Electronic Supplementary Information for Dalton Transactions

Supporting Information

Syntheses, Structures, and Photoluminescence of a Series of Silver(I) Sulfonates with Pyrazine Derivatives

Hai-Yan Liu,[a,b] Hua Wu,[a] Jian-Fang Ma,*[a] Jin Yang,*[a] and Ying-Ying Liu [a]

[a] *Key Lab of Polyoxometalate Science, Department of Chemistry, Northeast Normal University, Changchun 130024, People's Republic of China*

[b] *Department of Chemistry and Pharmaceutical Engineering, Suihua University, Suihua 152061, People's Republic of China*

* Correspondence authors

E-mail: jianfangma@yahoo.com.cn (J.-F. Ma)

E-mail: yangjinnenu@yahoo.com.cn (J. Yang)

Fax: +86-431-85098620 (J.-F. Ma)

Table S1. Selected bond lengths [Å] and angles [º] for 1–10 [a]

		Compound **1**	
Ag(1)-N(3)#1	2.312(2)	Ag(1)-N(2)	2.360(2)
Ag(1)-N(1)	2.481(3)	Ag(1)-O1W	2.550(3)
N(3)#1-Ag(1)-N(2)	162.13(8)	N(3)#1-Ag(1)-N(1)	103.97(8)
N(2)-Ag(1)-N(1)	92.78(8)	N(3)#1-Ag(1)-O1W	94.62(8)
N(2)-Ag(1)-O1W	91.15(8)	N(1)-Ag(1)-O1W	91.28(8)
		Compound **2**	
Ag(1)-N(2)	2.253(2)	Ag(1)-N(1)	2.293(2)
Ag(1)-N(3)#1	2.451(2)	Ag(1)-O(3)#2	2.784(2)
N(2)-Ag(1)-N(1)	156.19(8)	N(2)-Ag(1)-N(3)#1	106.54(7)
N(1)-Ag(1)-N(3)#1	95.80(8)	N(3)#1-Ag(1)-O(3)#2	86.18(7)
N(1)-Ag(1)-O(3)#2	97.21(8)	N(2)-Ag(1)-O(3)#2	92.51(8)
		Compound **3**	
Ag(1)-N(2)	2.263(2)	Ag(1)-N(3)	2.274(2)
Ag(1)-N(1)#1	2.457(2)	Ag(1)-O(1)	2.540(2)
N(2)-Ag(1)-N(3)	144.96(7)	N(2)-Ag(1)-N(1)#1	103.06(7)
N(3)-Ag(1)-N(1)#1	101.31(7)	N(2)-Ag(1)-O(1)	93.33(7)
N(3)-Ag(1)-O(1)	110.27(6)	N(1)#1-Ag(1)-O(1)	92.78(6)
		Compound **4**	
Ag(1)-N(3)#1	2.296(4)	Ag(1)-N(2)	2.308(4)
Ag(1)-N(1)#2	2.366(5)	Ag(1)-O(1)	2.38(2)
N(3)#1-Ag(1)-N(2)	113.7(2)	N(3)#1-Ag(1)-N(1)#2	132.9(2)
N(2)-Ag(1)-N(1)#2	105.8(2)	N(3)#1-Ag(1)-O(1)	104.8(6)
N(2)-Ag(1)-O(1)	102.9(8)	N(1)#2-Ag(1)-O(1)	90.0(4)
		Compound **5**	
Ag(1)-N(2)	2.321(2)	Ag(1)-N(3)	2.373(2)
Ag(1)-N(1)#1	2.401(2)	Ag(1)-O(1)	2.435(2)

N(2)-Ag(1)-N(3)	109.83(8)	N(2)-Ag(1)-N(1)#1	114.65(9)
N(3)-Ag(1)-N(1)#1	124.91(9)	N(2)-Ag(1)-O(1)	120.13(8)
N(3)-Ag(1)-O(1)	98.02(8)	N(1)#1-Ag(1)-O(1)	86.62(8)

Compound **6**

Ag(1)-N(3)	2.250(3)	Ag(1)-N(2)	2.270(3)
Ag(1)-N(1)	2.397(4)	Ag(1)-O(1)#1	2.521(3)
N(3)-Ag(1)-N(2)	148.8(1)	N(3)-Ag(1)-N(1)	101.9(1)
N(2)-Ag(1)-N(1)	103.9(1)	N(3)-Ag(1)-O(1)#1	97.5(1)
N(2)-Ag(1)-O(1)#1	95.7(1)	N(1)-Ag(1)-O(1)#1	98.7(1)

Compound **7**

Ag(1)-N(2)	2.203(2)	Ag(1)-N(3)#1	2.249(2)
Ag(1)-N(1)	2.433(2)	Ag(1)-O(3)	2.634(2)
N(2)-Ag(1)-N(3)#1	152.14(7)	N(2)-Ag(1)-N(1)	117.31(7)
N(3)#1-Ag(1)-N(1)	90.54(7)	N(1)-Ag(1)-O(3)	79.00(7)
N(2)-Ag(1)-O(3)	96.31(7)	N(3)#1-Ag(1)-O(3)	90.66(7)

Compound **8**

Ag(1)-N(2)	2.257(2)	Ag(1)-N(3)#1	2.284(2)
Ag(1)-N(1)	2.496(3)	Ag(1)-O(2)#4	2.640(3)
N(2)-Ag(1)-N(3)#1	148.09(9)	N(2)-Ag(1)-N(1)	116.96(9)
N(3)#1-Ag(1)-N(1)	92.24(9)	N(1)-Ag(1)-O(2)#4	93.34(9)
N(2)-Ag(1)-O(2)#4	104.82(8)	N(3)#1-Ag(1)-O(2)#4	84.77(8)

Compound **9**

Ag(1)-N(3)#1	2.222(2)	Ag(1)-N(2)	2.239(2)
Ag(1)-N(1)	2.520(2)	Ag(1)-O(2)	2.760(3)
Ag(1)-O(3)#3	2.827(2)		
N(3)#1-Ag(1)-N(2)	157.13(8)	N(3)#1-Ag(1)-N(1)	103.93(7)
N(2)-Ag(1)-N(1)	97.69(7)	O(2)-Ag(1)-N(1)	71.83(8)
N(1)-Ag(1)-O(3)#3	84.33(9)	N(3)#1-Ag(1)-O(3)#3	102.76(9)
N(2)-Ag(1)-O(3)#3	86.59(9)	O(2)-Ag(1)-O(3)#3	154.38(9)

Compound **10**

Ag(1)-N(3)	2.240(3)	Ag(1)-N(2)	2.307(3)
Ag(1)-N(1)	2.365(3)	Ag(1)-O(1)	2.831(3)
Ag(1)-O(3)#4	2.814(3)		
N(3)-Ag(1)-N(2)	127.0(1)	N(3)-Ag(1)-N(1)	129.8(1)
N(2)-Ag(1)-N(1)	96.9(1)	N(1)-Ag(1)-O(1)	70.2(1)
O(1)-Ag(1)-O(3)#4	146.0(1)	N(1)-Ag(1)-O(3)#4	85.9(1)
N(3)-Ag(1)-O(3)#4	95.0(1)	N(2)-Ag(1)-O(3)#4	114.5(1)

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

Table S2. 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**		
N(1)-H2B...O(2)#3	0.84(2)	2.23(2)	3.062(3)	169(3)
O1W-H(1B)...O(1)#4	0.89(3)	2.01(3)	2.900(3)	177(5)
O1W-H(1A)...O(3)#3	0.83(3)	2.03(3)	2.858(3)	177(4)
		Compound **2**		
N(1)-H(2N)...O(1)#3	0.83(3)	2.15(3)	2.977(3)	174(3)
		Compound **3**		
N(1)-HN2...O(2)#5	0.85(3)	2.05(3)	2.904(3)	179(3)
OW1-H(2A)...O(1)#6	0.85(4)	2.05(4)	2.876(3)	163(5)
OW1-H(1A)...O(3)#4	0.84(5)	2.12(5)	2.909(3)	158(5)
		Compound **4**		

N(1)-H(2N)...O(2)#5	0.85(1)	2.09(3)	2.89(2)	157(5)
Compound **5**				
N(1)-HN1...O(2)#4	0.88(3)	2.22(3)	3.065(3)	162(3)
N(1)-HN2...O(3)#5	0.84(3)	2.09(3)	2.917(4)	167(3)
Compound **6**				
N(1)-H(2N)...O(2)#5	0.77(7)	2.18(8)	2.925(5)	166(2)
N(1)-H(1N)...O(2)	0.98(6)	1.92(6)	2.754(5)	141(5)
Compound **7**				
N(1)-HN2...O(1)#3	0.82(2)	2.35(3)	2.955(3)	132(3)
N(1)-H(2N)...O(2)#3	0.82(2)	2.60(2)	3.034(3)	115(1)
N(1)-HN1...O(1)	0.87(2)	2.11(2)	2.842(3)	141(2)
Compound **8**				
N(1)-HN2...O(2)	0.86(6)	2.15(7)	2.899(4)	146(5)
Compound **9**				
N(1)-H(2N)...O(3)	0.86(2)	2.22(2)	2.951(3)	143(3)
N(1)-H(1N)...O(1)#3	0.82(4)	2.30(4)	2.998(3)	144(5)
Compound **10**				
N(1)-HN1...O(2)#3	0.85(4)	2.06(4)	2.848(4)	154(2)
OW1-H(2A)...O(2)	0.86(7)	2.16(6)	2.893(6)	142(9)
N(1)-HN2...O(3)	0.86(4)	2.37(4)	3.026(5)	134(4)

Symmetry operations: For **1**: #3 -x+1, -y+1, -z+1; #4 -x, -y+1, -z+1; For **2**: #3 x-1/2, -y+1/2, -z; For **3**: #4 x, y+1, z; #5 -x+1/2, y+1/2, -z+1/2; #6 x, -y+3, z+1/2; For **4**: #5 -x+1, -y+2, z+1/2; For **5**: #4 x, y+1, z; #5 -x+2, y+1/2, -z+1/2; For **6**: #5 -x+1/2, y+1/2, -z+3/2; For **7**: #3 -x+1, -y, z-1/2; For **9**: #3 -x+1, -y+1, z-1/2; For **10**: #3 -x+3/2, y+1/2, -z+1/2.

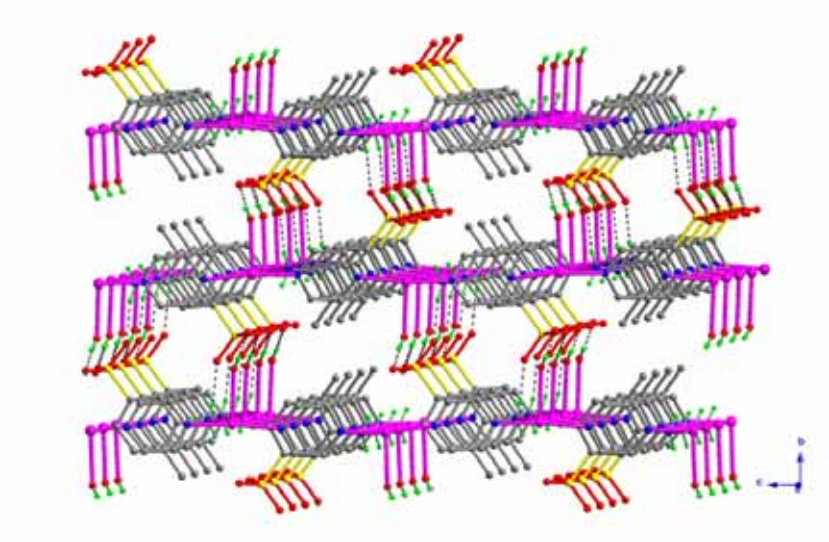
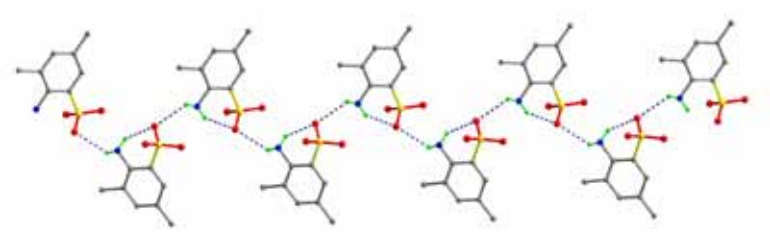
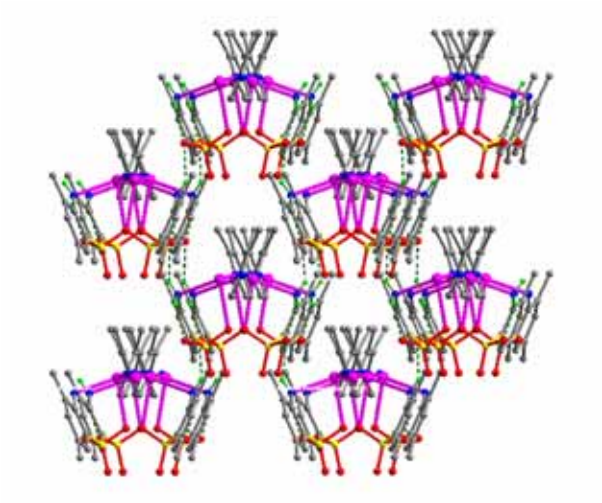


Fig. S1. View of the 3D supramolecular network in **1**.



(a)



(b)

Fig. S2. (a) An anionic chain *via* hydrogen bonds in **7**. (b) View of the 3D supramolecular network in **7**. H-bonds: dashed lines. Hydrogen atoms are omitted for clarity.

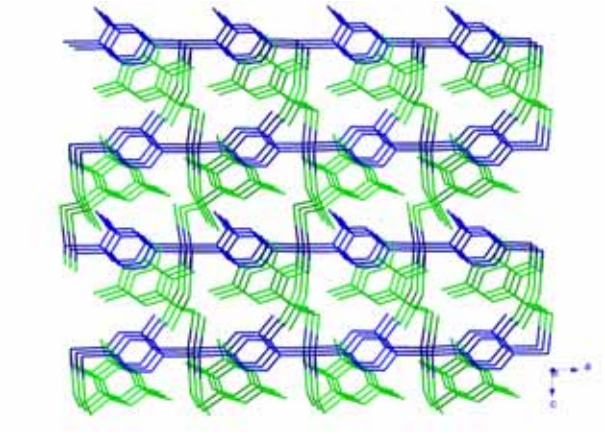


Fig. S3. Perspective view of 3D network for **9**.

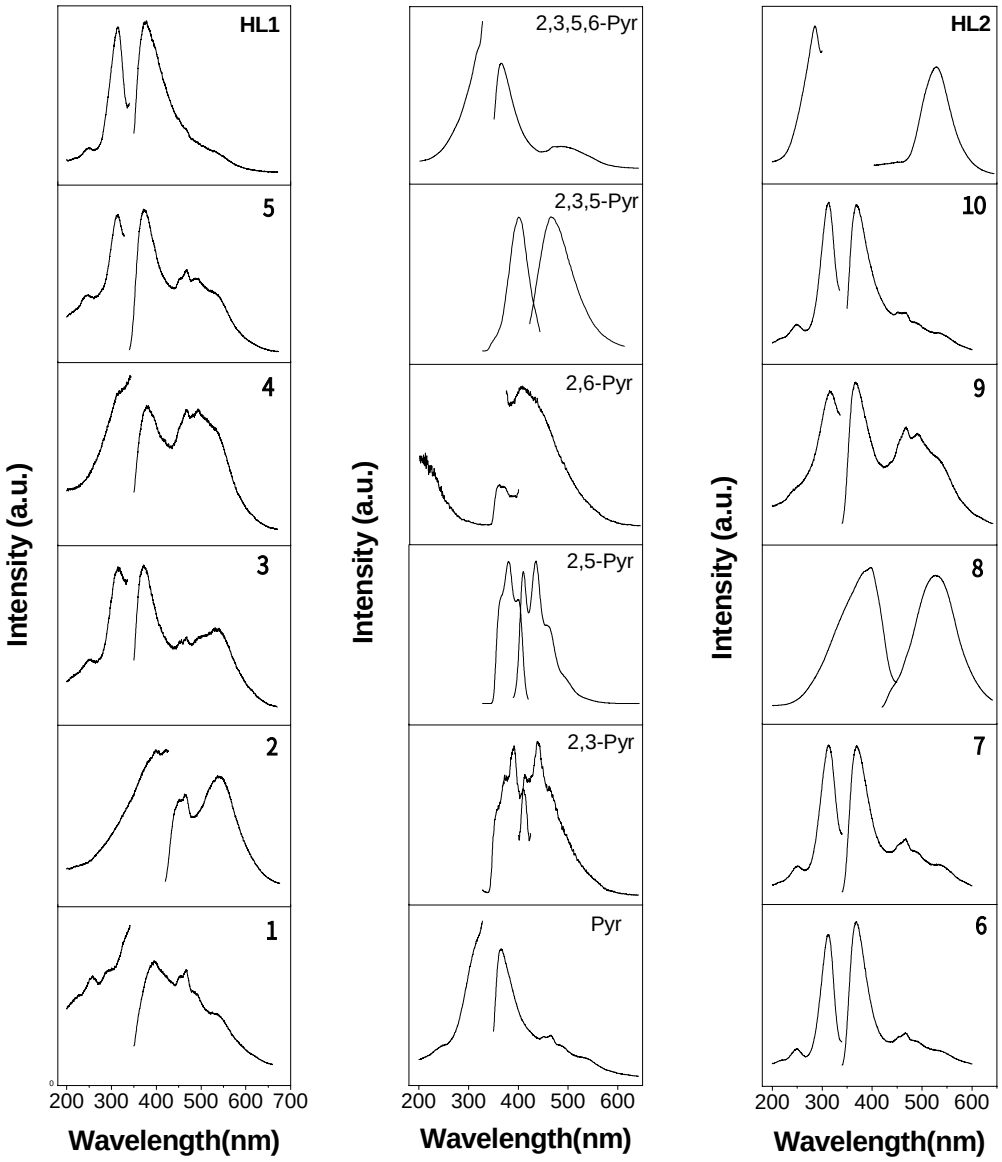


Fig. S4. The excitation-emission spectra of **1**–**10,** HL1, HL2, Pyr, 2,3-Pyr, 2,5-Pyr, 2,6-Pyr, 2,3,5-Pyr, and 2,3,5,6-Pyr at room temperature.