Supporting Information

Silver(I)–organic frameworks assembled with flexible supramolecular synthons with pendant ethynide arm attached to heteroaryl skeleton

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Table S1. X-ray Crystal Data and Structure Refinement for Complexes **1**–**4**.

Table S2. Selected Bond Lengths (Å) for Complexes **1**–**4**.

Table S1. X-ray Crystal Data and Structure Refinement for Complexes **1**–**4.**

	1	**2**	**3**	**4**
formula	$C_{17}H_6Ag_5F_{12}N_3O_9$	$C_{17}H_8Ag_5F_{12}N_3O_{10}$	$C_{83}H_{46}Ag_{14}F_{30}N_4O_{27}S_4$	$C_{70}H_{58}Ag_9N_9O_{22}S_7$
fw	1163.60	1181.61	3739.66	2572.50
cryst syst	triclinic	monoclinic	monoclinic	monoclinic
space group	$P\bar{1}$	$P2/c$	$P2_1/c$	Cc
a (Å)	8.9041(8)	16.0991(16)	8.0193(16)	15.346(3)
b (Å)	11.5928(7)	8.8039(10)	24.904(5)	24.558(5)
c (Å)	14.2517(10)	23.399(3)	26.491(5)	22.739(5)
α (deg)	71.388(6)	90	90	90
β (deg)	81.390(7)	120.917(7)	93.01(3)	109.46(3)
γ (deg)	88.826(6)	90	90	90
volume (Å^3)	1377.88(2)	2845.2(6)	5283.4(2)	8080(3)
Z	2	4	2	4
D_{calc} (g·cm^{-3})	2.805	2.758	2.351	2.115
F(000)	1088	2216	3560	5008
R(int)	0.0231	0.0542	0.0878	0.0358
GOF	1.065	1.006	1.116	1.081
R_1[a] [($I > 2\sigma(I)$)]	0.0511	0.0884	0.0988	0.0763
wR_2[b] [($I > 2\sigma(I)$)]	0.1309	0.1675	0.2915	0.2095
R_1[a] (all data)	0.0620	0.1510	0.1170	0.0827
wR_2[b] (all data)	0.1380	0.1955	0.3087	0.2161

[a] $R_1=\Sigma||F_o|-|F_c||/\Sigma|F_o|$; [b] $wR_2=\{\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$, $w = [\sigma^2(F_o^2)+(AP)^2+BP]^{-1}$, where $P = [\mathrm{Max}(F_o^2,0)+2F_c^2]/3$, and A and B are constants adjusted by the program.

Table S2. Selected Bond Lengths (Å) for Complexes **1**–**4.**

			1		
C1≡C2	1.202(7)	Ag1–C1	2.240(7)	Ag2–C1	2.287(7)
Ag3–C1	2.371(8)	Ag3–C2	2.934(8)	Ag4–C1	2.324(8)
Ag4–C2	2.698(8)	Ag1···Ag2	2.812(9)	Ag1···Ag3	2.917(10)
Ag1···Ag4	3.005(10)	Ag2···Ag2#2	2.812(1)	Ag2···Ag3	3.030(11)
Ag2···Ag4	3.153(10)	Ag6···Ag6#3	3.038(3)		
			2		
C1≡C2	1.206(1)	Ag1–C1	2.562(2)	Ag2–C1	2.655(2)
Ag1#1–C1	2.340(2)	Ag2#1–C1	2.28(2)	Ag4#2–C1	2.261(2)
Ag4#2–C2	3.066(2)	Ag1···Ag1#1	2.962(3)	Ag1···Ag4#2	3.176(2)
Ag1#1···Ag4#2	2.904(3)	Ag2#1···Ag4#2	2.936(2)	Ag1#1···Ag5#1	3.049(2)
Ag2#1···Ag5#1	3.024(3)				
			3		
C1≡C2	1.205(9)	Ag1–C1	2.375(1)	Ag1–C2	2.484(1)
Ag2–C3	2.188(1)	Ag3–C3	2.175(2)	Ag4–C1	2.304(1)
Ag4–C3	2.467(2)	Ag5–C1	2.162(1)	Ag6–C3	2.410(1)
Ag6–C4	2.496(1)	Ag7–C1	2.299(1)	Ag7–C2	2.884(1)
Ag1···Ag5	3.153(2)	Ag2···Ag3	2.842(2)	Ag2···Ag4	2.843(2)
Ag2···Ag6	3.399(2)	Ag3···Ag4	3.001(2)	Ag3···Ag6	3.131(2)
Ag4···Ag5	2.804(2)	Ag4···Ag7	2.980(2)	Ag5···Ag7	2.958(2)
			4		
C1≡C2	1.212(10)	C4≡C5	1.211(10)	C7≡C8	1.202(10)
C10≡C11	1.208(10)	Ag1–C1	2.077(2)	Ag1–C7	2.130(2)
Ag2–C4	2.108(3)	Ag2–C10	2.11(2)	Ag3–C10	2.36(3)
Ag3–C11	2.52(2)	Ag4–C1	2.34(2)	Ag4–C2	2.42(3)
Ag5–C7	2.40(2)	Ag5–C8	2.65(2)	Ag6–C4	2.321(3)
Ag6–C5	2.43(2)	Ag7–C7	2.18(3)	Ag7–C8	2.794(2)
Ag7–C10	2.14(3)	Ag7–C11	2.799(2)	Ag8–C7	2.47(3)
Ag8–C8	2.68(2)	Ag9–C1	2.31(2)	Ag9–C2	2.836(3)
Ag1···Ag4	3.277(9)	Ag1···Ag5	3.185(3)	Ag1···Ag7	3.018(9)
Ag1···Ag8	3.214(3)	Ag1···Ag9	2.935(3)	Ag2··Ag3	3.313(9)
Ag2··Ag7	2.864(3)	Ag2··Ag9	2.956(10)		

[a]Symmetry transformations used to generate equivalent atoms: #2 2 – *x*, 1 – *y*, – *z*; #3 2 – *x*, 2 – *y*, – *z* for **1**, #1 1 – *x*, – *y*, 2 – *z*; #2 *x*, – 1 + *y*, *z* for **2**.