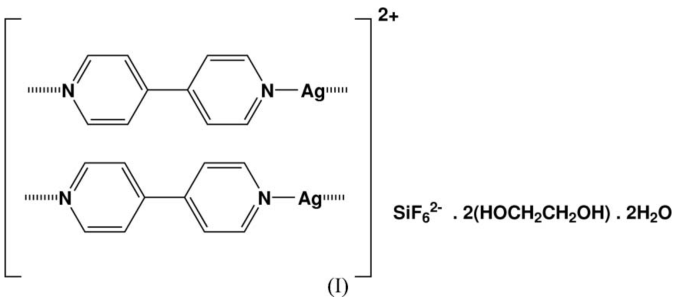
Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.016 Å
R factor = 0.042
wR factor = 0.093
Data-to-parameter ratio = 18.1

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

The structure of the title compound, $\{[Ag(C_{10}H_8N_2)]_2(SiF_6)\cdot 2H_2O\cdot 2C_2H_6O_2\}_n$, consists of two independent polymeric cationic chains containing Ag^I ions bridged by 4,4′-bipyridine ligands, hexafluorosilicate anions and cocrystallized ethylene glycol and water molecules. The Ag^I ion adopts a linear coordination geometry involving the N-donor ligands. A weak Ag⋯Ag interaction is observed, resulting in the formation of a double-chain structure. The hexafluorosilicate anions and the solvent molecules are linked by O—H⋯F, O—H⋯O and C—H⋯F hydrogen bonds to form a sheet-like structure parallel to the *bc* plane. The double $\{[Ag(4,4'\text{-bpy})]^+\}_n$ chains are linked to this two-dimensional network by C—H⋯O and C—H⋯F hydrogen bonds, forming a three-dimensional network.

Comment

The topologies and properties of polymeric silver complexes continue to attract considerable interest. It has been observed that the presence of Ag⋯Ag interactions is an important factor contributing to properties such as luminescence (Valencia *et al.*, 2005; Yeh *et al.*, 2005; Sun *et al.*, 2002). The reaction of $AgBF_4$ with 4,4′-bpy (4,4′-bpy is 4,4′-bipyridine) in water and/or acetonitrile has been shown to form three different crystal structures, all linear polymers (Carlucci *et al.*, 2002; Kokunov *et al.*, 2004; Blake *et al.*, 2000). We repeated this reaction in the presence of $(NH_4)_2SiF_6$ and obtained the title compound, (I).



(I)

In compound (I), two crystallographically nonequivalent Ag^I ions are each coordinated by two 4,4′-bpy ligands, resulting in the formation of parallel linear chains running along the *b* axis (Fig. 1). The Ag—N distances are in the range 2.113 (7)–2.159 (9) Å (Table 1) and agree with the average value of 2.14 Å found in other [Ag(4,4′-bpy)] systems (Wang *et al.*, 2004; Kokunov *et al.*, 2003, 2004; Sun *et al.*, 2003; Carlucci *et al.*, 2002; Blake *et al.*, 2000; Yaghi & Li, 1996). In the 4,4′-bpy ligands, the pyridine rings are twisted with respect to one

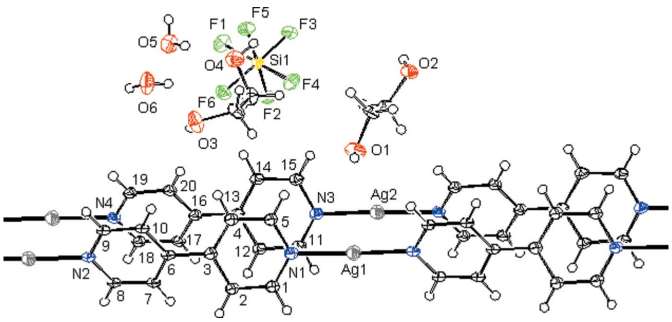


Figure 1
Part of the polymeric structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

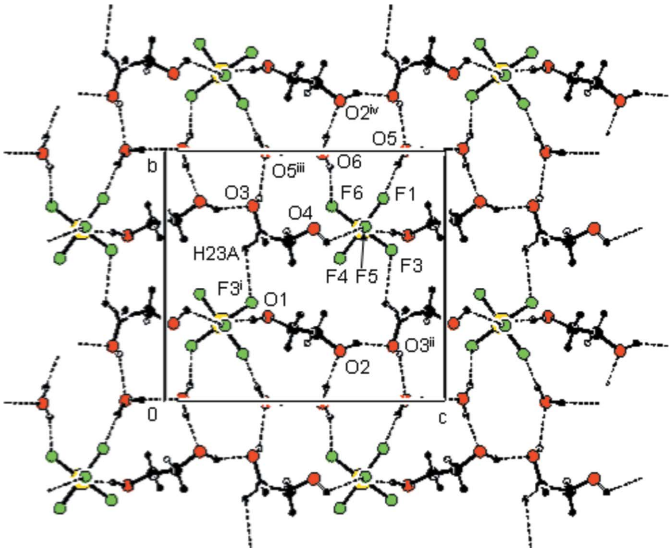


Figure 2
A view of the hydrogen-bonded two-dimensional network in (I), involving the SF_6^{2-} anions and solvent molecules. Hydrogen bonds are shown as dashed lines. Symmetry codes are as in Table 2.

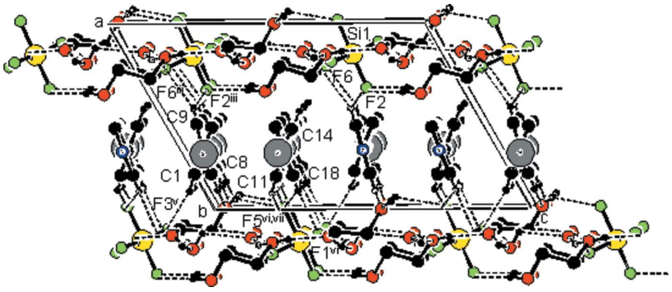


Figure 3
A crystal packing diagram for (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. Symmetry codes are as in Table 2.

another. The dihedral angle between the C1–C5/N1 and C6–C10/N2 rings is 36.7 (6)°, and that between the C11–C15/N3 and C16–C20/N4 rings is 39.3 (6)°.

A weak Ag···Ag interaction [Ag1···Ag2 3.4173 (9) Å] connects the chains, to form a double-chain structure. This contact distance is slightly shorter than twice the van der Waals radius of silver (1.72 Å; Spek, 2003), and slightly longer than the Ag···Ag distances (3.295 and 3.312 Å) found in the double-chain structure reported previously by Kokunov *et al.* (2004). A weak π–π stacking interaction is also observed between the 4,4′-bpy ligands in the double chain, the centroid–centroid distance between the approximately parallel pyridine rings (C6–C10/N2 and C16–C20/N4) being 3.656 (7) Å.

In the crystal structure of (I), the hexafluorosilicate anions and the solvent molecules form an extended two-dimensional hydrogen-bonding network parallel to the *bc* plane (Fig. 2 and Table 2). Four F atoms of the anion act as acceptors in strong O—H···F hydrogen bonds, while the water and ethylene glycol molecules act as both donor and acceptor in strong O—H···F and O—H···O hydrogen bonds. In addition, the $\{[Ag(4,4'\text{-bpy})]^+\}_n$ chains are linked to this two-dimensional network by C—H···O and C—H···F hydrogen bonds, resulting in the formation of a three-dimensional network (Fig. 3).

Experimental

Compound (I) was prepared by layering an ethylene glycol solution (5 ml) of 4,4′-bipyridine (1 mmol) with a water–ethylene glycol solution (1:3, 5 ml) of $AgBF_4$ (0.5 mmol) and $(NH_4)_2SiF_6$ (0.5 mmol) at room temperature. After two weeks, colourless needle-like crystals, suitable for X-ray analysis, appeared at the interface of the two solutions. Elemental analysis: calculated for $C_{24}H_{32}Ag_2O_6SiF_6N_4$: C 34.71, H 3.86, N 6.75%; found: C 34.66, H 4.03, N 6.62%. A thermogravimetric analysis performed in a nitrogen gas flow (150 ml min^{-1}) over the temperature range 298–523 K using aluminium crucibles gave the loss of two water molecules between 324 and 363 K (calculated: 4.34; found: 4.41%), two ethylene glycol molecules between 283 and 425 K (calculated: 14.94; found: 15.07%), and a silicon tetrafluoride molecule between 433 and 463 K (calculated: 12.54; found: 12.58%).

Crystal data

$[Ag(C_{10}H_8N_2)]_2(SiF_6)\cdot 2H_2O\cdot 2C_2H_6O_2$
M_r = 830.37
Monoclinic, *Pc*
a = 9.8887 (8) Å
b = 11.3492 (6) Å
c = 14.6304 (12) Å
β = 119.701 (9)°
V = 1426.2 (2) Å^3
Z = 2
D_x = 1.934 Mg m^{-3}
Mo *Kα* radiation
μ = 1.50 mm^{-1}
T = 153 (2) K
Needle, colourless
0.50 × 0.10 × 0.05 mm

Data collection

Stoe IPDS diffractometer
ω scans
Absorption correction: refined from ΔF (*PLATON*; Spek, 2003)
T_{min} = 0.252, T_{max} = 0.928
10905 measured reflections
5161 independent reflections
3559 reflections with $I > 2\sigma(I)$
R_{int} = 0.073
θ_{max} = 25.9°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.093
S = 0.84
5161 reflections
285 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0419P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.96 e Å^{-3}
Absolute structure: Flack (1983), with 2401 Friedel pairs
Flack parameter: 0.36 (6)

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Table 1
Selected geometric parameters (Å, °).

Ag1—N1	2.141 (9)	Ag2—N3	2.159 (9)
Ag1—N2^{i}	2.113 (7)	Ag2—N4^{i}	2.135 (8)
N2^{i}—Ag1—N1	174.0 (7)	N4^{i}—Ag2—N3	175.1 (7)
C2—C3—C6—C7	−37.3 (17)	C12—C13—C16—C17	−36.1 (17)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···F2^{ii}	0.84	1.89	2.721 (14)	173
O2—H2A···O3^{iii}	0.84	1.86	2.630 (11)	151
O3—H3···O5^{iv}	0.84	2.16	2.733 (11)	126
O4—H4A···F5	0.84	2.40	2.719 (14)	103
O5—H1O···F1	0.83 (11)	1.93 (10)	2.761 (11)	173 (11)
O6—H3O···F6	0.85 (11)	1.92 (9)	2.696 (12)	152 (10)
O6—H4O···O2^{v}	0.86 (10)	1.81 (8)	2.605 (11)	153 (14)
C23—H23A···F3^{ii}	0.99	2.52	3.049 (12)	113
C1—H1···F3^{vi}	0.95	2.38	3.052 (13)	127
C8—H8···O4^{vii}	0.95	2.42	3.208 (14)	140
C9—H9···F2^{iv}	0.95	2.46	3.199 (12)	134
C9—H9···F6^{iv}	0.95	2.52	3.437 (16)	161
C11—H11···F5^{viii}	0.95	2.54	3.280 (12)	135
C12—H12···O2^{viii}	0.95	2.43	3.349 (16)	164
C14—H14···F6	0.95	2.27	3.204 (14)	168
C18—H18···F1^{vii}	0.95	2.47	3.410 (17)	172
C18—H18···F5^{vii}	0.95	2.52	3.231 (13)	131

Symmetry codes: (ii) $x, -y+1, z-\frac{1}{2}$; (iii) $x, -y+1, z+\frac{1}{2}$; (iv) $x, -y, z-\frac{1}{2}$; (v) $x, y-1, z$; (vi) $x-1, y, z-1$; (vii) $x-1, -y, z-\frac{1}{2}$; (viii) $x-1, -y+1, z-\frac{1}{2}$.

The H atoms of the water molecules were located in a difference Fourier map and refined with the O—H distances restrained to 0.84 (3) Å and $U_{\rm iso}$(H) = $1.5U_{\rm eq}$(O). Other H atoms were placed in calculated positions and allowed to ride on their parent atoms, with C—H = 0.95–0.99 Å and O—H = 0.84 Å, and with $U_{\rm iso}$(H) = $1.2U_{\rm eq}$($C_{\rm methylene}$) or $1.5U_{\rm eq}$(O,$C_{\rm methyl}$). Compound (I) crystallizes in the non-centrosymmetric space group *Pc* and was refined as an inversion twin, with components in the ratio 0.64 (6):0.36 (6). Attempts to solve the structure in the centrosymmetric space group *P*2/*c* were unsuccessful. The maximum and minimum electron-density peaks lie next to the Ag1 atom.

Data collection: *EXPOSE* (Stoe & Cie, 2000); cell refinement: *CELL* (Stoe & Cie, 2000); data reduction: *INTEGRATE* (Stoe & Cie, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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