Supplementary Material (ESI) for CrystEngComm

Supporting Information File

A series of metal-organic frameworks based on polydentate Schiff-base ligands derived from benzil dihydrazone: synthesis, crystal structures and luminescent properties

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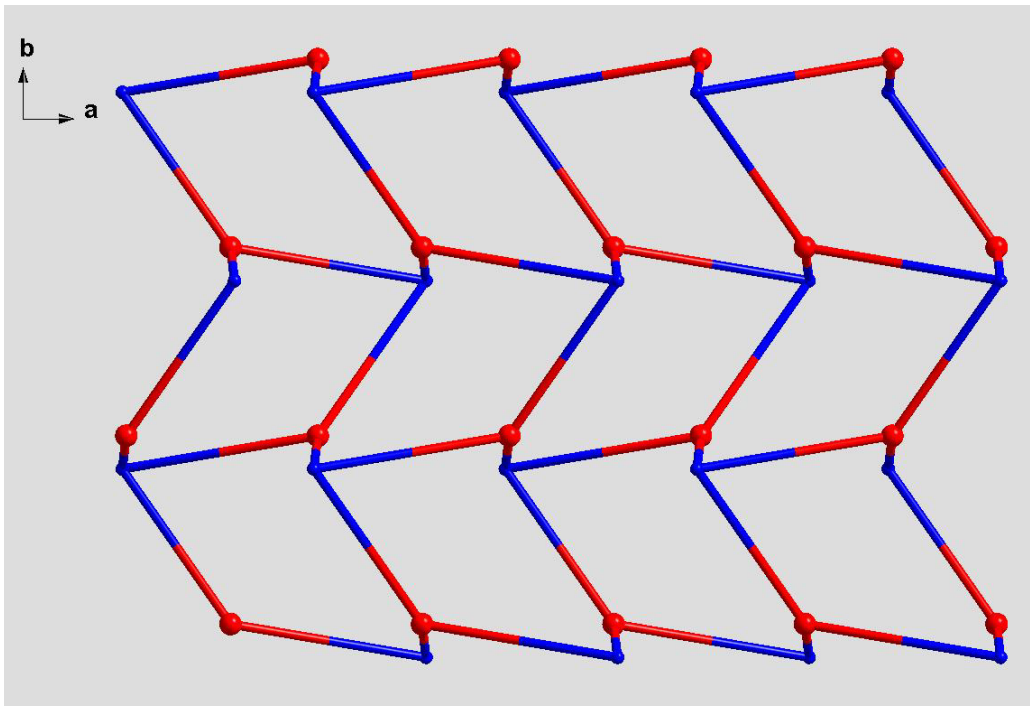
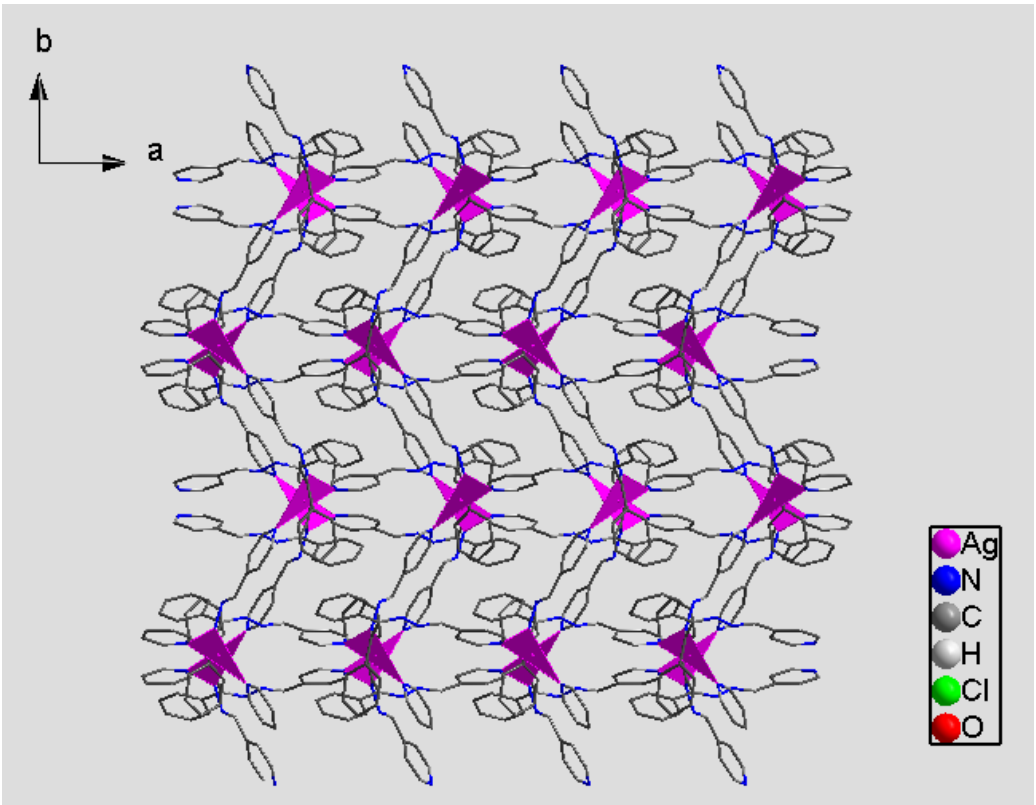


(a)



(b)

Figure S1. (a) Schematic illustration of such 2D motif. (b)View of 3D supramolecular structure of **1**.

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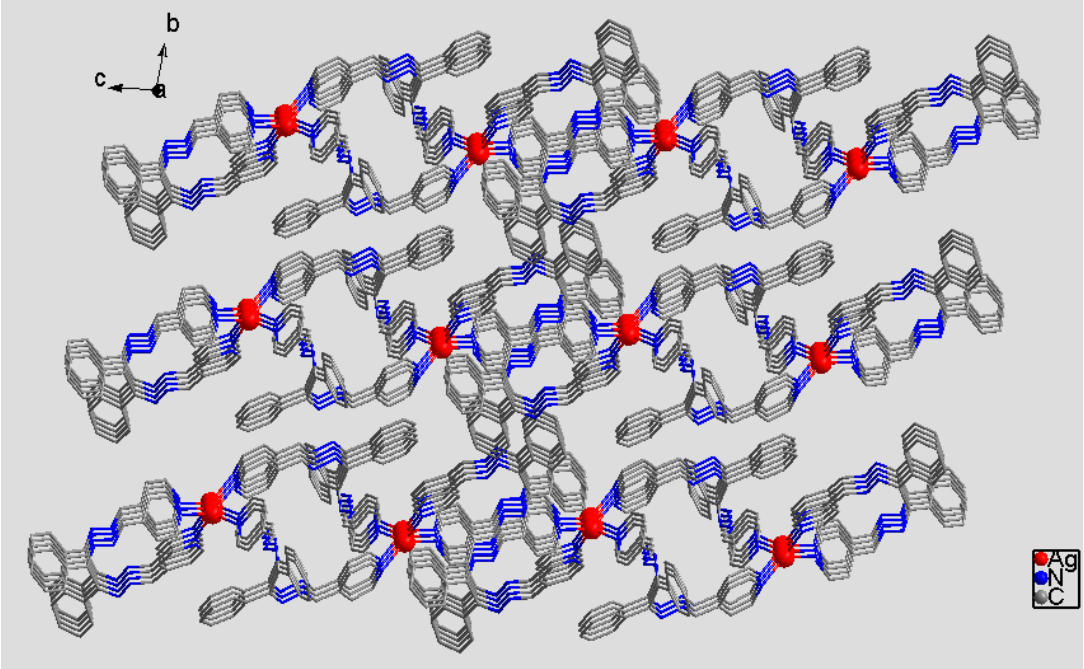

Figure S2. View of 3D supramolecular structure of **2**.

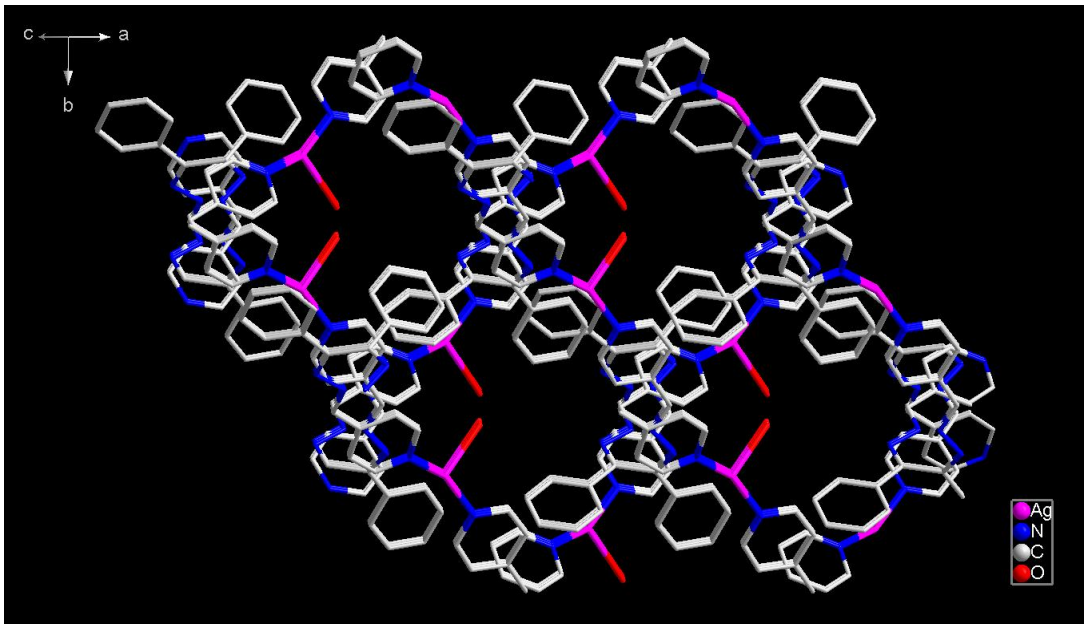

Figure S3. View of 3D supramolecular structure of **3**. The N atoms and uncoordinated oxygen atoms of nitrate anions and solvent molecules are omitted for clarity.

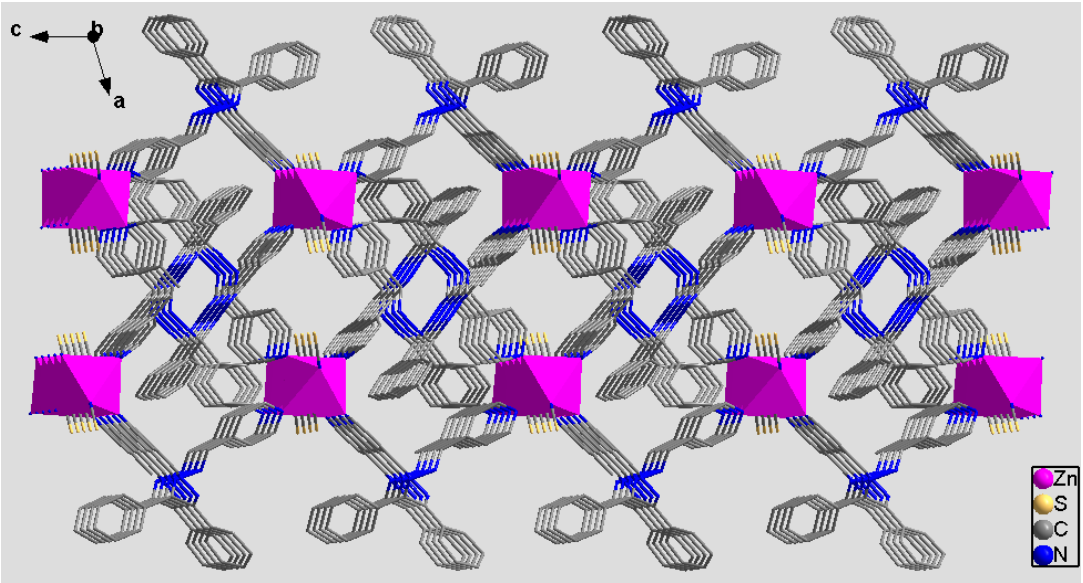

Figure S4. View of 3D supramolecular structure of **4.**

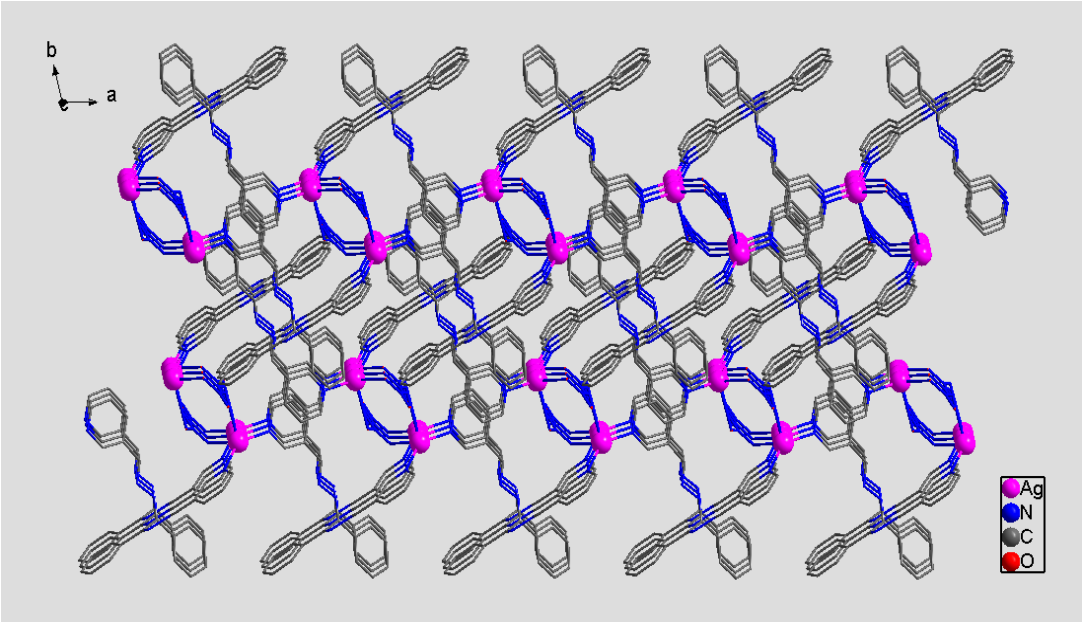

Figure S5. View of 3D supramolecular structure of **5**.

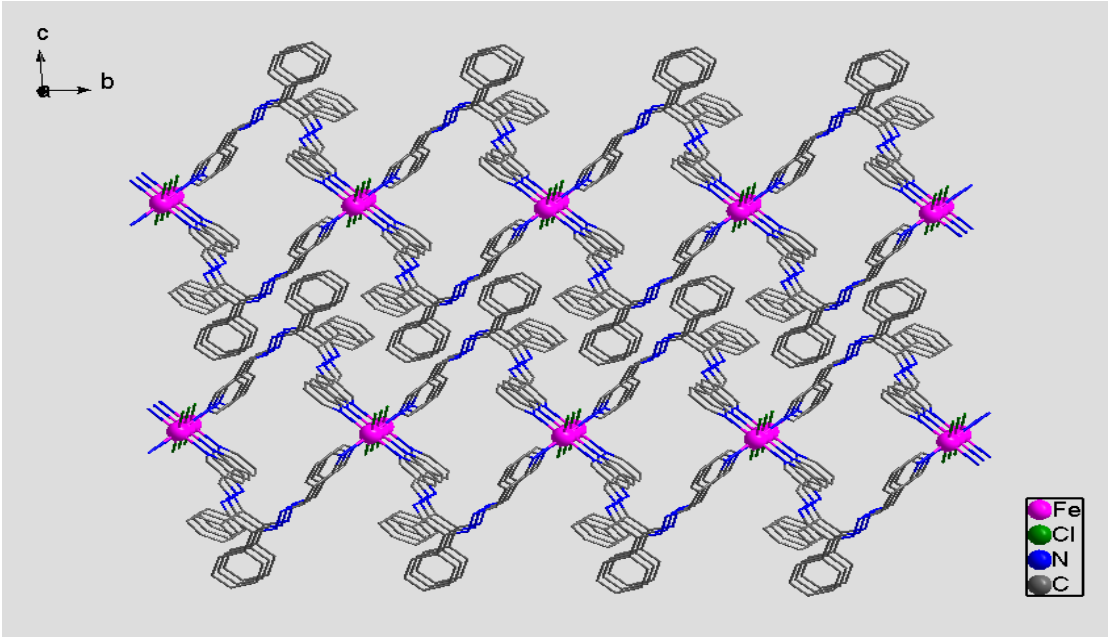

Figure S6. View of 3D supramolecular structure of **6**.

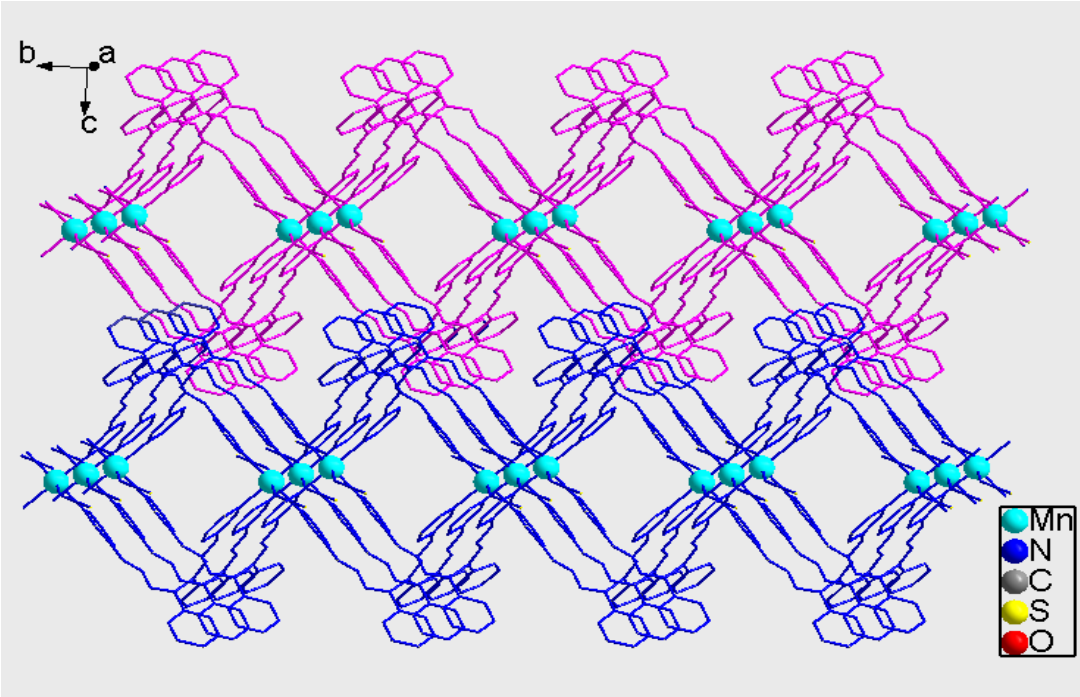

Figure S7. View of 3D supramolecular structure of **7**.

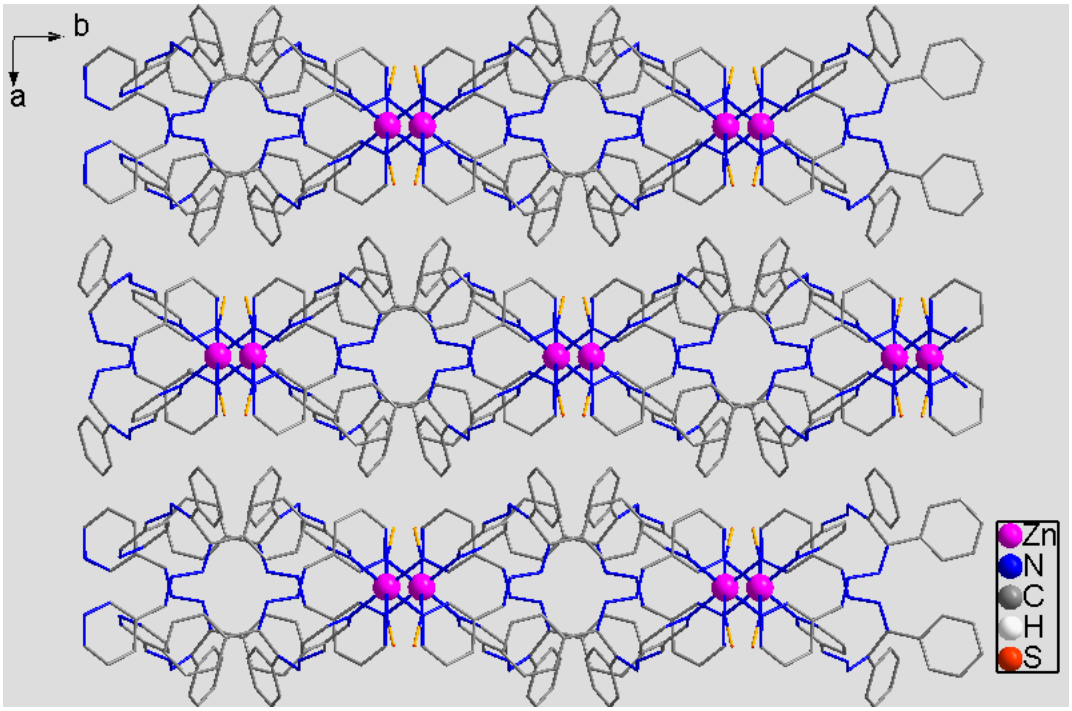

Figure S8. View of 3D supramolecular structure of **8** along c-axis.

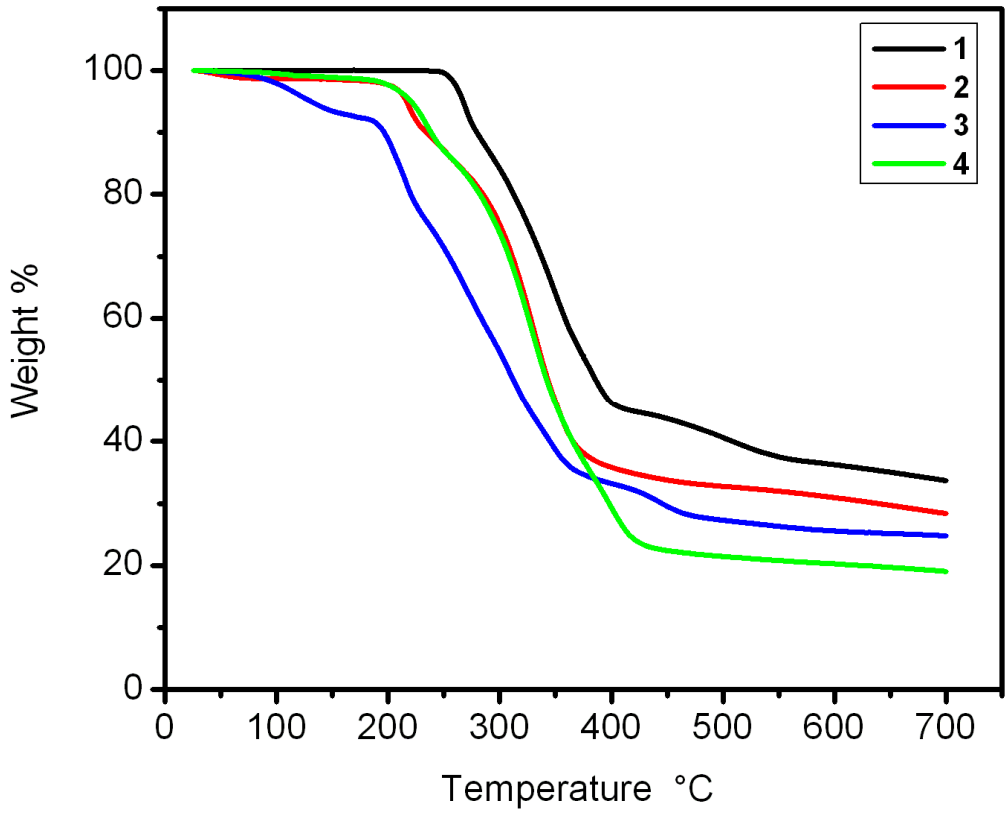

Figure S9. TGA curves for **1**–**4** polymers.

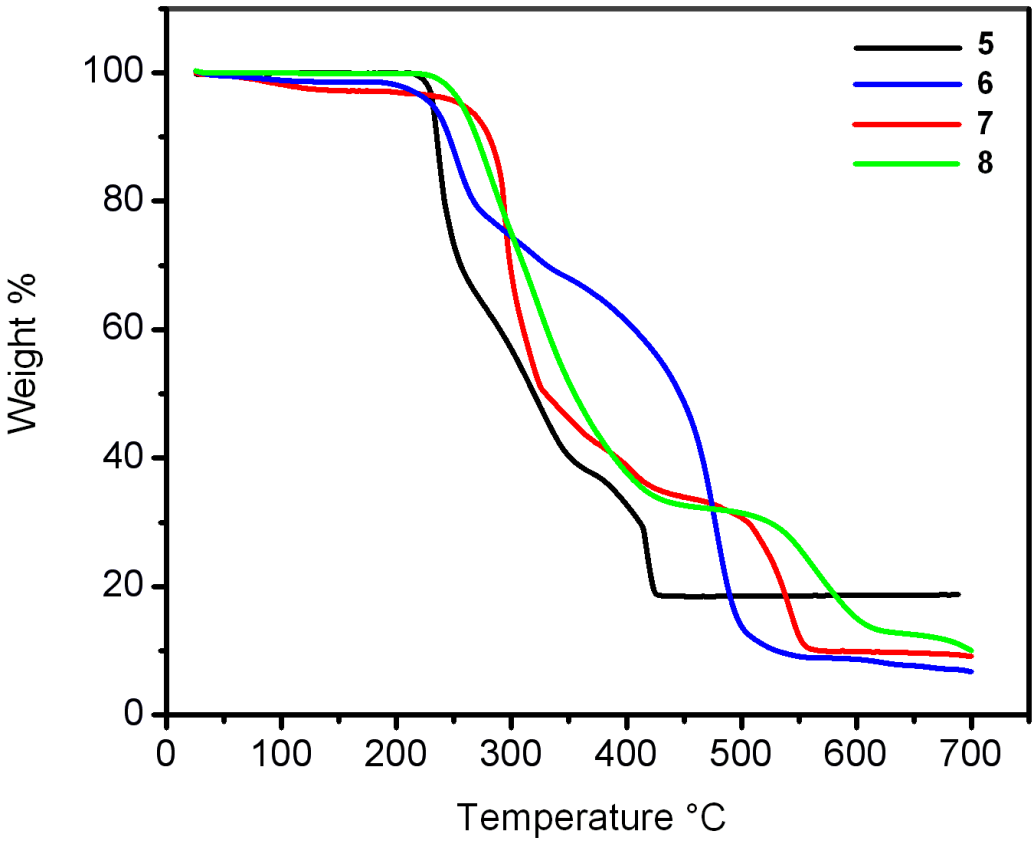

Figure S10. TGA curves for **5–8** polymers.

Table S1. Selected Bond Distances (Å) and Bond Angles (°) for **1**–**4**.

Compound **1**			
Ag(1)–N(1B)	2.202(2)	Ag(1)–N(3C)	2.375(2)
Ag(1)–N(6)	2.230(2)		
N(1B)–Ag(1)–N(3C)	123.68(7)	N(1B)–Ag(1)–N(6)	132.26(8)
N(6)–Ag(1)–N(3C)	104.03(8)		
Compound **2**			
Ag(1)–N(1)	2.336(2)	Ag(1)–N(6A)	2.366(2)
Ag(1)–N(7)	2.285(2)	Ag(1)–N(12B)	2.441(2)
N(1)–Ag(1)–N(6A)	96.25(9)	N(1)–Ag(1)–N(12B)	90.70(8)
N(6A)–Ag(1)–N(12B)	126.52(9)	N(7)–Ag(1)–N(1)	136.55(9)
N(7)–Ag(1)–N(6A)	110.83(9)	N(7)–Ag(1)–N(12B)	98.83(9)
Compound **3**			
Ag(1)–N(1)	2.179(5)	Ag(1)–N(6A)	2.158(6)
Ag(1)–O(2)	2.706(17)		
N(6A)–Ag(1)–N(1)	155.9(2)	N(6A)–Ag(1)–O(2)	118.8(5)
N(1)–Ag(1)–O(2)	85.2(5)		
Compound **4**			
Zn(1)–N(1)	2.221(5)	Zn(1)–N(6A)	2.210(5)
Zn(1)–N(7)	2.232(5)	Zn(1)–N(12B)	2.216(4)
Zn(1)–N(13)	2.108(5)	Zn(1)–N(14)	2.072(5)
N(1)–Zn(1)–N(6A)	92.17(17)	N(1)–Zn(1)–N(7)	178.18(17)
N(1)–Zn(1)–N(12B)	95.54(17)	N(7)–Zn(1)–N(6A)	86.93(17)
N(12B)–Zn(1)–N(6A)	171.02(16)	N(12B)–Zn(1)–N(7)	85.49(16)
N(13)–Zn(1)–N(1)	89.45(18)	N(13)–Zn(1)–N(6A)	86.59(17)
N(13)–Zn(1)–N(7)	92.07(18)	N(13)–Zn(1)–N(12B)	88.89(17)
N(14)–Zn(1)–N(1)	90.14(18)	N(14)–Zn(1)–N(6A)	93.18(18)
N(14)–Zn(1)–N(7)	88.33(18)	N(14)–Zn(1)–N(12B)	91.39(18)
N(14)–Zn(1)–N(13)	179.5(2)		

Symmetry transformations used to generate equivalent atoms: **1**: B 1/2 – *x*, 1/2 + *y*, *z*; C –1/2 + *x*, *y*, 1/2 – *z*; **2**: A 1+x, y, z, B –x, 2–y, 2–z; **3**: A –1 + *x*, –*y*, –1/2 + *z*; **4**: A *x*, 3/2 – *y*, 1/2 + *z*; B *x*, 5/2 – *y*, –1/2 + *z*.

Table S2. Selected Bond Distances (Å) and Bond Angles (°) for **5**–**8.**

Compound **5**			
Ag(1)–N(1)	2.192(3)	Ag(1)–N(6A)	2.170(3)
Ag(1)–O(3)	2.625(3)	Ag(1)–O(1B)	2.720(4)
N(6A)–Ag(1)–N(1)	144.32(10)	N(6A)–Ag(1)–O(3)	102.24(11)
N(1)–Ag(1)–O(3)	96.55(11)	N(6A)–Ag(1)–O(1B)	121.80(11)
N(1)–Ag(1)–O(1B)	90.07(10)	O(3)–Ag(1)–O(1B)	83.48(11)
Compound **6**			
Fe(1)–N(1)	2.320(2)	Fe(1)–N(6B)	2.226(2)
Fe(1)–Cl(1)	2.435(1)		
N(6B)–Fe(1)–N(1)	86.20(7)	N(6C)–Fe(1)–N(1)	93.80(7)
N(1)–Fe(1)–Cl(1)	89.27(5)	N(1)–Fe(1)–Cl(1A)	90.73(5)
N(6B)–Fe(1)–Cl(1)	88.94(5)	N(6C)–Fe(1)–Cl(1)	91.06(5)
Compound **7**			
Mn(1)–N(1)	2.308(2)	Mn(1)–N(6B)	2.366(2)
Mn(1)–N(7)	2.151(2)		
N(1)–Mn(1)–N(6B)	86.50(8)	N(1)–Mn(1)–N(6C)	93.50(8)
N(7)–Mn(1)–N(1)	89.37(9)	N(7A)–Mn(1)–N(1)	90.63(9)
N(7)–Mn(1)–N(6B)	90.49(8)	N(7)–Mn(1)–N(6C)	89.51(8)
Compound **8**			
Zn(1)–N(1)	2.230(2)	Zn(1)–N(6B)	2.186(2)
Zn(1)–N(7)	2.086(2)		
N(7)–Zn(1)–N(7A)	179.12(12)	N(7)–Zn(1)–N(6C)	90.85(8)
N(7A)–Zn(1)–N(6C)	89.78(8)	N(6B)–Zn(1)–N(6C)	87.58(10)
N(1)–Zn(1)–N(1A)	89.65(10)	N(6B)–Zn(1)–N(1)	91.39(7)
N(7)–Zn(1)–N(1)	89.56(8)	N(7)–Zn(1)–N(1A)	89.82(8)
N(6C)–Zn(1)–N(1)	178.88(7)	N(6B)–Zn(1)–N(1)	91.39(7)

Symmetry transformations used to generate equivalent atoms: **5**: A − 1 + *x*, *y*, *z*; B − 1 − *x*, 2 − *y*, 2 − *z*; **6**: A −1− *x*, −1 − *y*, −1− *z*; B −1+ *x*, −1 + *y*, *z* ; C − *x*, − *y*, −1− *z*； **7**: A − *x*, 2 − *y*, 1 − *z*; B −1 + *x*, 1 + *y*, *z* ; C 1 − *x*, 1 − *y*, 1 − *z* ； **8**: A − *x*, *y*, 1/2 − *z*; B − *x*, − *y*, 1 − *z*; C *x*, − *y*, −1/2 + *z*.

Table S3. Hydrogen Bonding Interactions (A˚ and °) of **1**–**6**.

D–H···A	D–H	H···A	D···A	∠DHA	Symmetry Codes
Compound **1**					
C(2)–H(2)···O(1)	0.94	2.51	3.210(4)	132	3/2 – *x*, – 1/2 + *y*, *z*
C(2)–H(2)···O(3)	0.94	2.52	3.339(4)	146	3/2 – *x*, – 1/2 + *y*, *z*
C(6)–H(6)···O(1)	0.94	2.54	3.413(4)	155	–1/2 + *x*, *y*, 1/2 – *z*
C(24)–H(24)···O(2)	0.94	2.59	3.242(5)	127	–1/2 + *x*, *y*, 1/2 – *z*
Compound **2**					
C(26)–H(26)···F(1)	0.93	2.42	3.280(4)	154	– *x*, 2 – *y*, 1 – *z*
C(29)–H(29)···F(2)	0.93	2.42	3.282(4)	153	– *x*, 1 – *y*, 1 – *z*
C(38)–H(38)···F(4)	0.93	2.44	3.320(4)	159	1 + *x*, *y*, 1 + *z*
C(42)–H(42)···N(9)	0.93	2.60	3.438(3)	151	1 – *x*, 1 – *y*, 2 – *z*
Compound **3**					
O(4)–H(4B)···O(1)	0.85	2.05	2.88(2)	166	
O(4)–H(4B)···O(2)	0.85	2.50	3.12(2)	131	
O(4)–H(4B)···O(2')	0.85	2.59	3.20(3)	130	
C(12)–H(12A)···O(2')	0.93	2.56	3.30(3)	136	1/2 + *x*, – 1/2 – *y*, 1/2 + *z*
C(12)–H(12A)···O(3')	0.93	2.56	3.44(3)	160	1/2 + *x*, – 1/2 – *y*, 1/2 + *z*
C(17)–H(17A)···O(1')	0.93	2.49	3.27(3)	142	*x*, – 1 + *y*, *z*
C(21)–H(21A)···O(4)	0.93	2.49	3.276(14)	142	*x*, – *y*, 1/2 + *z*
C(24)–H(24A)···O(1)	0.93	2.54	3.30(2)	139	1/2 + *x*, 1/2 – *y*, 1/2 + *z*
C(24)–H(24A)···O(1')	0.93	2.54	3.20(2)	128	1/2 + *x*, 1/2 – *y*, 1/2 + *z*
C(25)–H(25A)···O(3')	0.93	2.24	2.92(3)	129	1 + *x*, –*y*, 1/2 + *z*
Compound **4**					
C(2)–H(2A)···N(14)	0.93	2.53	3.090(9)	119	
C(3)–H(3A)···N(13)	0.93	2.58	3.160(8)	121	
C(18)–H(18A)···N(15')	0.93	2.54	3.24(2)	132	– 2 – *x*, 2 – *y*, – 1 – *z*
C(25)–H(25A)···N(13)	0.93	2.51	3.023(8)	115	*x*, 3/2 – *y*, – 1/2 + *z*
C(50)–H(50A)···N(13)	0.93	2.51	3.077(8)	119	*x*, 5/2 – *y*, 1/2 + *z*
Compound **5**					
C(1)–H(1A)···O(1)	0.93	2.49	3.258(6)	140	– 1 – *x*, 2 – *y*, 2 – *z*
C(3)–H(3A)···O(2)	0.93	2.53	3.268(5)	137	1 + *x*, *y*, *z*
C(16)–H(16A)···N(3)	0.93	2.54	3.390(4)	152	– *x*, 1 – *y*, 1 – *z*
Compound **6**					
C(1)–H(1A)···Cl(1)	0.93	2.60	3.291(3)	131	– 1 – *x*, – 1 – *y*, – 1 – *z*
C(2)–H(2A)···Cl(1)	0.93	2.67	3.330(2)	128	