Electronic Supplementary Information for Dalton Transactions

Supporting Information

Influence of Sulfonate Anions on the Solid-structures of Silver Complexes Supported by 4,4'-Bipyridine Bridge

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Table S1. Hydrogen-bond geometries for compounds **1**–**10** (Å,°)

D–H···A	D–H [Å]	H···A [Å]	D···A [Å]	<D–H···A [°]
		Compound **1**		
OW1-H(1B)...O(1)#3	0.81(3)	2.03(2)	2.813(3)	165(3)
OW1-H(1A)...O(3)	0.82(2)	2.07(2)	2.838(3)	154(3)
N(4)-HN2...OW1#4	0.85(3)	2.17(3)	2.985(4)	160(3)
		Compound **2**		
OW2-HW2B...O(3)#3	0.84(4)	2.02(5)	2.858(9)	177(10)
OW1-HW1A...O(1)	0.78(4)	2.27(6)	3.027(9)	165(15)
OW1-HW1B...OW2#4	0.84(4)	2.14(5)	2.965(10)	168(11)
		Compound **3**		
OW2-HW2B...O(2)#5	0.846(10)	1.991(10)	2.825(3)	169(2)
OW2-HW2A...OW1	0.842(10)	1.932(10)	2.770(3)	173(2)
OW1-HW1A...O(4)#6	0.851(10)	1.884(14)	2.689(4)	157(3)
O(5)-H(7A)...O(3)	0.84(3)	1.67(4)	2.454(4)	153(4)
OW1-HW1B...O(1)#7	0.852(10)	1.956(15)	2.752(4)	155(3)
		Compound **4**		
OW1-HW1B...O(2)#3	0.85(3)	1.87(3)	2.681(4)	160(4)
OW1-HW1A...O(3)#4	0.79(3)	1.98(4)	2.770(4)	175(5)
N(1)-HN1...OW1#5	0.94(4)	2.04(4)	2.984(5)	173(3)
		Compound **6**		
N(3)-HN3B...O(1)#4	0.84(4)	2.13(4)	2.977(8)	175(7)
		Compound **7**		
OW1-HW1...O(1)	0.869(10)	2.024(11)	2.887(3)	172(3)
OW1-HW2...O(1)#2	0.872(10)	2.051(10)	2.920(3)	175(3)
		Compound **8**		
OW1-HW2...O(3)#4	0.79(3)	2.02(4)	2.798(5)	170(6)
OW1-HW1...O(5)#5	0.83(4)	1.99(4)	2.795(4)	163(5)

OW2-HW4...O(4)#3	0.85(4)	2.22(4)	2.986(5)	149(6)
OW2-HW3...O(2)	0.82(4)	2.10(4)	2.886(5)	160(6)
		Compound **9**		
OW1-HW1A...O(1)#5	0.81(5)	2.07(5)	2.872(11)	169(13)
OW2-HW2A...O(5)#6	0.86(5)	2.00(5)	2.858(13)	171(10)
OW2-HW2B...O(4)#7	0.85(5)	2.00(5)	2.848(13)	174(14)
OW1-HW1B...O(3)	0.83(5)	2.18(5)	3.000(11)	170(13)
		Compound **10**		
OW2-H(2A)...O(5)#3	0.96(5)	1.87(5)	2.794(5)	160(9)
OW2-H(2B)...O(7)	0.83(5)	2.10(9)	2.788(6)	140(11)
OW3-H(3B)...O(2)	1.00(5)	2.18(8)	2.901(5)	128(7)
OW3-H(3A)...OW4	0.87(5)	1.93(6)	2.747(7)	156(10)
OW6-H(6A)...O(4)#3	0.88(5)	1.91(6)	2.768(6)	163(10)
OW6-H(6B)...O(8)	0.88(5)	2.03(6)	2.853(6)	154(10)

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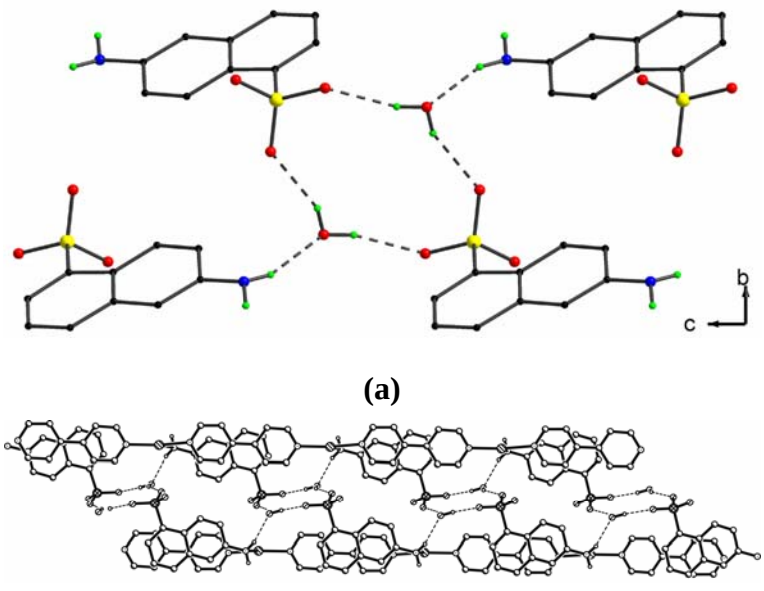
[a] Symmetry operations: for **1**: #3 –x + 1, -y + 1, -z; #4 –x + 1, -y + 1, -z + 1; for **2**: #1 x, y, z + 1; #2 x, y, z - 1; #3 –x + 5/4, y + 1/4, z + 1/4; #4 –x + 3/2, -y + 3/2, z; for **3**: #1 x - 1, y, z - 1; #2 -x, -y + 1, -z; #3 x + 1, y, z + 1; #4 x, -y + 1/2, z; #5 x - 1, y, z + 1; #6 x - 1, y, z; #7 x, y, z + 1; for **4**: #1 x - 1, y, z - 1; #2 x + 1, y, z + 1; #3 x, y - 1, z; #4 -x, -y + 1, -z; #5 –x + 1, -y + 1, -z + 1; for **6**: #1 x - 1/2, -y + 1/2, z - 1/2; #2 -x, -y + 1, -z + 2; #3 x + 1/2, -y + 1/2, z + 1/2; #4 –x + 1/2, y + 1/2, -z + 1/2; for **7**: #1 -x, y, -z + 1/2; #2 –x + 2, -y + 1, -z + 2; for **8**: #1 x - 1, y + 1, z; #2 –x - 1, -y + 2, -z + 2; #3 x + 1, y - 1, z; #4 x - 1, y, z; #5 -x, -y + 1, -z + 2; for **9**: #1 x, y - 1, z; #2 x, y + 1, z; #3 –x + 1, -y + 1, -z + 2; #4 -x, -y + 1, -z; #5 -x, -y + 1, -z + 1; #6 –x + 1, y - 1/2, -z + 3/2; #7 x, -y + 1/2, z + 1/2; for **10**: #1 x - 1/2, -y + 3/2, z - 1/2; #2 x + 1/2, -y + 3/2, z + 1/2; #3 x - 1, y, z; #4 x + 1, -y + 1, z - 1/2.

Table S2. Selected Bond Lengths [Å] and Angles [deg] for **1**–**10**. [a]

		Compound **1**	
Ag(1)-N(2)#1	2.166(2)	Ag(1)-N(1)	2.188(2)
Ag(1)-N(4)	2.550(2)	N(2)#1-Ag(1)-N(1)	161.25(8)
N(2)#1-Ag(1)-N(4)	107.98(8)	N(1)-Ag(1)-N(4)	90.23(8)
		Compound **2**	
Ag(1)-N(1)	2.132(8)	Ag(1)-N(2)#1	2.169(8)
N(1)-Ag(1)-N(2)#1	179.4(2)		
		Compound **3**	
Ag(1)-N(2)	2.154(2)	Ag(1)-N(1)#1	2.154(1)
Ag(1)-Ag(1)#3	3.3323(9)	N(2)-Ag(1)-N(1)#1	173.37(7)
Ag(1)-OW(2)#2	2.681(3)		
		Compound **4**	
Ag(1)-N(2)	2.184(2)	Ag(1)-N(3)#1	2.188(2)
Ag(1)-O(1)	2.70(2)	Ag(1)-O(1)#2	2.64(1)
N(2)-Ag(1)-N(3)#1	165.95(10)		
		Compound **5**	
Ag(1)-N(2)	2.195(3)	Ag(1)-N(3)#1	2.199(3)
Ag(1)-O(1)	2.576(3)	Ag(1)-O(1)#2	2.586(3)
N(2)-Ag(1)-N(3)#1	166.5(1)	N(2)-Ag(1)-O(1)	95.8(1)
N(3)#1-Ag(1)-O(1)	91.0(1)	N(2)-Ag(1)-O(1)#2	91.1(1)
N(3)#1-Ag(1)-O(1)#2	101.3(1)	O(1)-Ag(1)-O(1)#2	83.2(1)
		Compound **6**	
Ag(1)-N(2)#1	2.181(4)	Ag(1)-N(1)	2.181(4)
Ag(1)-O(2)	2.833(9)	Ag(1)-O(2)#4	2.833(9)
N(2)#1-Ag(1)-N(1)	166.7(2)	O(2)-Ag(1)-O(2)#4	72.77(3)
		Compound **7**	
Ag(1)-N(3)	2.143(2)	Ag(1)-N(3)#1	2.143(2)
Ag(2)-N(2)	2.160(2)	Ag(2)-N(1)	2.188(2)
Ag(2)-O(4)	2.511(2)	Ag(1)-O(2)#3	2.678(7)
Ag(1)-O(2)#2	2.678(7)	N(3)-Ag(1)-N(3)#1	173.0(1)
N(2)-Ag(2)-N(1)	171.50(8)	N(2)-Ag(2)-O(4)	106.64(8)
N(1)-Ag(2)-O(4)	70.37(7)	N(1)-Ag(2)-O(4)	70.37(7)
		Compound **8**	
Ag(1)-N(4)#1	2.160(2)	Ag(1)-N(3)	2.170(3)
Ag(1)-O(1)#2	2.67(4)	Ag(2)-N(2)	2.195(3)
Ag(2)-N(1)	2.205(3)	Ag(2)-O(5)	2.512(3)
Ag(2)-OW1	2.560(3)	N(4)#1-Ag(1)-N(3)	175.36(11)
N(2)-Ag(2)-N(1)	153.91(12)	N(2)-Ag(2)-O(5)	128.66(10)
N(1)-Ag(2)-O(5)	70.40(10)	N(2)-Ag(2)-OW1	85.45(12)
N(1)-Ag(2)-OW1	112.25(12)	O(5)-Ag(2)-OW1	96.52(11)

		Compound **9**	
Ag(1)-N(4)#1	2.132(6)	Ag(1)-N(3)	2.171(8)
Ag(2)-N(1)	2.143(6)	Ag(2)-N(2)	2.177(8)
Ag(1)-O(3)#5	2.87(2)	Ag(1)-OW2	2.71(3)
Ag(2)-O(4)	2.83(2)	Ag(2)-OW1	2.74(3)
N(4)#1-Ag(1)-N(3)	175.9(3)	N(1)-Ag(2)-N(2)	175.9(3)
		Compound **10**	
Ag(1)-N(6)#1	2.141(5)	Ag(1)-N(5)	2.150(5)
Ag(2)-N(4)#2	2.164(5)	Ag(2)-N(3)	2.169(5)
Ag(3)-N(2)	2.151(5)	Ag(3)-N(1)#1	2.153(5)
Ag(1)-O(9)#3	2.789(3)	Ag(1)-O(6)	2.851(3)
Ag(3)-O(2)#4	2.784(4)	N(4)#2-Ag(2)-N(3)	176.0(1)
N(6)#1-Ag(1)-N(5)	178.3(2)	N(2)-Ag(3)-N(1)#1	174.0(2)

[a] Symmetry operations: for **1**: #1 x, y, z + 1; for **2**: #1 x, y, z + 1; #2 x, y, z – 1; for **3**: #1 x – 1, y, z – 1; #2 –x, –y + 1, –z; #3 –x, 1 – y, 2 – z; for **4**: #1 x – 1, y, z – 1 #2 –x, 1 – y, z; for **5**: #1 x, y + 1, z; #2 –x + 2, –y + 2, –z + 1; for 6: #1 x – 1/2, –y + 1/2, z – 1/2; #4 1 – x, 1 – y, –z; for **7**: #1 –x, y, –z + 1/2; #2 1 – x, 1 – y, 1 – z; #3 x – 1, 1 – y, z + 1/2; for **8**: #1 x – 1, y + 1, z; #2 x + 1, y – 1, z; for **9**: #1 x, y – 1, z; #5 x, 1/2 – y, 1/2 + z; for **10**: #1 x – 1/2, –y + 3/2, z – 1/2; #2 x + 1/2, –y + 3/2, z + 1/2; #3 1.5 + x, y + 1/2, z; #4 x + 1/2, y + 1/2, z; #5 x,1 – y, z + 0.5.



(a)

(b)

Figure S1. (a) The hydrogen-bonding ring in **1**. (b) A 1D double chain via hydrogen bonds in **1**.

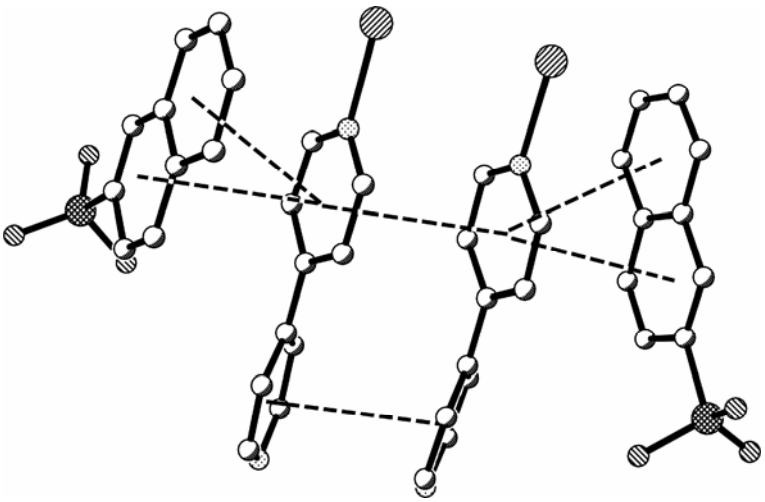


Figure S2: The π–π stacking styles of **2**.

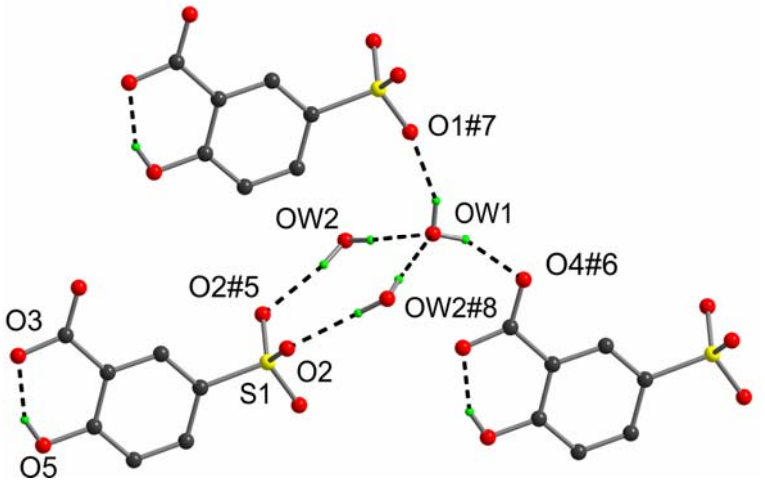
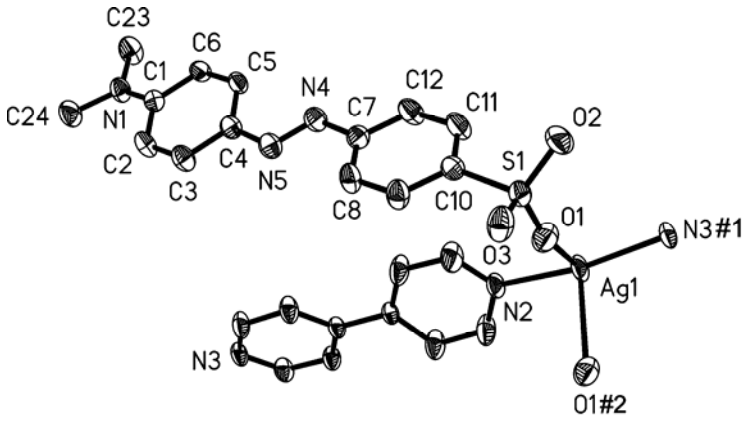
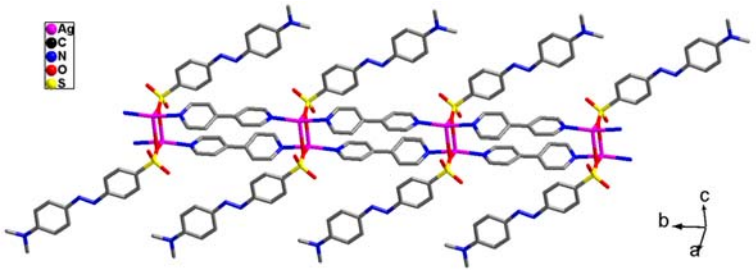


Figure S3. The hydrogen bonds in **3**.



(a)



(b)

Figure S4. (a) ORTEP view of environment of the Ag(I) in **5** showing 30% thermal probability ellipsoids. (b) The double chain in **5**. In **5**, Each silver cation is four-coordinated by two nitrogen atoms from two bipy ligands, and two oxygen atoms from different sulfonate anions. The silver cations are bridged by bipy ligands to form a 1D infinite polymeric chain, and the chains are further bridged by sulfonate anions to form an infinite polymeric double chain as shown.

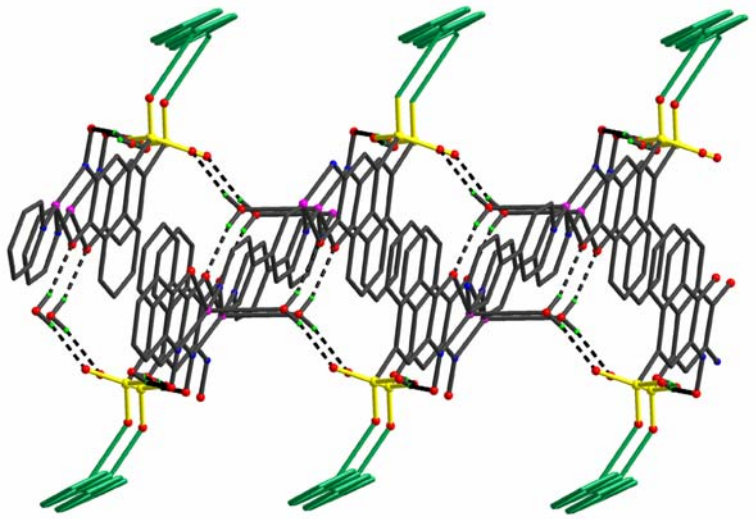


Figure S5. The 2D supramolecuar layer through hydrogen bonds in **8**.

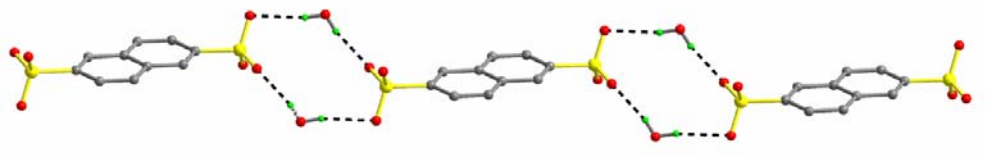


Figure S6. An anionic chain in **9** via hydrogen bonds. H bonds: dashed lines.

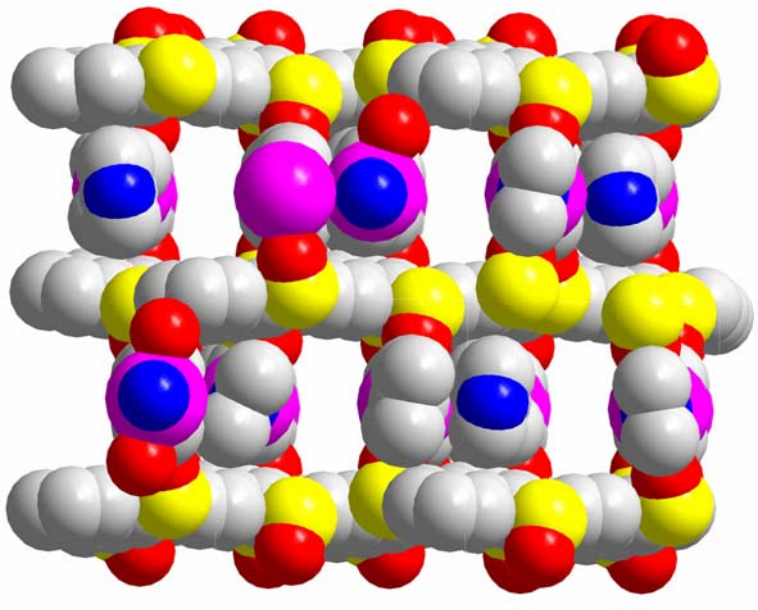


Figure S7. The three-dimensional porous framework with rectangle channels. The isolated Ag-bipy chains are omitted.