Electronic Supporting Information for:

Solvothermal In-situ Synthesis of Cyanide-contained Ternary Silver(I) Coordination Polymers and their Phosphorescent Properties

Yun Ling, Fu-Peng Zhai, Ming-Li Deng, Dong Wu, Zhen-Xia Chen, Xiao-Feng Liu, Ya-Ming Zhou,* Lin-Hong Weng

Shanghai Key Laboratory of Molecular Catalysis and Innovative Materials, Department of Chemistry, Fudan University, Shanghai (200433), China.

* To whom corresponding: Dr. Y.M. Zhou, E-mail: ymzhou@fudan.edu.cn;

Fax: +86 21 65643925; Tel: +86 21 65642261

Table S1. Selected bond length (Å) and angles (°) for **1**, **2**, **3**, **4**

1			
Ag1–N1	2.226(10)	Ag1–C5	2.083(13)
Ag1–N5 ^{i}	2.318(12)	Ag2–N3	2.171(11)
Ag2–N6 ^{ii}	2.166(10)	Ag3–N2	2.162(12)
Ag3–N4	2.165(12)	Ag3–N7 ^{iii}	2.630(14)
N7–C5	1.122(19)		
N1–Ag1–C5	137.7(5)	N1–Ag1–N5 ^{i}	95.2(4)
N5 ^{i}–Ag1–C5	126.8(5)	N3–Ag2–N6 ^{ii}	165.9(5)
N2–Ag3–N4	171.0(4)		
2			
Ag1–N1	2.127(3)	Ag2–N2	2.191(3)
Ag2–C7/N4	2.126(4)	Ag2–N3 ^{iv}	2.261(3)
C7–N4	1.118(7)		
N1–Ag1–N1 ^{v}	153.27(11)	N2–Ag2–C7/N4	128.00(14)
N2–Ag2–N3 ^{iv}	115.00(10)	N3^{iv}–Ag2–C7/N4	116.67(13)
3			
Ag1–N1	2.075(11)	Ag1–C18 ^{vi}	2.026(14)
Ag2–N2	2.201(11)	Ag2–N4	2.182(10)
Ag2–N7	2.118(11)	Ag3–N3	2.231(10)
Ag3–N5	2.234(11)	Ag3–N8	2.173(12)
Ag4–N6	2.082(10)	Ag4–C17 ^{vii}	2.057(13)
N7–C17	1.143(17)	N8–C18	1.149(18)
N1–Ag1–C18 ^{vi}	174.8(5)	N2–Ag2–N4	117.4(4)
N2–Ag2–N7	119.9(4)	N4–Ag2–N7	122.1(4)
N3–Ag3–N5	117.4(4)	N3–Ag3–N8	121.3(4)
N5–Ag3–N8	116.9(4)	N6–Ag4–C17 ^{vii}	174.4(5)
4			
Ag1–N2	2.074(10)	Ag1–N4	2.083(8)
Ag2–N5	2.350(8)	Ag2–C18/N8	2.085(11)
Ag2–N6 ^{viii}	2.165(8)	Ag3–N1	2.220(10)
Ag3–C17/N7	2.066(16)	Ag3–N3^{ix}	2.225(10)
C17–N7	1.14(2)	C18–N8	1.15(2)
N2–Ag1–N4	178.0(3)	N5–Ag2–C18	111.2(4)
N5–Ag2–N6 ^{viii}	105.0(3)	N6^{viii}–Ag2–C18	143.8(4)
N1–Ag3–C17	128.1(5)	N1–Ag3–N3 ^{ix}	105.3(4)
N3^{ix}–Ag3–C17	126.6(5)		

Symmetry code used: i: -x, 1-y, 2-z; ii: 1+x,1+y,-1+z; iii: -1+x,1+y,z; iv : 1/2-x,1/2-y,1-z; v: -x,y,3/2-z; vi: 2-x,-1/2+y,1/2-z; vii: 1-x,1/2+y,3/2-z; viii: 1/2-x,-1/2+y,z; ix: 1/2-x,1/2+y,z

Fig. S1. the PXRD patterns for **1** (a), **2** (b), **3** (c), **4** (d) compared with its simulated one (I: the simulated data from CIF, II: the solvothermal in-situ product, III: the product obtained using AgCN as the source.)

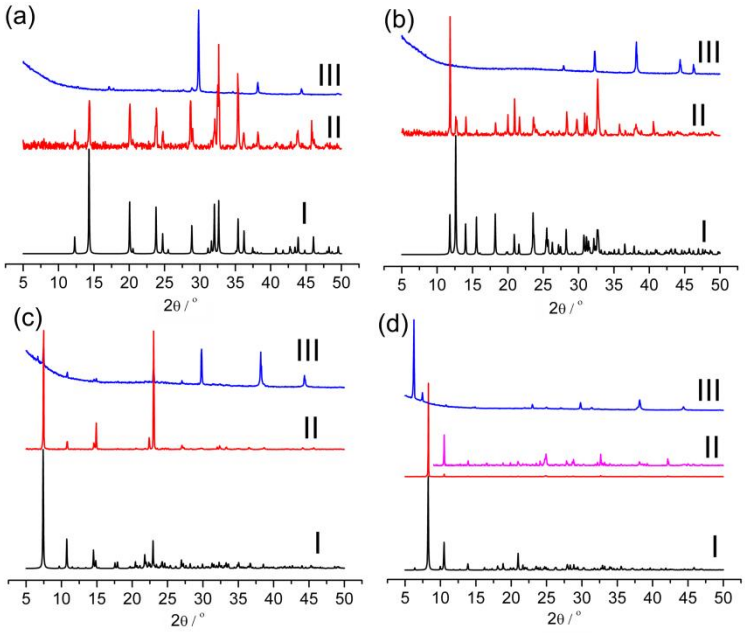

Fig. S2. the IR spectra of **1**, **2**, **3**, **4** and $[Ag_3(dmtrz)_2CN]_n$ showing characteristic absorption bands of CN- group

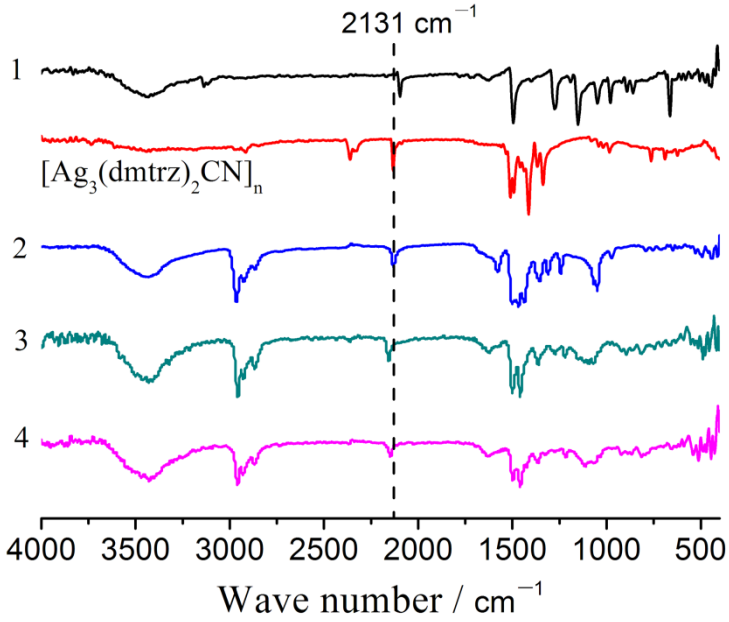

Fig. S3. the TGA data of **1(a)**, **2(b)**, **3(c)** ,**4(d)** and $[Ag_3(dmtrz)_2CN]_n$.

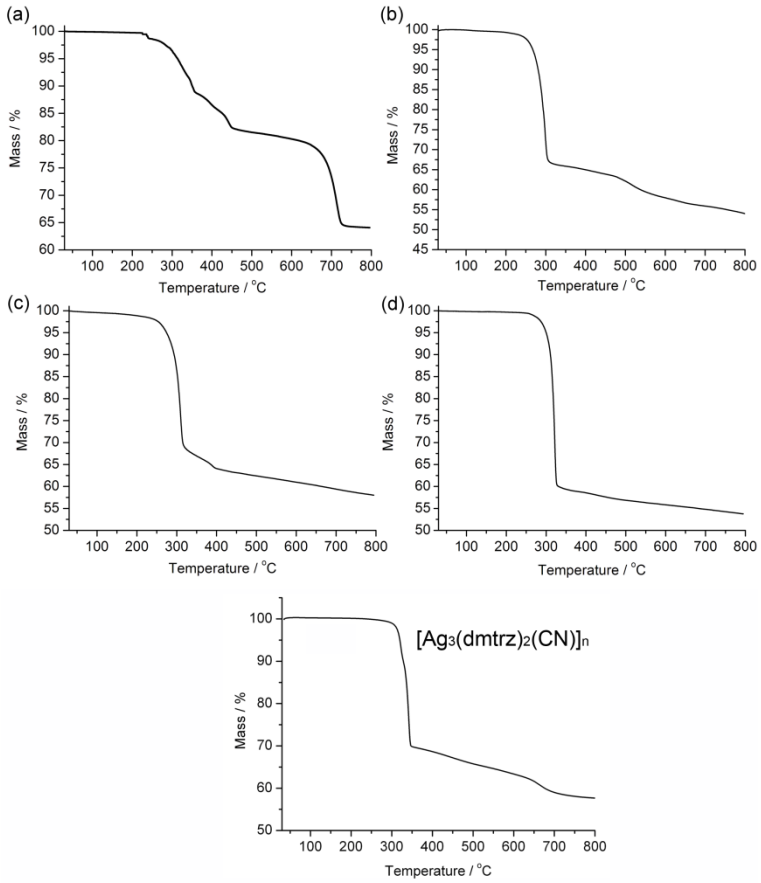

Fig. S4. (a) the 2D layer structure of **1** generated by connecting neighboring 1D chain structures through Ag(3)···N(7) interactions (*ca.* distance 2.603 Å); (b) 3D packing structure generated by connecting neighboring 2D layers through argentophilic interactions

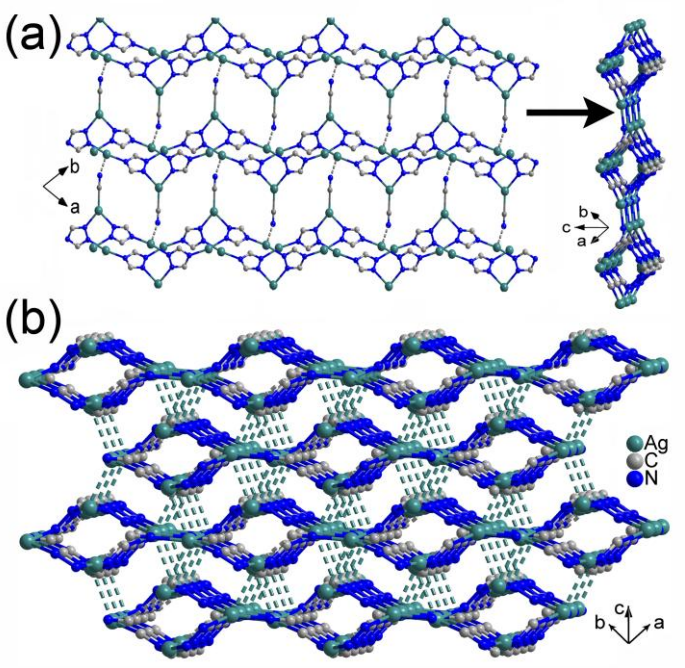

Fig. S5. the phosphorescent property of **1** (dot-line: excitation spectra; red solid-line: emission spectra at room temperature, blue solid-line: emission spectra at 77K)

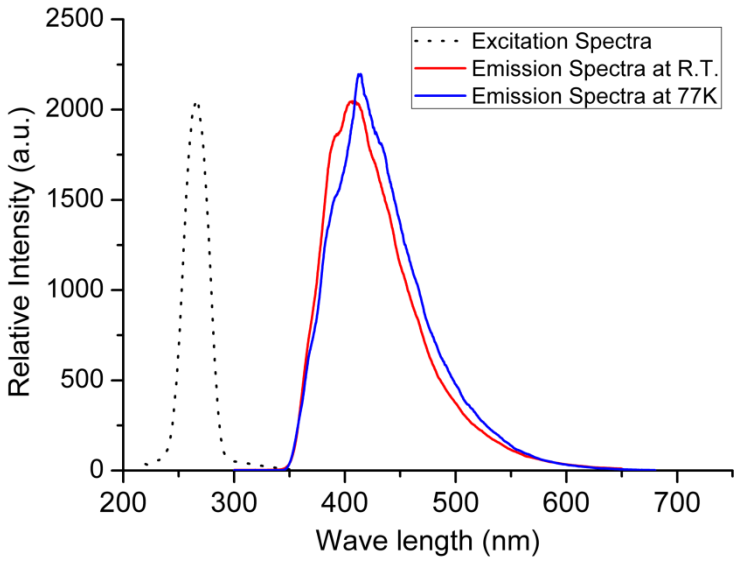

Fig. S6. the phosphorescent property of **2** (dot-line: excitation spectra; red solid-line: emission spectra at room temperature, blue solid-line: emission spectra at 77K)

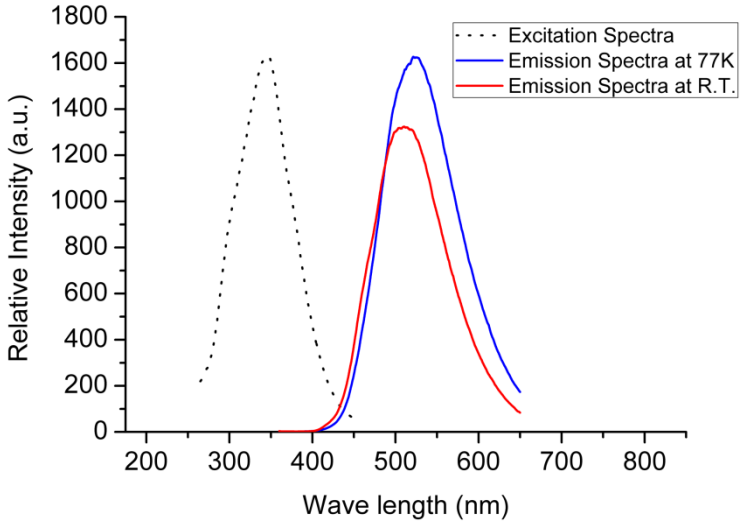

Fig. S7. the phosphorescent property of **3** (red solid-line: emission spectra at room temperature, blue solid-line: emission spectra at 77K, exictated by 340 nm)

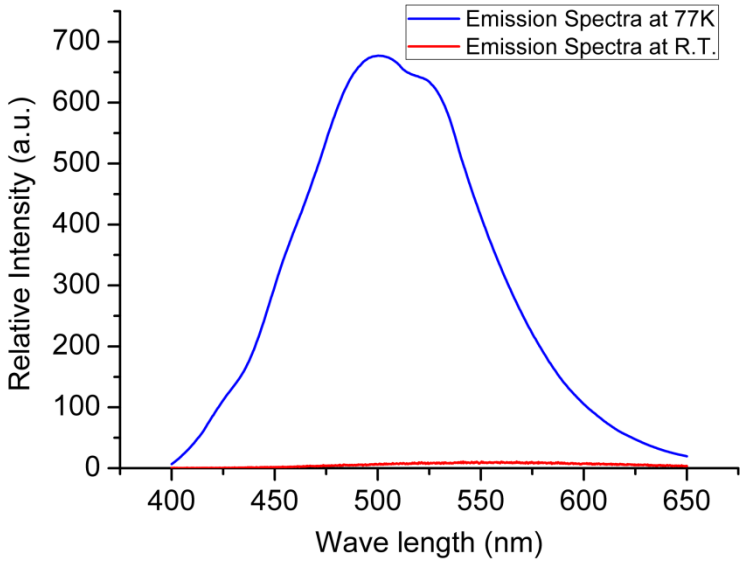

Fig. S8. the phosphorescent property of **4** (red solid-line: emission spectra at room temperature, blue solid-line: emission spectra at 77K, exictated by 340 nm)

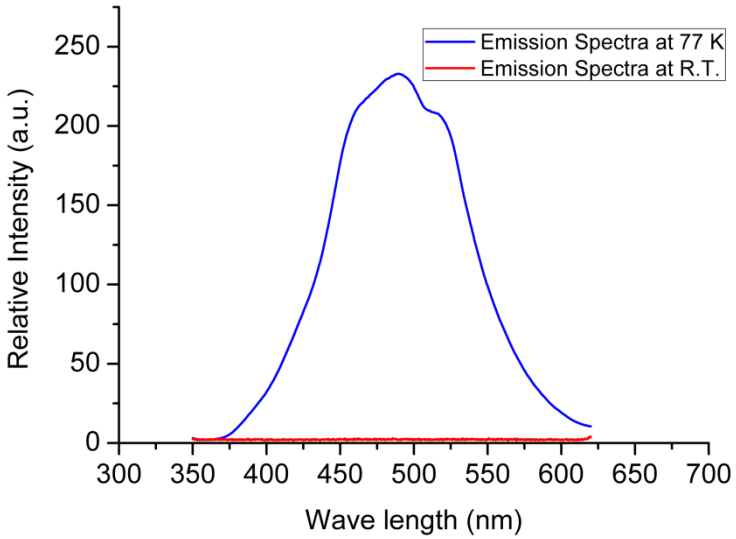

Fig. S9. Energy band structures and density of states (total and partial) of **1** (a and c) and $[Ag(trz)]_n$ (b and d) (theoretical calculation of the electronic band structure of **1** and $[Ag(trz)]_n$ along with density of states has been carried out with the DMol^3 code. the Fermi level is set at 0 Ha. The calculated energy gaps for **1** and $[Ag(trz)]_n$ are 0.151 and 0.149 Ha, respectively, which are very close. 1Ha = 27.2114 ev)