Electronic Supplementary Material (ESI) for CrystEngComm

Assembly of Organometallic Networks with Multinuclear Silver(I)-Ethynediide Supramolecular Synthon, Trifluoroacetate and Ligands Derived from Isomeric Dicyanobenzenes

Supporting Information

Table S1. X-ray crystal data and structure refinement parameters.

Compound	**1**	**2**	**3**	**4**	**5**	**6**
Empirical formula	$C_{48}H_{12}Ag_{14}F_{30}N_6O_{20}$	$C_{56}H_{16}Ag_{15}F_{30}N_9O_{23}$	$C_{22}H_{12}Ag_6F_6O_{13}$	$C_{22}H_9Ag_6F_6NO_{10}$	$C_{26}H_{16}Ag_8F_{12}N_2O_{16}$	$C_{56}H_{20}Ag_{16}F_{18}N_4O_{24}$
Formula weight	3072.82	3370.83	1245.54	1208.52	1703.37	3200.68
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Triclinic	Monoclinic
Space group	$P2_1/c$ (No.14)	$C2/c$ (No. 15)	$P2_1/n$ (No.14)	$P2_1/c$ (No.14)	P-1 (No. 2)	$P2_1/n$ (No.14)
a [Å]	8.300(5)	19.894(9)	6.904(5)	18.999(3)	8.222(7)	27.310(3)
b [Å]	31.638(2)	26.220(1)	18.743(2)	17.422(2)	16.225(1)	8.465(8)
c [Å]	27.360(2)	17.945(1)	22.419(2)	8.262(1)	16.461(1)	32.750(3)
α [°]	90	90	90	90	93.275(2)	90
β [°]	95.450(1)	119.636(1)	97.687(1)	96.619(2)	95.797(1)	109.776(2)
γ [°]	90	90	90	90	97.895(1)	90
V[Å^3]	7151.7(7)	8136.4(8)	2875.0(4)	2716.4(6)	2158.4(3)	7124.2(1)
Z	4	4	4	4	2	4
D_{calc}(g/cm3)	2.854	2.752	2.878	2.955	2.565	2.984
μ(Mo-Kα)(mm^{-1})	3.888	3.664	4.112	4.340	3.660	4.413
F(000)	5720	6296	2336	2256	1556	5960
Reflections collected	101304	56209	26954	17852	32274	107180

Independent reflections	17086	9793	6962	4893	10298	17155
Observed reflections [I>2s(I)]	14658	8515	5746	3899	8480	13555
Parameters	1063	601	456	408	552	1063
Goodness-of-fit	1.099	1.070	1.022	1.077	1.052	1.114
R_1[I>2s(I)][a]	0.080	0.054	0.048	0.098	0.090	0.085
wR_2(all data)[b]	0.204	0.157	0.136	0.247	0.244	0.236

[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 **1–6**.

1					
C(1)≡C(2)	1.245(1)	C(3)≡C(4)	1.238(1)	Ag(1)-C(1)	2.308(8)
Ag(4)-C(1)	2.505(8)	Ag(5)-C(1)	2.255(9)	Ag(6)-C(1)	2.176(8)
Ag(1)-C(2)	2.648(8)	Ag(2)-C(2)	2.273(8)	Ag(3)-C(2)	2.138(8)
Ag(4)-C(2)	2.396(8)	Ag(7)-C(2)	2.517(8)	Ag(1)-C(3)#1	2.661(8)
Ag(7)-C(3)	2.555(8)	Ag(8)-C(3)	2.163(7)	Ag(9)-C(3)	2.404(8)
Ag(12)-C(3)	2.186(8)	Ag(7)-C(4)	2.559(8)	Ag(10)-C(4)	2.170(8)
Ag(11)-C(4)	2.158(8)	Ag(1)···Ag(2)	2.923(1)	Ag(1)···Ag(8)#1	2.952(9)
Ag(1)···Ag(11)#1	3.115(1)	Ag(1)···Ag(5)	3.198(1)	Ag(2)···Ag(3)	2.898(1)
Ag(2)···Ag(7)	3.022(1)	Ag(2)···Ag(11)#1	3.308(1)	Ag(3)···Ag(7)	3.109(9)
Ag(3)···Ag(4)	3.113(1)	Ag(4)···Ag(5)	2.896(9)	Ag(4)···Ag(10)#1	3.050(1)
Ag(4)···Ag(11)#1	3.299(1)	Ag(5)···Ag(6)	2.816(9)	Ag(5)···Ag(12)#1	3.079(9)
Ag(6)···Ag(8)	3.107(9)	Ag(6)···Ag(9)	3.191(9)	Ag(6)···Ag(7)	3.251(1)
Ag(7)···Ag(8)	2.859(9)	Ag(7)···Ag(9)	3.094(1)	Ag(8)···Ag(12)	2.836(9)
Ag(9)···Ag(10)	2.991(9)	Ag(9)···Ag(12)	3.041(9)	Ag(10)···Ag(11)	2.793(1)
2					
C(1)≡C(2)	1.245(8)	Ag(1)-C(1)	2.220(5)	Ag(6)-C(1)#1	2.618(5)
Ag(5)-C(1)	2.548(5)	Ag(2)-C(1)	2.414(5)	Ag(4)-C(1)	2.151(6)
Ag(1)-C(2)	2.187(5)	Ag(7)-C(2)	2.302(5)	Ag(5)-C(2)	2.417(5)
Ag(1)···Ag(6)	2.834(6)	Ag(1)···Ag(7)	2.896(6)	Ag(1)···Ag(2)	3.294(5)
Ag(7)···Ag(3)	3.195(7)	Ag(7)···Ag(6)	3.372(7)	Ag(3)···Ag(4)	2.757(7)
Ag(2)···Ag(3)	3.133(5)	Ag(3)···Ag(6)#1	3.327(7)	Ag(6)···Ag(6)#1	2.859(9)
Ag(6)···Ag(5)	3.081(7)	Ag(5)···Ag(4)	3.013(7)		

3

C(1)≡C(2)	1.238(8)	Ag(4)-C(1)	2.982(7)	Ag(2)-C(1)	2.188(5)
Ag(3)-C(1)	2.427(6)	Ag(6)-C(1)	2.575(5)	Ag(4)-C(2)	2.494(6)
Ag(4)-C(2)#2	2.643(6)	Ag(3)-C(2)#3	2.372(5)	Ag(5)-C(2)	2.119(6)
Ag(6)-C(2)	2.603(5)	Ag(4)···Ag(3)#1	2.928(6)	Ag(4)···Ag(1)	2.982(7)
Ag(4)···Ag(4)#2	3.083(9)	Ag(4)···Ag(5)#2	3.106(7)	Ag(4)···Ag(5)	3.298(7)
Ag(4)···Ag(6)	3.327(1)	Ag(1)···Ag(2)	2.971(7)	Ag(1)···Ag(3)	3.156(7)
Ag(2)···Ag(6)	2.846(8)	Ag(2)···Ag(3)	3.136(6)	Ag(3)···Ag(3)#3	2.824(9)
Ag(3)···Ag(4)#4	2.928(6)	Ag(3)···Ag(5)#4	3.043(6)	Ag(5)···Ag(6)	3.308(8)

4

C(1)≡C(2)	1.231(2)	Ag(1)-C(1)	2.328(1)	Ag(2)-C(1)#1	2.670(1)
Ag(2)-C(1)	2.707(1)	Ag(5)-C(1)	2.362(1)	Ag(6)-C(1)	2.085(1)
Ag(2)-C(2)	2.360(1)	Ag(3)-C(2)	2.181(1)	Ag(4)-C(2)	2.169(1)
Ag(5)-C(2)	2.624(1)	Ag(1)···Ag(6)	2.865(2)	Ag(1)···Ag(2)	2.893(1)
Ag(1)···Ag(2)#2	3.004(1)	Ag(1)···Ag(3)#1	3.047(2)	Ag(2)···Ag(4)	3.230(2)
Ag(2)···Ag(3)	3.257(2)	Ag(2)···Ag(3)#1	3.268(2)	Ag(2)···Ag(5)	3.281(2)
Ag(2)···Ag(6)#1	3.290(2)	Ag(3)···Ag(4)	2.810(2)	Ag(3)···Ag(5)#2	3.257(2)
Ag(4)···Ag(5)	2.863(2)	Ag(4)···Ag(6)#4	3.025(2)	Ag(5)···Ag(6)	3.213(2)

5

C(1)≡C(2)	1.220(1)	Ag(1)-C(1)	2.300(8)	Ag(2)-C(1)	2.178(9)
Ag(3)-C(1)	2.299(9)	Ag(6)-C(1)	2.257(9)	Ag(1)-C(2)#1	2.384(9)
Ag(3)-C(2)	2.480(1)	Ag(4)-C(2)	2.169(1)	Ag(5)-C(2)	2.155(1)
Ag(6)-C(2)	2.673(1)	Ag(1)···Ag(1)#1	2.745(1)	Ag(1)···Ag(4)#1	3.276(9)
Ag(2)···Ag(3)	2.983(1)	Ag(2)···Ag(6)	2.997(1)	Ag(2)···Ag(4)#2	3.025(1)
Ag(2)···Ag(5)#2	3.077(1)	Ag(3)···Ag(4)	2.918(1)	Ag(3)···Ag(5)#2	3.037(1)
Ag(3)···Ag(6)#2	3.279(1)	Ag(4)···Ag(5)	2.870(1)	Ag(4)···Ag(6)#2	3.068(1)

Ag(5)···Ag(6)	2.871(1)				
6					
C(1)≡C(2)	1.243(1)	C(3)≡C(4)	1.221(1)	Ag(1)-C(1)	2.124(1)
Ag(2)-C(1)	2.149(1)	Ag(5)-C(1)	2.610(1)	Ag(6)-C(1)#2	2.481(9)
Ag(6)-C(1)	2.591(1)	Ag(3)-C(2)#2	2.181(1)	Ag(4)-C(2)#2	2.294(1)
Ag(5)-C(2)	2.283(1)	Ag(6)-C(2)	2.456(9)	Ag(6)-C(2)#2	2.461(9)
Ag(11)-C(3)#3	2.493(1)	Ag(15)-C(3)	2.395(9)	Ag(15)-C(3)#3	2.491(9)
Ag(16)-C(3)#3	2.120(9)	Ag(11)-C(4)#3	2.359(1)	Ag(12)-C(4)	2.251(1)
Ag(13)-C(4)	2.160(1)	Ag(15)-C(4)#3	2.445(9)	Ag(15)-C(4)	2.518(9)
Ag(1)···Ag(2)	2.788(1)	Ag(1)···Ag(4)	3.017(1)	Ag(1)···Ag(3)	3.076(1)
Ag(1)···Ag(5)	3.132(1)	Ag(1)···Ag(6)#1	3.302(1)	Ag(2)···Ag(3)	3.061(1)
Ag(3)···Ag(4)	2.951(1)	Ag(3)···Ag(5)#2	2.989(1)	Ag(3)···Ag(6)#2	3.346(1)
Ag(4)···Ag(5)	3.073(1)	Ag(5)···Ag(6)#1	3.334(1)	Ag(5)···Ag(6)#1	3.335(1)
Ag(11)···Ag(13)#3	3.149(1)	Ag(11)···Ag(15)	3.176(1)	Ag(11)···Ag(16)	3.179(1)
Ag(11)···Ag(12)	3.210(1)	Ag(12)···Ag(13)	2.844(1)	Ag(12)···Ag(16)	2.997(1)
Ag(13)···Ag(14)	3.082(1)	Ag(13)···Ag(16)	3.094(1)	Ag(14)···Ag(16)	2.807(1)
Ag(14)···Ag(15)	3.202(1)	Ag(15)···Ag(16)#4	3.130(1)		

[a] Symmetry transformations used to generate equivalent atoms:

For **1**: #1 $x - 1, y, z$.

For **2**: #1 $-x + 2, -y + 2, -z$.

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

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

For **5**: #1 $-x + 1, -y + 1, -z + 1$; #2 $-x + 2, -y + 1, -z + 1$; #3 $-x + 1, -y + 2, -z + 1$.

For **6**: #1 $-x - ½, y - ½, -z + ½$; #2 $-x - ½, y + ½, -z + ½$; #3 $-x + ½, y - ½, -z + ½$; #4 $-x + ½, y + ½, -z + ½$.