Supporting Information

Crystal Structures and Physical Properties of Ag(I) Coordination Polymers with Unsymmetrical Dipyridyl Ligand

Eunji Lee, Hyunsoo Ryu, Suk-Hee Moon,[†] and Ki-Min Park[*]

Department of Chemistry and Research Institute of Natural Science, Gyeongsang National University, Jinju 660-701, Korea
[*]E-mail: kmpark@gnu.ac.kr
[†]Department of Food and Nutrition, Kyungnam College of Information and Technology, Busan 617-701, Korea
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Table S1. Crystal data and structure refinement for **1**, **2** and **3**

Identification code	**1**	**2**	**3**
Empirical formula	$C_{13}H_{17}AgClN_3O_5S$	$C_{13}H_{17}AgBF_4N_3OS$	$C_{13}H_{17}AgF_6N_3OPS$
Formula weight	470.68	458.04	516.20
Temperature (K)	298(2)	298(2)	298(2)
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/n$	$P2_1/n$	$P2_1/n$
a (Å)	8.7565(12)	8.7419(8)	9.1009(10)
b (Å)	12.9289(17)	12.8229(13)	13.2298(15)
c (Å)	15.402(2)	15.1970(14)	15.6584(8)
°	90	90	90
°	99.827(3)	99.536(2)	98.642(2)
°	90	90	90
Volume (Å^3)	1718.1(4)	1680.0(3)	1863.9(4)
Z	4	4	4
Density (calculated) (Mg/m^3)	1.820	1.811	1.839
Absorption coefficient (mm^{-1})	1.479	1.370	1.344
F(000)	997	912	1024
Crystal size (mm^3)	0.20×0.20×0.10	0.30×0.20×0.20	0.50×0.40×0.40
Theta range for data collection	2.07 to 25.99°	2.09 to 26.00°	2.02 to 26.00°
Reflections collected	9668	9399	10387
Independent reflections	3372 [R(int) = 0.1146]	3290 [R(int) = 0.0813]	3667 [R(int) = 0.0589]
Completeness to theta = 26.00°	100.0%	99.9%	100.0%
Absorption correction	None		
Refinement method	Full-matrix least-squares on F^2		
Data / restraints / parameters	3372 / 0 / 236	3290 / 0 / 236	3667 / 0 / 253
Goodness-of-fit on F^2	1.034	1.007	1.045
R_1, wR_2 [$I > 2\sigma(I)$]	0.0517, 0.1252	0.0504, 0.1145	0.0487, 0.1317
R_1, wR_2 [all data]	0.1425, 0.1656	0.1141, 0.1491	0.0859, 0.1586
Largest diff. peak and hole (e.Å^{-3})	0.733 and -1.022	0.879 and -0.775	0.552 and -0.788

Table S2. Hydrogen bond geometries (Å, °) for **1**, **2**, and **3**

D-H···A	*d*(D-H)	*d*(H···A)	*d*(D···A)	<(DHA)	Symmetry code on A atom
Compound **1**					
N3-H3···O5	0.86	2.19	2.963(9)	149.5	*x*, *y*, *z*
C9-H9···O3	0.93	2.57	3.417(12)	150.9	–*x*, –*y*, –*z*+1
C12-H12A···O4	0.96	2.32	3.16(3)	146.4	*x*, *y*, *z*
C13-H13D···O2	0.96	2.50	3.398(13)	155.4	*x*+1/2, –*y*+1/2, *z*–1/2
Compound **2**					
N3-H3···O5	0.86	2.21	2.965(7)	147.1	*x*, *y*, *z*
C12-H12A···F4	0.96	2.28	3.11(2)	144.9	*x*, *y*, *z*
C12-H12B···F3	0.96	2.51	3.47(2)	177.0	–*x*+1, –*y*, –*z*+1
C13-H13F···F1	0.96	2.46	3.335(12)	151.9	*x*+1, *y*, *z*
C13-H13D···F2	0.96	2.50	3.398(11)	155.6	*x*+1/2, –*y*+1/2, *z*–1/2
Compound **3**					
N3-H3···O5	0.86	2.13	2.937(6)	156.2	*x*, *y*, *z*
C3-H3A···F5	0.93	2.42	3.201(9)	141.6	*x*–1/2, –*y*+1/2, *z*–1/2
C12-H12A···F2	0.96	2.41	3.33(2)	159.1	*x*, *y*, *z*
C12'-H12E···F4	0.96	2.59	3.45(2)	149.1	*x*+1, *y*, *z*

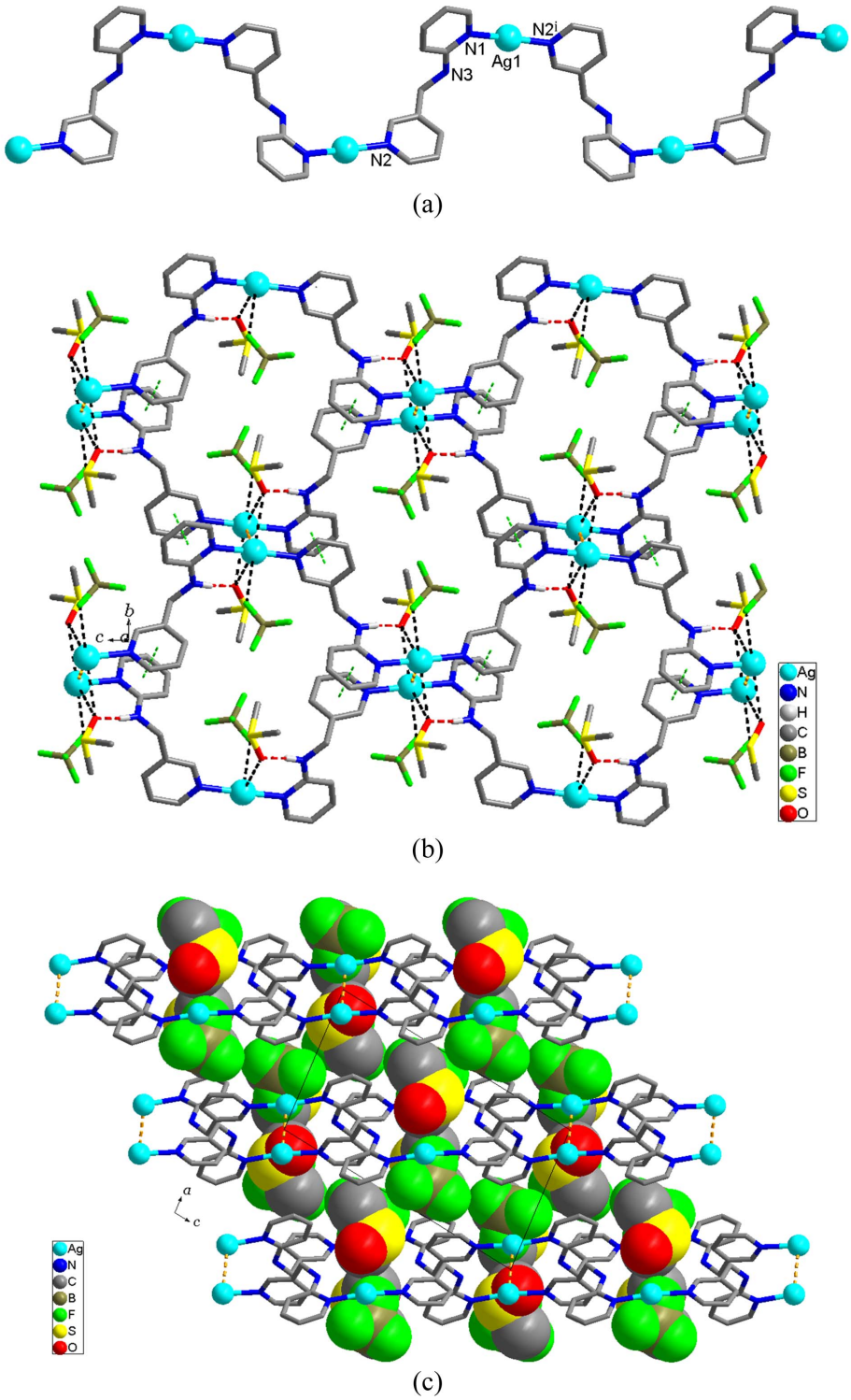

Figure S1. Honeycomb type 2-D network structure of **2**, $\{[Ag(L)]\cdot(BF_4)\cdot(DMSO)\}_n$: (a) 1-D zigzag chain showing coordination environment, (b) 2-D framework showing several interactions (dashed lines): Ag···Ag interactions (yellow), Ag···O interactions (black), N-H···O hydrogen bonds (red), and π···π stacking interactions (green), and (c) side view of packing arrangement of 2-D layers. H atoms and the disordered part of DMSO molecules are omitted. [Symmetry codes: (i) 0.5+*x*, 0.5-*y*, 0.5+*z*; (ii) -0.5+*x*, 0.5-*y*, -0.5+*z*].

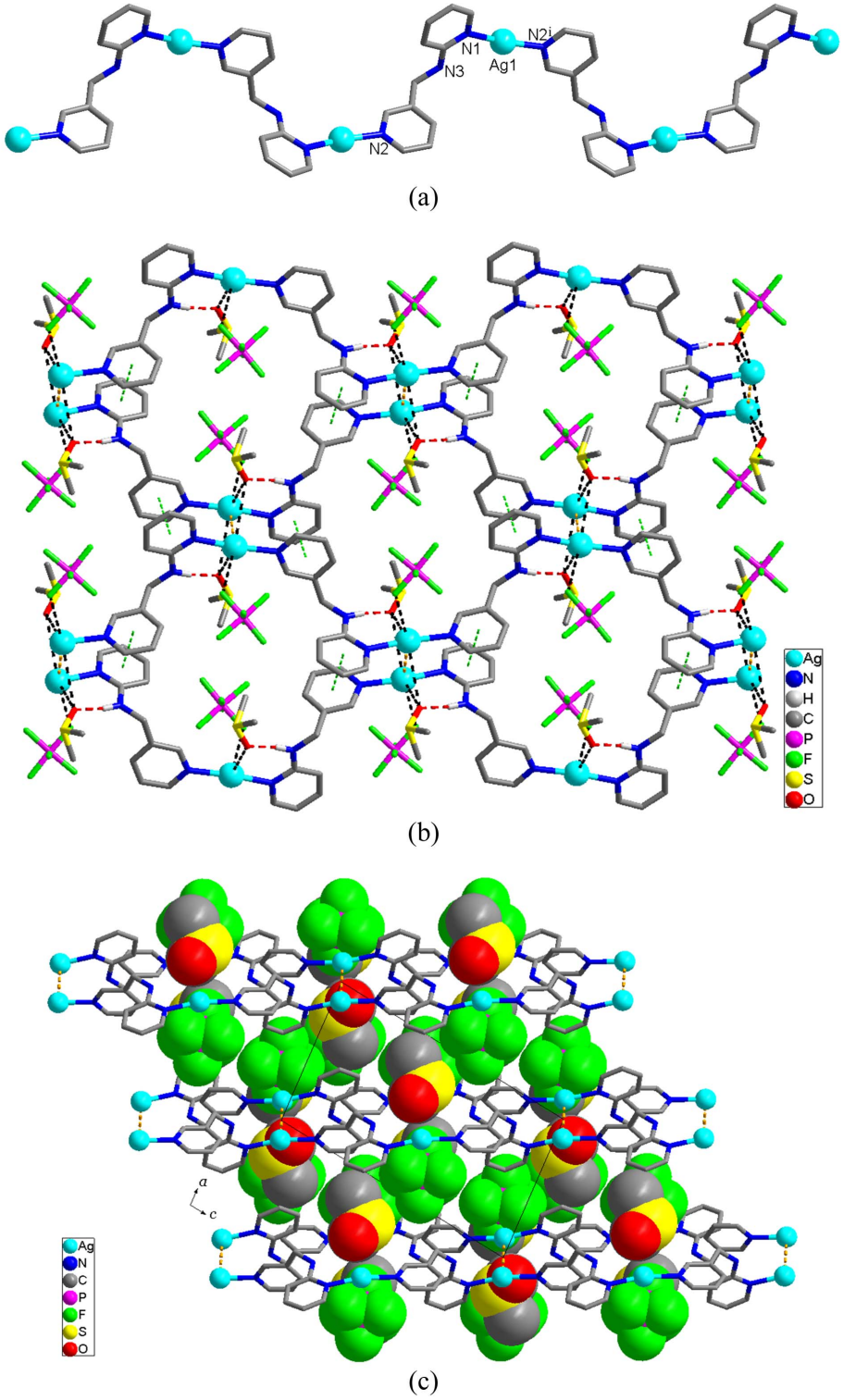

Figure S2. Honeycomb type 2-D network structure of **3**, $\{[Ag(L)]\cdot(PF_6)\cdot(DMSO)\}_n$: (a) 1-D zigzag chain showing coordination environment, (b) 2-D framework showing several interactions (dashed lines): Ag···Ag interactions (yellow), Ag···O interactions (black), N-H···O hydrogen bonds (red), and π···π stacking interactions (green), and (c) side view of packing arrangement of 2-D layers. H atoms and the disordered part of DMSO molecules are omitted. [Symmetry codes: (i) 0.5+*x*, 0.5-*y*, 0.5+*z*; (ii) -0.5+*x*, 0.5-*y*, -0.5+*z*].

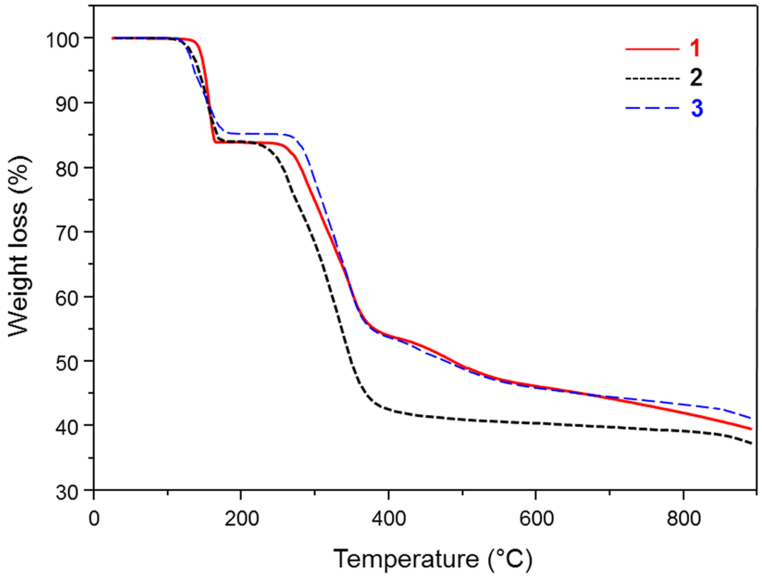

Figure S3. TGA curves of complexes 1-**3**.