Structure Diversity of $C_2@Ag_n$ Cages Consolidated by Heteroaromatic *N*-donor Ligands in Silver Ethynediide Complexes

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Supporting Information

Table S1. X-ray crystal data and structure refinement for compounds **1**–**7**.

Compound	**1**	**2**	**3**	**4**	**5**	**6**	**7**
Formula	$C_{22}H_{11}Ag_6F_{15}N_2O_{11}$	$C_{46}H_{29}Ag_9F_{36}N_4O_{28}$	$C_{38}H_{24}Ag_{12}F_{24}N_{12}O_{16}$	$C_{10}H_8Ag_3F_6N_2O_4$	$C_7H_3Ag_3F_6N_3O_4$	$C_{28}H_{14}Ag_6F_{15}N_3O_{10}$	$C_{82}H_{57}Ag_{12}F_{36}N_{16}O_{27}$
FW	1411.55	2740.56	2655.13	657.79	630.73	1484.64	3676.88
Crystal system	Monoclinic	Triclinic	Triclinic	Orthorhombic	Orthorhombic	Monoclinic	Monoclinic
Space group	*C*2/*c* (No. 15)	*P*-1 (No. 2)	*P*-1 (No. 2)	*P*ccn (No. 56)	*P*bn (No. 0)	$P2_1/c$ (No.14)	*C*2/*c* (No. 15)
a (Å)	32.896(2)	14.992(1)	9.228(2)	14.970(2)	15.366(9)	8.006(7)	28.548(2)
b (Å)	8.295(4)	15.837(1)	13.386(2)	26.147(3)	17.267(1)	26.240(2)	11.543(5)
c (Å)	28.617(1)	18.853(2)	27.285(5)	8.596(1)	9.884(6)	18.095(2)	35.637(2)

α (°)	90	79.380(2)	89.373(3)	90	90	90	90
β (°)	122.446(7)	70.681(2)	80.450(3)	90	90	102.567(2)	112.064(1)
γ (°)	90	62.268(1)	77.505(3)	90	90	90	90
Volume (Å^3)	6590.0(5)	3736.5(6)	3244.0(1)	3364.4(7)	2622.5(3)	3710.1(6)	10883.3(1)
Z	8	2	2	8	8	4	4
D_{calc} (g·cm^{-3})	2.846	2.436	2.718	2.597	3.195	2.658	2.244
T (K)	296	296	296	296	296	296	296
μ [mm^{-1}]	3.641	2.474	3.672	3.538	4.533	3.240	2.247
F(000)	5296.0	2608.0	2488.0	2472	2344	2800	7060
$R_1[(I > 2\sigma(I))]$	0.064	0.050	0.094	0.048	0.042	0.053	0.072
$wR_2[(I > 2\sigma(I))]$	0.181	0.130	0.272	0.113	0.112	0.112	0.183
R_1 (all data)[a]	0.070	0.072	0.124	0.073	0.046	0.099	0.093
wR_2 (all data)[b]	0.191	0.146	0.294	0.132	0.116	0.134	0.200
GOF	1.087	1.009	1.042	1.035	0.983	1.005	1.033
The number of restraints imposed during refinements	18	0	20	0	0	0	13

[a] $R_1 = \sum||F_o| - |F_c||/\sum|F_o|$. [b] $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum[w(F_o^2)^2]\}^{1/2}$

Table S2. Selected Bond Lengths (Å) for Complexes 1–7.

1					
C(1)≡C(1)#1	1.182(2)	C(2)≡C(2)#1	1.206(2)	Ag(1)-C(1)	2.211(8)
Ag(2)-C(1)	2.129(9)	Ag(3)-C(1)	2.632(8)	Ag(3)-C(1)#1	2.651(9)
Ag(6)-C(1)#2	2.493(9)	Ag(3)-C(2)	2.477(8)	Ag(4)-C(2)	2.134(9)
Ag(5)-C(2)	2.308(8)	Ag(6)-C(2)	2.357(9)	Ag(1)···Ag(6)#3	2.820(3)
Ag(1)···Ag(3)#1	2.901(1)	Ag(1)···Ag(4)	3.277(2)	Ag(2)···Ag(6)#3	2.840(7)
Ag(2)···Ag(3)	3.289(2)	Ag(3)···Ag(5)	3.081(2)	Ag(3)···Ag(4)	3.152(1)
Ag(3)···Ag(4)#1	3.309(2)	Ag(3)···Ag(3)#1	3.372(2)	Ag(4)···Ag(5)	2.803(1)
Ag(4)···Ag(6)	3.280(5)	Ag(5)···Ag(6)	3.121(7)	Ag(6)···Ag(6)#1	2.760(7)
2					
C(1)≡C(2)	1.195(8)	Ag(1)-C(1)	2.433(6)	Ag(2)-C(1)	2.189(6)
Ag(3)-C(1)	2.448(5)	Ag(5)-C(1)	2.299(5)	Ag(6)-C(1)	2.401(6)
Ag(3)-C(2)	2.455(6)	Ag(4)-C(2)	2.458(6)	Ag(7)-C(2)	2.208(5)
Ag(8)-C(2)	2.223(6)	Ag(9)-C(2)	2.462(6)	Ag(1)···Ag(5)	2.905(7)
Ag(1)···Ag(2)	2.942(7)	Ag(1)···Ag(4)	3.013(7)	Ag(1)···Ag(8)	3.273(7)
Ag(2)···Ag(6)	2.943(7)	Ag(2)···Ag(3)	3.089(7)	Ag(2)···Ag(5)	3.160(8)

Ag(3)···Ag(7)	3.033(7)	Ag(3)···Ag(6)	3.158(7)	Ag(3)···Ag(4)	3.239(7)
Ag(4)···Ag(7)	2.976(7)	Ag(4)···Ag(8)	2.965(6)	Ag(5)···Ag(6)	2.968(7)
Ag(5)···Ag(9)	3.222(8)	Ag(6)···Ag(9)	2.929(7)	Ag(7)···Ag(8)	2.900(7)
Ag(7)···Ag(9)	2.905(6)	Ag(8)···Ag(9)	2.980(6)		

3

C(1)≡C(2)	1.19(2)	C(3)≡C(4)	1.18(2)	Ag(1)-C(1)	2.468(2)
Ag(2)-C(1)	2.570(2)	Ag(3)-C(1)	2.073(2)	Ag(4)-C(1)	2.540(2)
Ag(5)-C(1)	2.697(2)	Ag(6)-C(1)	2.507(2)	Ag(2)-C(2)	2.549(2)
Ag(5)-C(2)	2.415(2)	Ag(6)-C(2)	2.497(2)	Ag(7)-C(2)	2.611(2)
Ag(8)-C(2)	2.077(2)	Ag(4)-C(3)	2.440(2)	Ag(7)-C(3)	2.500(2)
Ag(9)-C(3)	2.066(2)	Ag(10)-C(3)	2.672(2)	Ag(12)-C(3)	2.587(2)
Ag(2)-C(4)#1	2.363(2)	Ag(10)-C(4)	2.326(2)	Ag(11)-C(4)	2.134(2)
Ag(12)-C(4)	2.370(2)	Ag(1)···Ag(2)	2.895(2)	Ag(1)···Ag(12)#1	3.086(2)
Ag(1)···Ag(3)	3.160(2)	Ag(1)···Ag(6)	3.190(2)	Ag(1)···Ag(9)#1	3.214(2)
Ag(2)···Ag(11)#1	2.828(2)	Ag(2)···Ag(10)#1	3.115(2)	Ag(2)···Ag(12)#1	3.127(2)
Ag(2)···Ag(5)	3.131(2)	Ag(3)···Ag(4)	2.955(2)	Ag(4)···Ag(7)	2.876(2)
Ag(4)···Ag(6)	3.053(2)	Ag(4)···Ag(9)	3.072(2)	Ag(4)···Ag(5)	3.139(2)

Ag(4)···Ag(12)	3.173(2)	Ag(5)···Ag(7)	3.052(2)	Ag(6)···Ag(7)	3.076(2)
Ag(6)···Ag(9)	3.250(2)	Ag(7)···Ag(8)	2.933(2)	Ag(7)···Ag(10)	3.126(2)
Ag(7)···Ag(9)	3.171(2)	Ag(10)···Ag(11)	3.181(2)	Ag(12)···Ag(1)#2	3.086(2)
Ag(12)···Ag(2)#2	3.127(2)				
4					
C(1)≡C(1)#1	1.215(1)	Ag(1)-C(1)	2.095(7)	Ag(2)-C(1)	2.399(7)
Ag(2)-C(1)#1	2.600(8)	Ag(2)-C(1)#3	2.616(8)	Ag(3)-C(1)	2.420(7)
Ag(1)···Ag(2)#2	2.899(1)	Ag(1)···Ag(3)#2	3.141(1)	Ag(1)···Ag(2)	3.163(9)
Ag(1)···Ag(3)	3.281(1)	Ag(2)···Ag(3)#2	3.023(1)	Ag(2)···Ag(3)#3	3.055(1)
Ag(2)···Ag(2)#1	3.084(1)	Ag(2)···Ag(3)#1	3.238(1)	Ag(3)···Ag(2)#4	3.023(1)
Ag(3)···Ag(2)#2	3.055(1)	Ag(3)···Ag(1)#4	3.141(1)	Ag(3)···Ag(2)#1	3.238(1)
5					
C(1)≡C(1)#1	1.220(9)	Ag(1)-C(1)	2.338(4)	Ag(1)-C(1)#1	2.555(5)
Ag(2)-C(1)	2.191(4)	Ag(3)-C(1)	2.155(5)	Ag(1)···Ag(1)#1	3.057(7)
Ag(1)···Ag(3)#2	3.102(6)	Ag(2)···Ag(3)	2.867(6)	Ag(2)···Ag(2)#1	3.190(9)
6					
C(1)≡C(2)	1.206(1)	Ag(2)-C(1)	2.227(1)	Ag(2)-C(1)#1	2.514(1)

Ag(3)-C(1)#2	2.562(9)	Ag(4)-C(1)	2.331(9)	Ag(6)-C(1)	2.255(1)
Ag(1)-C(2)	2.100(9)	Ag(3)-C(2)	2.411(1)	Ag(3)-C(2)#2	2.587(9)
Ag(5)-C(2)	2.262(9)	Ag(1)···Ag(3)	3.028(1)	Ag(1)···Ag(5)	3.208(1)
Ag(2)···Ag(2)#1	2.784(2)	Ag(2)···Ag(6)	2.882(1)	Ag(2)···Ag(4)	3.122(1)
Ag(2)···Ag(4)#1	3.344(1)	Ag(3)···Ag(3)#2	2.839(2)	Ag(3)···Ag(5)	2.895(1)
Ag(4)···Ag(5)	2.924(1)	Ag(4)···Ag(6)	3.025(1)	Ag(5)···Ag(6)	3.178(1)
7					
C(1)≡C(2)	1.06(3)	Ag(2)-C(1)	2.642(1)	Ag(3)-C(1)	2.191(2)
Ag(5)-C(1)	2.677(1)	Ag(2)-C(2)	2.384(5)	Ag(4)-C(2)	2.310(2)
Ag(5)-C(2)	2.321(3)	Ag(1)···Ag(2)	2.896(2)	Ag(1)···Ag(3)#1	2.917(1)
Ag(1)···Ag(5)#1	3.365(1)	Ag(2)···Ag(4)	2.600(2)	Ag(2)···Ag(5)#1	3.017(1)
Ag(2)···Ag(4)#1	3.129(2)	Ag(3)···Ag(5)	3.141(1)	Ag(3)···Ag(3)#1	3.164(2)
Ag(4)···Ag(4)#1	1.045(3)	Ag(4)···Ag(5)	2.782(2)	Ag(4)···Ag(2)#1	3.129(2)
Ag(4)···Ag(5)#1	3.313(2)				

[a] Symmetry transformations used to generate equivalent atoms:

For **1**: #1 -x, y, -z + ½; #2 x, y – 1, z; #3 x, y + 1, z.

For **3**: #1 x – 1, y, z; #2 1 + x, y, z.

For **4**: #1 –x + 3/2, -y + ½, z; #2 x, -y + ½, z + ½; #3 x, -y + ½, z – ½; #4 –x + 3/2, y, z + ½.

For **5**: #1 -x, y, -z + ½; #2 x, -y, z + ½.

For **6**: #1 –x, -y + 1, -z + 1; #2 –x + 1, -y + 1, -z + 1.

For **7**: #1 –x + 1, y, -z + ½.