Supporting information

Coordination Assemblies of seven Metal-Organic Frameworks based on a long bent connector under different conditions: structural diversity and properties

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Table S1. Selected bond lengths (Å) and bond angles (°) for 1

1			
Bond lengths (Å)			
Zn(1)-O(4)	1.949(3)	Zn(2)-O(8)	1.972(3)
Zn(1)-O(1)	1.955(3)	Zn(2)-N(9)#1	1.997(3)
Zn(1)-N(22)	2.017(4)	Zn(2)-N(1)#2	2.038(4)
Zn(1)-N(8)	2.041(4)	N(1)-Zn(2)#2	2.038(4)
Zn(2)-O(6)	1.945(3)	N(9)-Zn(2)#5	1.997(3)
Bond angles (°)			
O(4)-Zn(1)-O(1)	112.93(16)	O(6)-Zn(2)-O(8)	103.48(17)
O(4)-Zn(1)-N(22)	96.59(16)	O(6)-Zn(2)-N(9)#1	115.88(16)
O(1)-Zn(1)-N(22)	131.63(16)	O(8)-Zn(2)-N(9)#1	128.28(16)
O(4)-Zn(1)-N(8)	117.81(16)	O(6)-Zn(2)-N(1)#2	101.22(15)
O(1)-Zn(1)-N(8)	99.83(15)	O(8)-Zn(2)-N(1)#2	96.33(16)
N(22)-Zn(1)-N(8)	98.76(15)	N(9)#1-Zn(2)-N(1)#2	106.81(14)
Symmetry transformations used to generate equivalent atoms: #1 x+2,y,z-1; #2 -x+4,-y+2,-z+1; #3 -x+1,-y+2,-z+1; #4 -x+3,-y+2,-z; #5 x-2,y,z+1			

Table S2. Selected bond lengths (Å) and bond angles (°) for 3

3			
Bond lengths (Å)			
Zn(1)-O(4)#1	1.939(4)	Zn(1)-N(8)#2	2.028(5)
Zn(1)-O(1)	1.952(4)	N(8)-Zn(1)#3	2.028(5)
Zn(1)-N(1)	1.996(5)	O(4)-Zn(1)#4	1.939(4)
Bond angles (°)			
O(4)#1-Zn(1)-O(1)	99.75(18)	O(4)#1-Zn(1)-N(8)#2	102.6(2)
O(4)#1-Zn(1)-N(1)	115.3(2)	O(1)-Zn(1)-N(8)#2	112.8(2)
O(1)-Zn(1)-N(1)	111.10(19)	N(1)-Zn(1)-N(8)#2	114.19(18)
Symmetry transformations used to generate equivalent atoms: #1 x-1/2,-y+1/2,z-1/2; #2 x-1,y,z+1; #3 x+1,y,z-1; #4 x+1/2,-y+1/2,z+1/2			

Table S3. Selected bond lengths (Å) and bond angles (°) for 4

4			
Bond lengths (Å)			
Zn(1)-O(1)	1.940(2)	Zn(1)-N(8)#2	2.020(3)
Zn(1)-O(4)#1	1.945(2)	N(8)-Zn(1)#3	2.020(3)
Zn(1)-N(1)	2.007(3)	O(4)-Zn(1)#4	1.945(2)
Bond angles (°)			
O(1)-Zn(1)-O(4)#1	105.15(10)	O(1)-Zn(1)-N(8)#2	115.25(11)
O(1)-Zn(1)-N(1)	111.67(11)	O(4)#1-Zn(1)-N(8)#2	100.80(11)
O(4)#1-Zn(1)-N(1)	118.70(11)	N(1)-Zn(1)-N(8)#2	105.21(11)
Symmetry transformations used to generate equivalent atoms: #1 -x+1,y+3/2,-z-1/2; #2 -x+2,y+3/2,-z+1/2; #3 -x+2,y-3/2,-z+1/2; #4 -x+1,y-3/2,-z-1/2			

Table S4. Selected bond lengths (Å) and bond angles (°) for 5

5			
Bond lengths (Å)			
Co(1)-O(1)	1.947(2)	Co(1)-N(1)	2.020(3)
Co(1)-O(5)#1	1.959(3)	N(8)-Co(1)#3	2.021(3)
Co(1)-N(8)#2	2.021(3)	O(5)-Co(1)#4	1.960(3)
Bond angles (°)			
O(1)-Co(1)-O(5)#1	101.98(11)	O(1)-Co(1)-N(1)	116.53(11)
O(1)-Co(1)-N(8)#2	100.59(11)	O(5)#1-Co(1)-N(1)	113.60(12)
O(5)#1-Co(1)-N(8)#2	118.51(11)	N(8)#2-Co(1)-N(1)	105.41(12)
Symmetry transformations used to generate equivalent atoms: #1 -x,y-3/2,-z-1/2; #2 -x+1,y+3/2,-z+1/2; #3 -x+1,y-3/2,-z+1/2; #4 -x,y+3/2,-z-1/2			

Table S5. Selected bond lengths (Å) and bond angles (°) for 6

6			
Bond lengths (Å)			
Cd(1)-N(8)	2.266(4)	Cd(1)-N(3)	2.427(4)
Cd(1)-N(1)	2.282(4)	Cd(1)-O(1)	2.439(4)
Cd(1)-O(2)	2.316(3)	Cd(1)-O(5)	2.451(4)
Bond angles (°)			
N(8)-Cd(1)-N(1)	135.18(14)	O(2)-Cd(1)-O(1)	54.84(12)
N(8)-Cd(1)-O(2)	85.86(13)	N(3)-Cd(1)-O(1)	88.36(14)
N(1)-Cd(1)-O(2)	136.89(14)	N(8)-Cd(1)-O(5)	88.27(14)
N(8)-Cd(1)-N(3)	84.41(14)	N(1)-Cd(1)-O(5)	84.75(13)
N(1)-Cd(1)-N(3)	97.43(13)	O(2)-Cd(1)-O(5)	84.04(12)
O(2)-Cd(1)-N(3)	99.67(13)	N(3)-Cd(1)-O(5)	171.51(13)
N(8)-Cd(1)-O(1)	138.13(12)	O(1)-Cd(1)-O(5)	99.98(12)
N(1)-Cd(1)-O(1)	86.62(13)		
Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z+1; #2 -x,-y,-z; #3 -x,-y+1,-z+1			

Table S6. Selected bond lengths (Å) and bond angles (°) for 7

7			
Bond lengths (Å)			
Cd(1)-N(6)#1	2.230(3)	Cd(1)-O(4)#3	2.598(2)
Cd(1)-N(8)	2.271(3)	N(6)-Cd(1)#4	2.230(3)
Cd(1)-O(2)	2.300(2)	O(4)-Cd(1)#5	2.327(2)
Cd(1)-O(4)#2	2.327(2)	O(4)-Cd(1)#6	2.598(2)
Cd(1)-O(1W)	2.402(2)		
Bond angles (°)			
N(6)#1-Cd(1)-N(8)	164.91(10)	O(2)-Cd(1)-O(1W)	85.37(9)
N(6)#1-Cd(1)-O(2)	105.62(10)	O(4)#2-Cd(1)-O(1W)	170.91(9)
N(8)-Cd(1)-O(2)	84.85(10)	N(6)#1-Cd(1)-O(4)#3	82.32(9)
N(6)#1-Cd(1)-O(4)#2	103.62(9)	N(8)-Cd(1)-O(4)#3	86.21(9)
N(8)-Cd(1)-O(4)#2	84.84(9)	O(2)-Cd(1)-O(4)#3	169.89(8)
O(2)-Cd(1)-O(4)#2	99.73(8)	O(4)#2-Cd(1)-O(4)#3	84.12(8)
N(6)#1-Cd(1)-O(1W)	82.03(9)	O(1W)-Cd(1)-O(4)#3	89.65(8)
N(8)-Cd(1)-O(1W)	88.15(10)		
Symmetry transformations used to generate equivalent atoms: #1 x-1,y-1,z; #2 x,-y+1/2,z+1/2; #3 -x+1,y-1/2,-z+1/2; #4 x+1,y+1,z; #5 x,-y+1/2,z-1/2; #6 -x+1,y+1/2,-z+1/2			

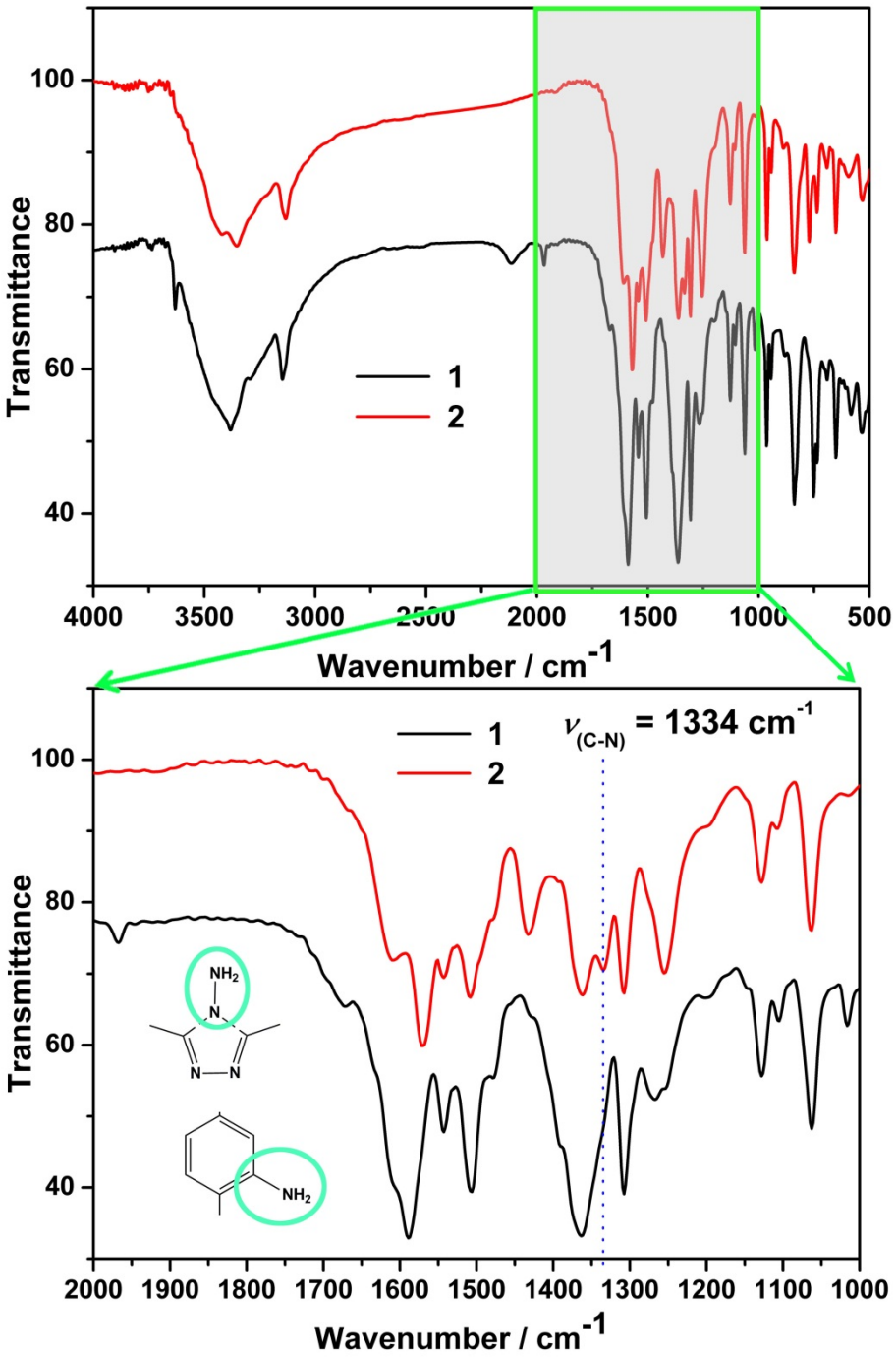

Fig. S1 Infrared spectrums of compounds **1** and **2**. Both **1** and **2** contain the N-rich ligand **L** (4-amino-3,5-bis(4-imidazol-1-ylphenyl)-1,2,4-triazole) in which one NH_2 group is connected to the 4-positioned nitrogen atom of the triazole core. Therefore, the characteristic bands corresponding to the asymmetrical (ν_{asym}(-NH_2)) and symmetrical stretchings of the amine moieties (ν_{sym}(-NH_2)) as well as the characteristic bands ascribed to the medium N-H bending (scissoring) vibration (δ(-NH_2)) can't be used as evidences for the presence of 2-amino-1,4-benzenedicarboxylic acid (NH_2-BDC) in **2** (up). Fortunately, in **L**, the –NH_2 is linked

to a nitrogen atom while in NH_2-BDC the $–NH_2$ group is connected to carbon atom (bottom inset). Thus, after comparing the IR spectra of **1** with that of **2**, the C-N stretching absorption distinctive of aromatic amines at 1334 cm^{-1} evidently proves the presence of NH_2-BDC in **2**.[1]

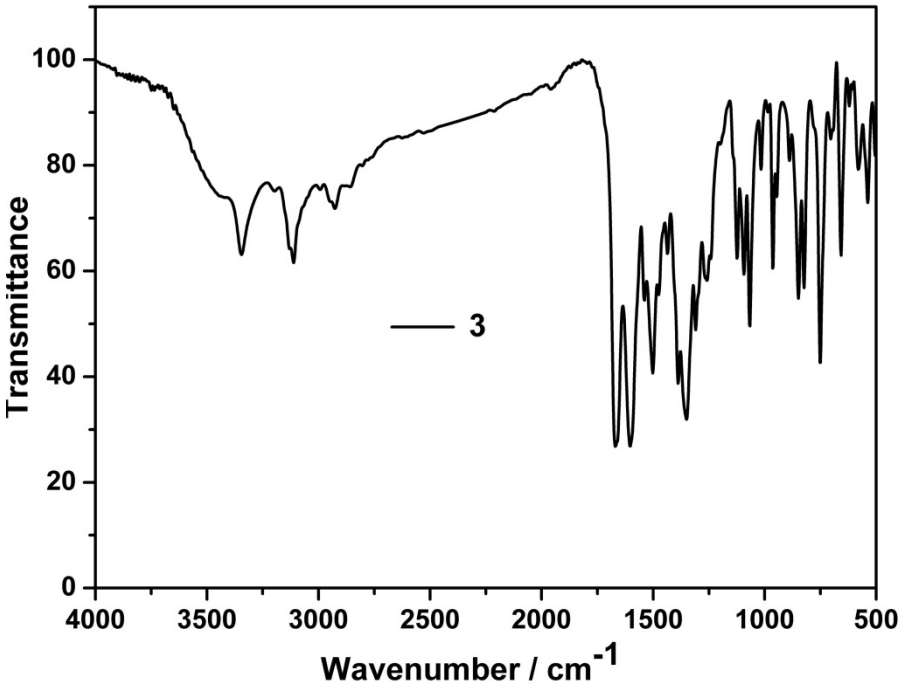

Fig. S2 Infrared spectrum of compound **3**.

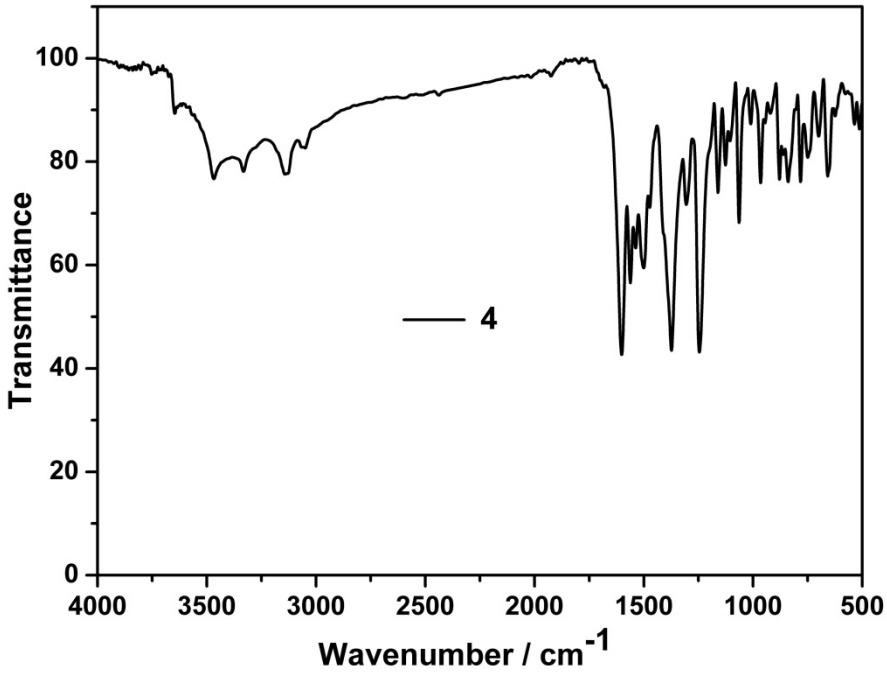

Fig. S3 Infrared spectrum of compound **4**.

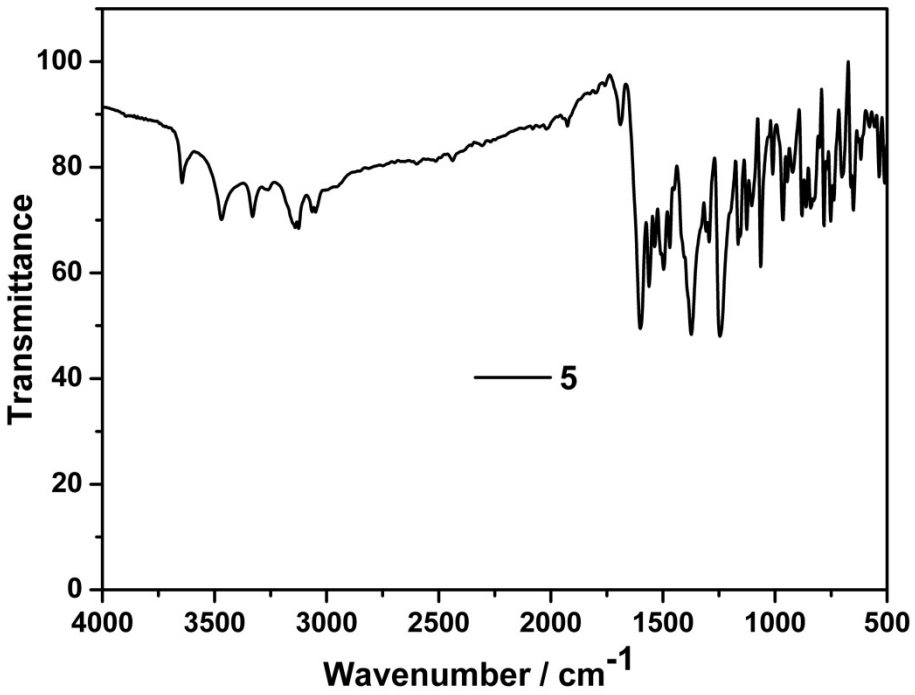

Fig. S4 Infrared spectrum of compound **5**.

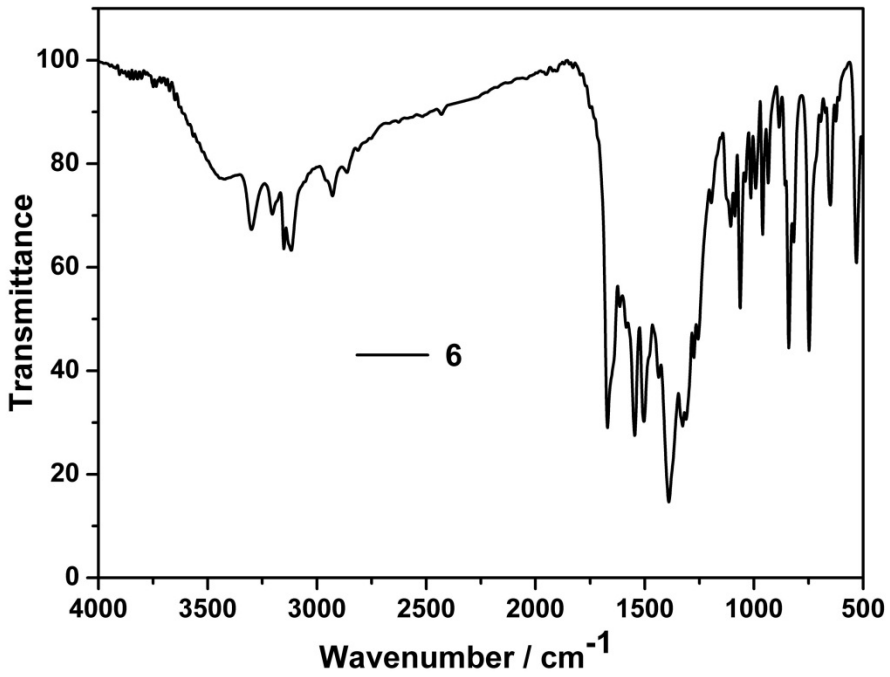

Fig. S5 Infrared spectrum of compound **6**.

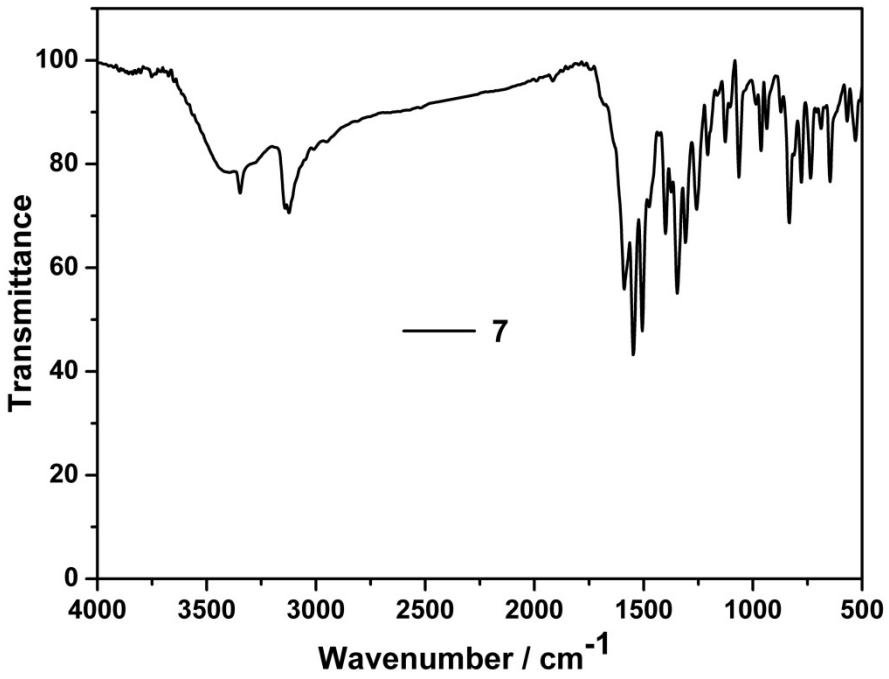

Fig. S6 Infrared spectrum of compound **7**.

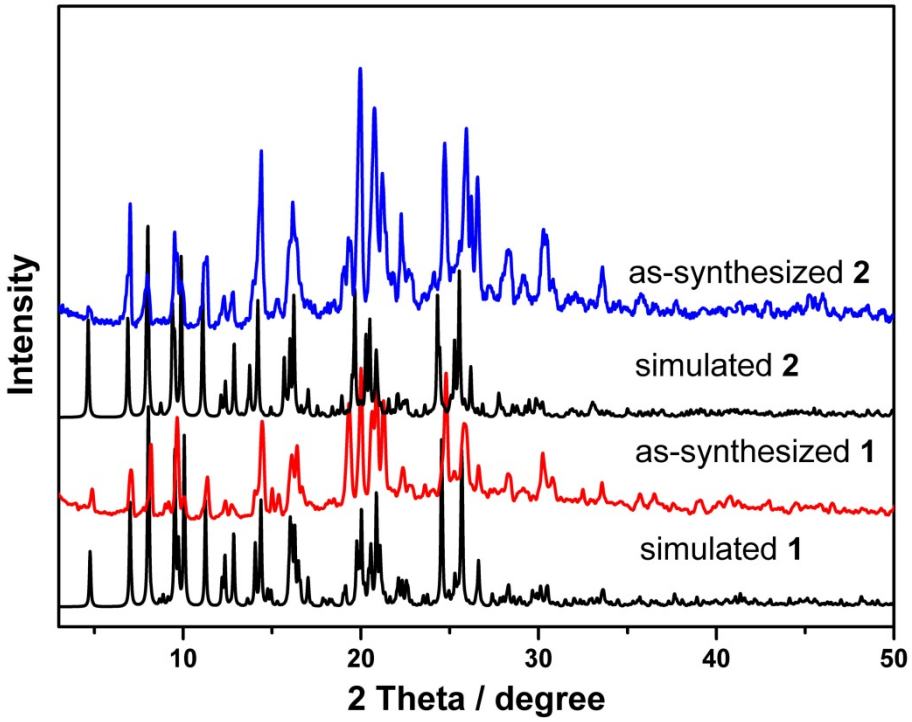

Fig. S7 PXRD profiles of as-synthesized (**1** and **2**) and the simulated ones.

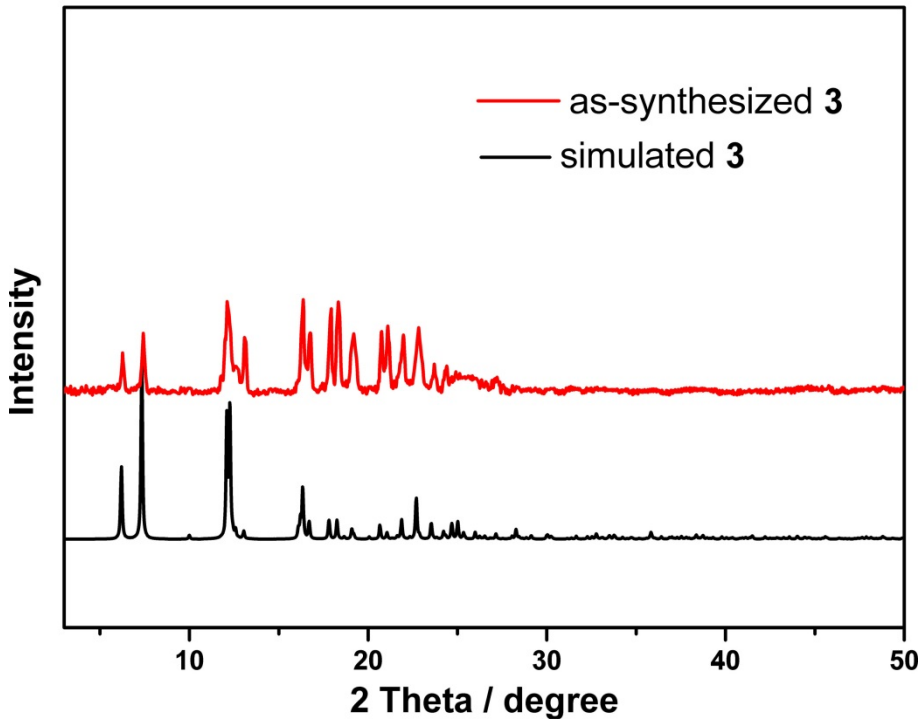

Fig. S8 PXRD profile of as-synthesized **3** and the simulated one.

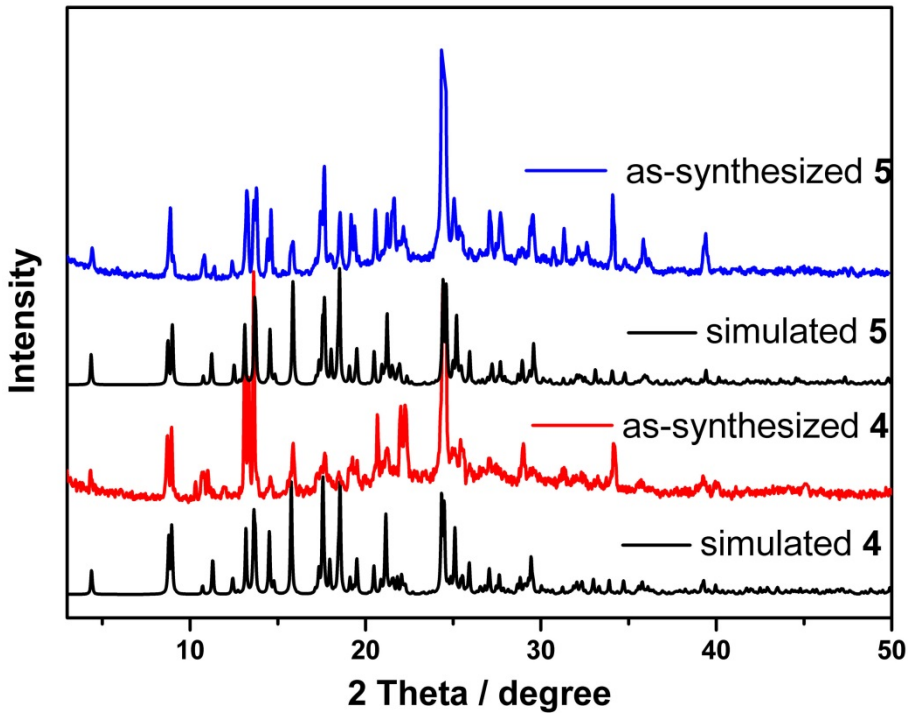

Fig. S9 PXRD profiles of as-synthesized (**4** and **5**) and the simulated ones.

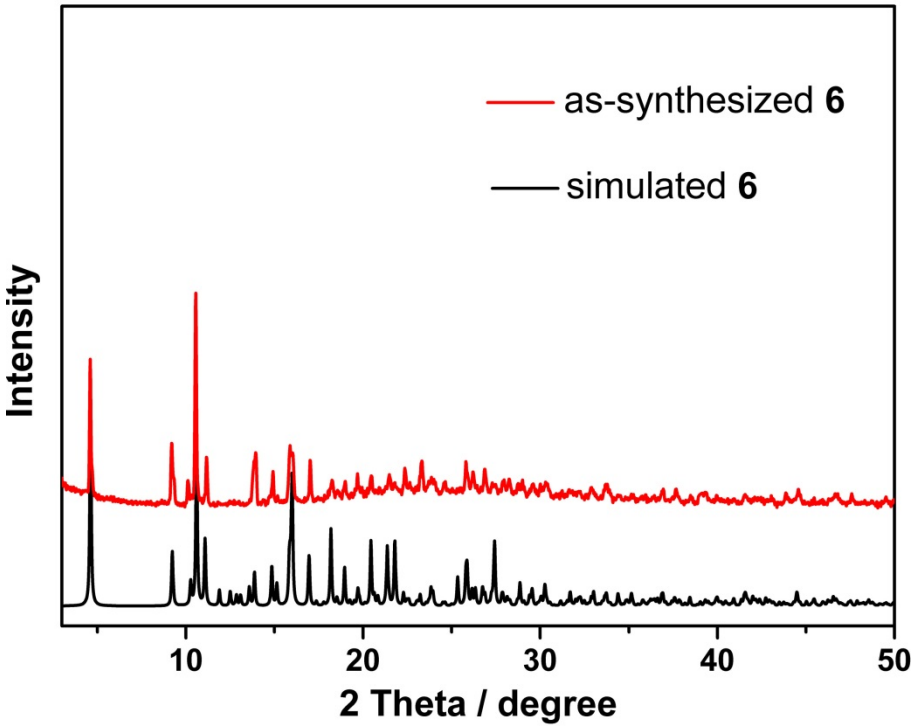

Fig. S10 PXRD profile of as-synthesized **6** and the simulated one.

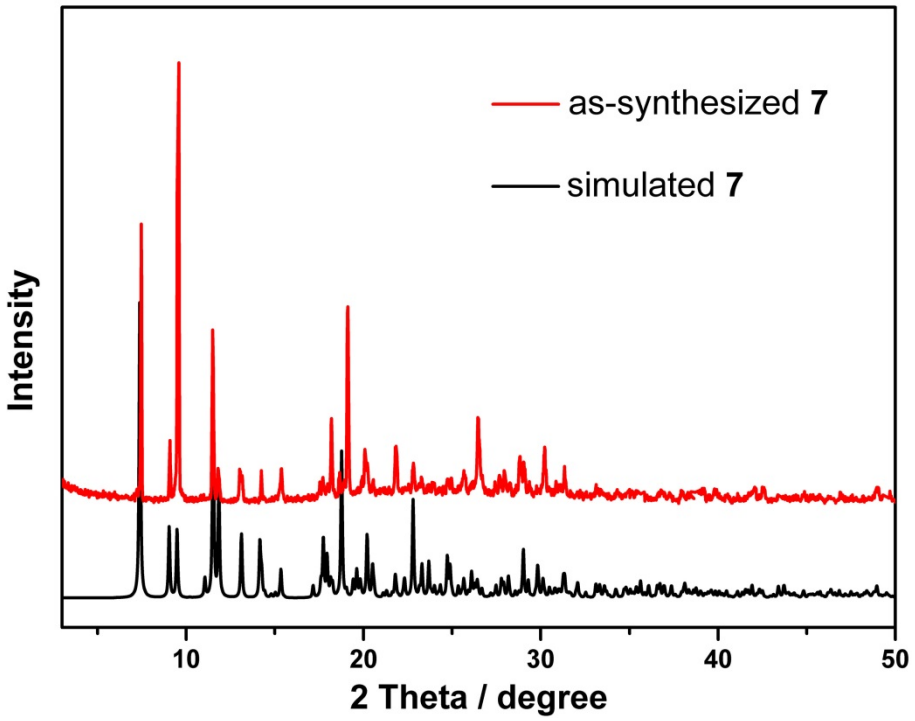

Fig. S11 PXRD profile of as-synthesized **7** and the simulated one.

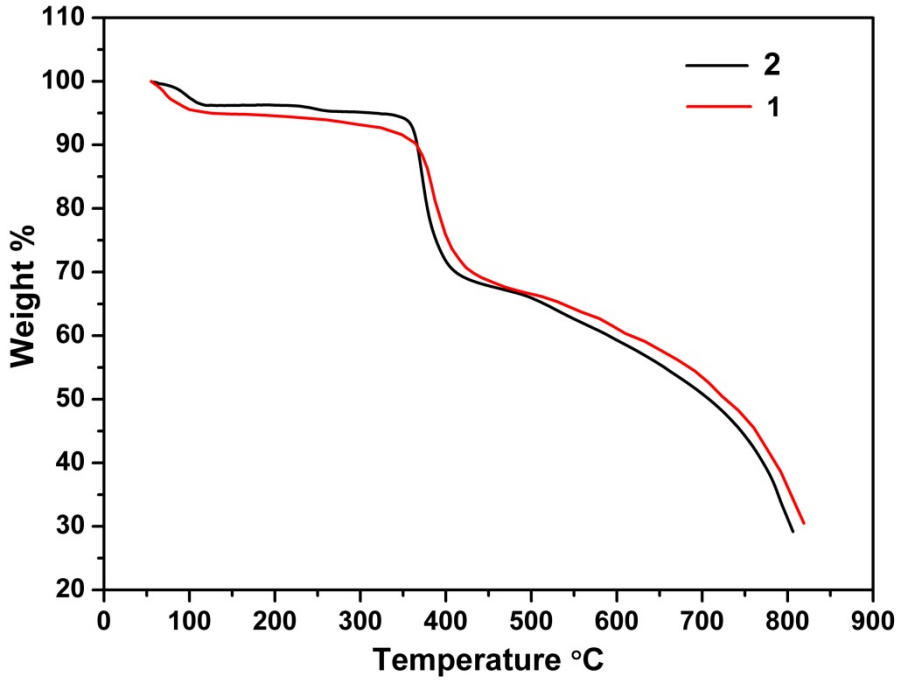

Fig. S12 TGA curves of compound **1** and **2**.

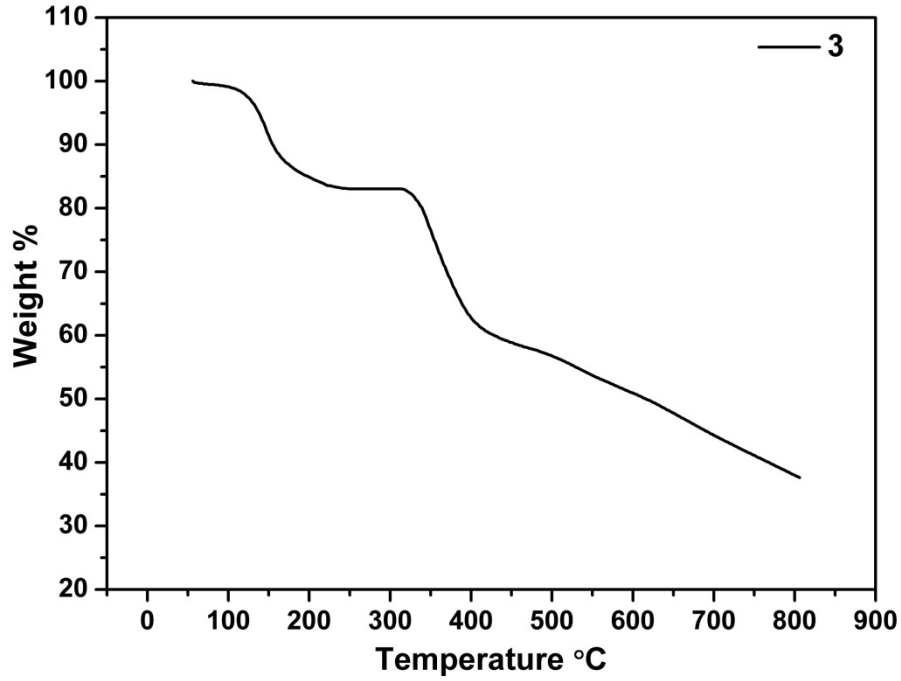

Fig. S13 TGA curves of compound **3**.

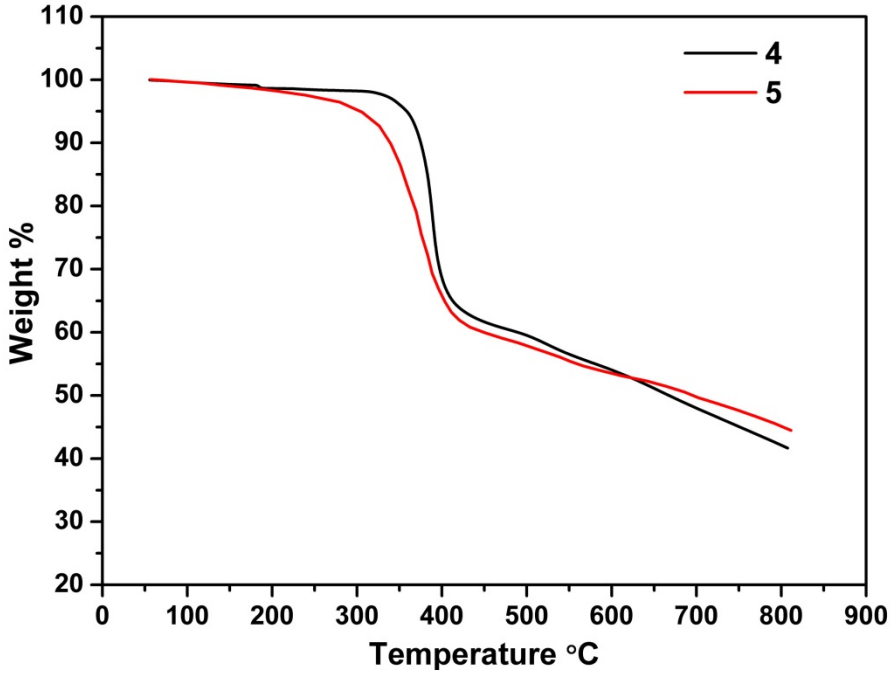

Fig. S14 TGA curves of compound **4** and **5**.

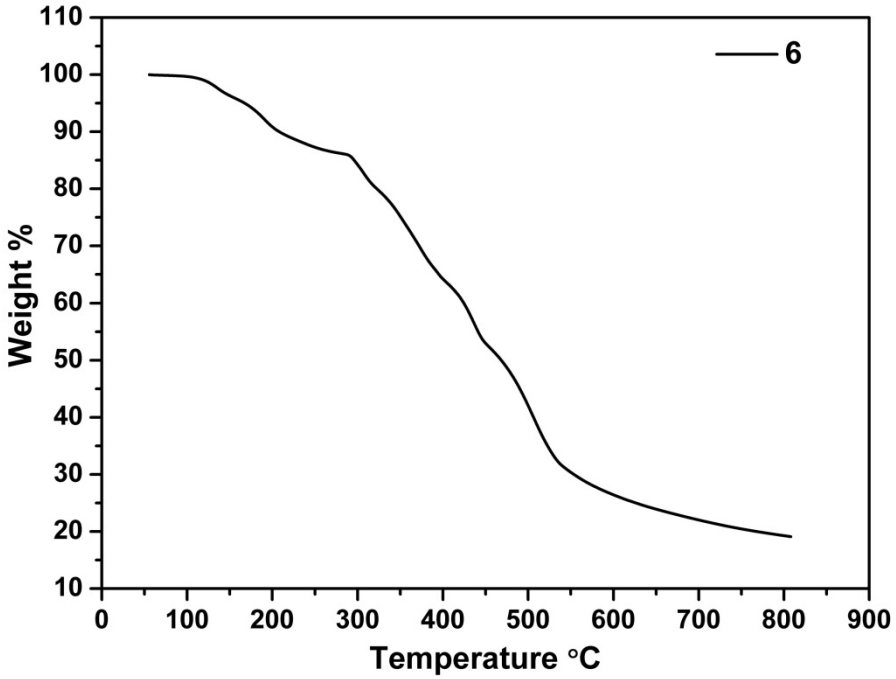

Fig. S15 TGA curves of compound **6**.

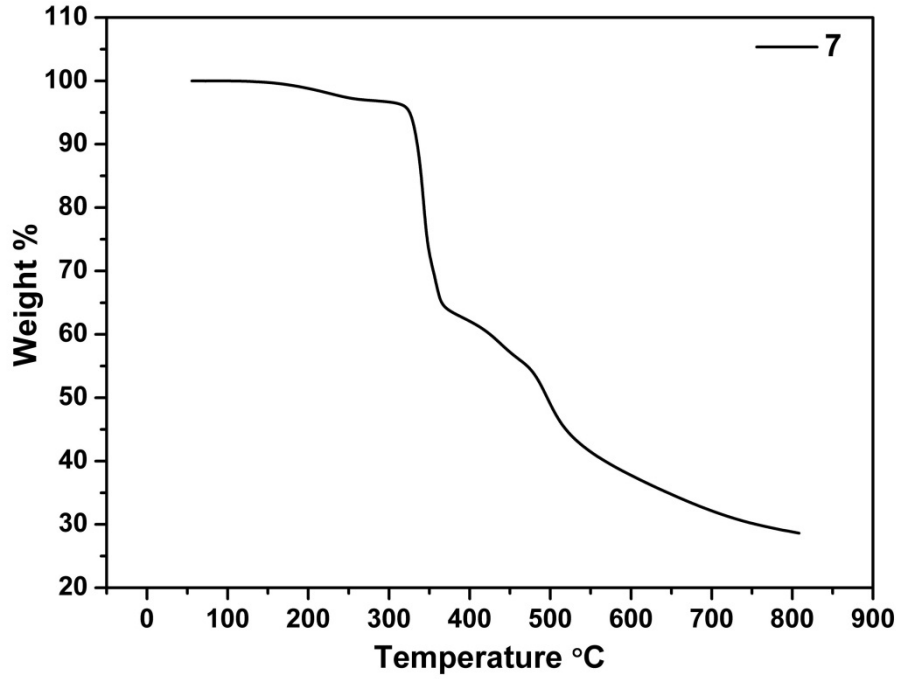

Fig. S16 TGA curves of compound **7**.

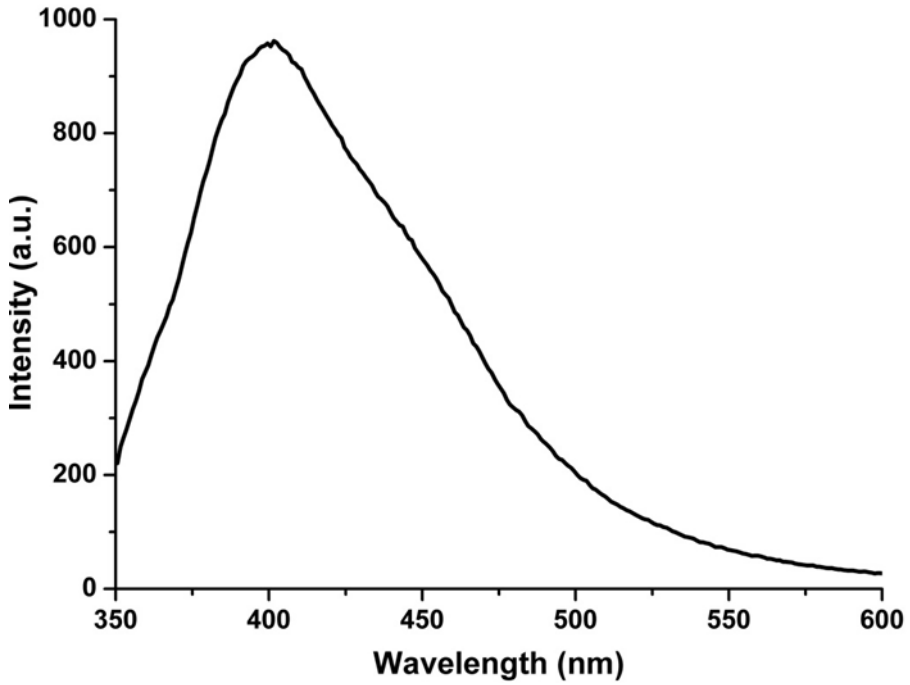

Fig. S17 Photoluminescent spectra of 4-amino-3,5-bis(4-imidazol-1-ylphenyl) -1,2,4-triazole (**L**) in solid state at room temperature (λ_{ex} = 330 nm).

References

1 (a) M. Kandiah, M. H. Nilsen, S. Usseglio, S. Jakobsen, U. Olsbye, M. Tilset, C. Larabi, E. A. Quadrelli, F. Bonino and K. P. Lillerud, *Chem. Mater.*, 2010, **22**, 6632; (b) P. Serra-Crespo, E. V. Ramos-Fernandez, J. Gascon and F. Kapteijn, *Chem. Mater.*, 2011, **23**, 2565; (c) E. Haque, V. Lo, A. I. Minett, A. T. Harris and T. L. Church, *Journal of Materials Chemistry A*, 2014, **2**, 193.