Electronic Supplementary Information for

Temperature and pH driven self-assembly of Zn(II) coordination polymers: crystal structures, supramolecular isomerism, and photoluminescence

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Table S1. Selected Bond Lengths (Å) and Angles (°) for **1-5**.

1			
Zn(1)-O(1)	1.9838(15)	Zn(1)-O(4)#1	1.9848(15)□
Zn(1)-N(1)	2.017(2)	Zn(1)-N(4)	2.018(2)
O(1)-Zn(1)-O(4)#1	100.17(6)□	O(1)-Zn(1)-N(1)	110.51(7)
O(4)#1-Zn(1)-N(1)	114.13(7)	O(1)-Zn(1)-N(4)	106.90(7)□
O(4)#1-Zn(1)-N(4)	111.23(7)	N(1)-Zn(1)-N(4)	112.94(8)
2			
Zn(1)-O(1)#1	1.9884(15)	Zn(1)-O(2)	2.0067(14)□
Zn(1)-N(7)	2.0307(18)	Zn(1)-O(7)#2	2.058(2)
Zn(1)-O(8)#2	2.295(2)		
Zn(2)-O(5)	1.9349(15)□	Zn(2)-N(1)	2.0167(18)
Zn(2)-O(3)	2.0398(15)□	Zn(2)-N(6)#3	2.0654(18)
O(2)-Zn(1)-N(7)	99.75(7)	O(1)#1-Zn(1)-N(7)	103.82(7)
O(2)-Zn(1)-O(7)#2	139.83(7)	O(1)#1-Zn(1)-O(7)#2	111.51(7)
N(7)-Zn(1)-O(7)#2	101.18(7)□	O(2)-Zn(1)-O(8)#2	85.86(7)
O(1)#1-Zn(1)-O(8)#2	105.92(8)	N(7)-Zn(1)-O(8)#2	148.95(8)
O(7)#2-Zn(1)-O(8)#2	59.38(8)	O(1)#1-Zn(1)-O(2)	96.08(6)

O(5)-Zn(2)-O(3)	110.36(7)□	O(5)-Zn(2)-N(1)	123.57(7)
N(1)-Zn(2)-O(3)	112.68(7)□	O(5)-Zn(2)-N(6)#3	110.98(7)
N(1)-Zn(2)-N(6)#3	101.42(7)	O(3)-Zn(2)-N(6)#3	93.03(7)
3			
Zn(1)-O(4)#1	1.950(3)	Zn(1)-O(2)	1.975(3)
Zn(1)-N(1)	2.022(4)	Zn(1)-N(6)#2	2.056(4)
O(4)#1-Zn(1)-O(2)	105.38(12)□	O(4)#1-Zn(1)-N(1)	115.04(14)□
O(2)-Zn(1)-N(1)	114.82(14)	O(4)#1-Zn(1)-N(6)#2	108.74(14)
O(2)-Zn(1)-N(6)#2	103.50(14)□	N(1)-Zn(1)-N(6)#2	108.62(15)
4			
Zn(1)-O(2)	1.965(2)	Zn(1)-O(4)#1	1.9794(19)□
Zn(1)-O(6)	1.988(2)	Zn(1)-N(1)	2.018(2)
O(2)-Zn(1)-O(4)#1	102.15(8)	O(2)-Zn(1)-O(6)	99.36(9)
O(4)#1-Zn(1)-O(6)	106.26(10)	O(2)-Zn(1)-N(1)	121.69(9)
O(4)#1-Zn(1)-N(1)	113.29(9)□	O(6)-Zn(1)-N(1)	112.23(10)
5			
Zn(1)-O(4)#1	1.9649(17)	Zn(1)-O(1)	1.9740(18)
Zn(1)-O(6)	2.0012(19)	Zn(1)-N(1)	2.012(2)
O(4)#1-Zn(1)-O(1)	102.03(7)	O(4)#1-Zn(1)-O(6)	106.46(8)
O(1)-Zn(1)-O(6)	106.04(8)	O(4)#1-Zn(1)-N(1)	117.31(8)□
O(1)-Zn(1)-N(1)	114.32(8)	O(6)-Zn(1)-N(1)	109.76(8)

Symmetry codes: **1**: #1 x, y+1, z; **2**: #1: -x+2, y-1/2, -z+1/2; #2: -x+2, -y, -z+1; #3: -x+1, y-1/2, -z+1/2; **3**: #1: x, y+1, z; #2: -x+2, -y+2, -z+1; **4**: #1: x+1/2, y+1/2, z; **5**: #1: x-1/2, y-1/2, z.

Table S2. Hydrogen bonds for complexes **1** and **3**-**5**. (Å, º)

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
1				
O(5)-H(2W)...O(3)	0.85	1.98	2.802(3)	163.4□
O(5)-H(1W)...O(6)#4	0.85	2.15	2.977(8)	164.1
O(5)-H(1W)...O(6')#4	0.85	2.16	2.959(9)	155.9

O(6')-H(5W)...O(2)#5	0.85	1.92	2.657(6)	144.7
O(6)-H(3W)...O(2)#5	0.85	2.07	2.709(6)	131.9
3				
O(6)-H(1W)...O(7)	0.78	2.44	3.006(13)	129.9
O(6)-H(2W)...O(3)	0.85	2.01	2.855(7)	178.1
O(7)-H(4W)...O(1)	0.83	1.97	2.743(7)	156.3
4				
O(7)-H(4W)...N(3)#3	0.85	2.32	3.109(4)	154.1
O(7)-H(3W)...O(1)	0.85	1.95	2.727(3)	152.0
O(6)-H(2W)...O(3)#4	0.85	1.80	2.651(3)	173.3□
O(6)-H(1W)...O(7)#4	0.85	1.89	2.708(3)	159.7
5				
O(6)-H(1W)...O(2)#4	0.82	1.93	2.718(3)	161.2□
O(6)-H(2W)...O(7)#5	0.97	1.67	2.632(3)	169.8
O(7)-H(3W)...N(3)#6	0.92	2.24	3.072(3)	150.2
O(7)-H(3W)...O(5)#7	0.92	2.64	3.168(3)	117.1
O(7)-H(4W)...O(3)#8	0.85	1.89	2.728(3)	169.2

Symmetry transformations used to generate equivalent atoms: **1**: #4: x-1, y, z; #5: x+1, y, z; **4**: #3: -x+1, y, -z+3/2; #4: -x+1/2, y+1/2, -z+3/2; **5**: #4: -x+3/2, -y+1/2, -z+1; #5: x-1/2, y+1/2, z+1; #6: x, -y, z-1/2; #7: x-1/2, y+1/2, z+1; #8: -x+3/2, -y+1/2, -z+2.

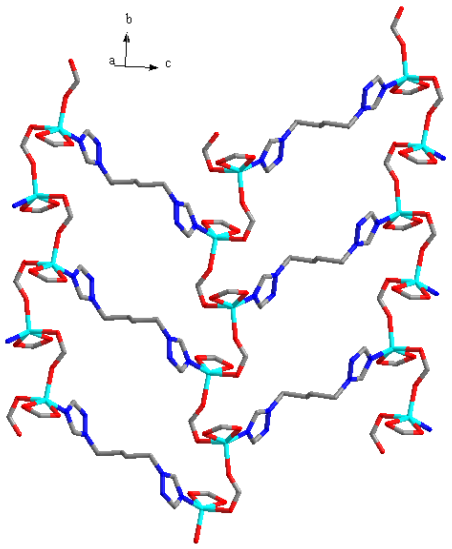


Fig. S1. View of the 2D layer of **2**.

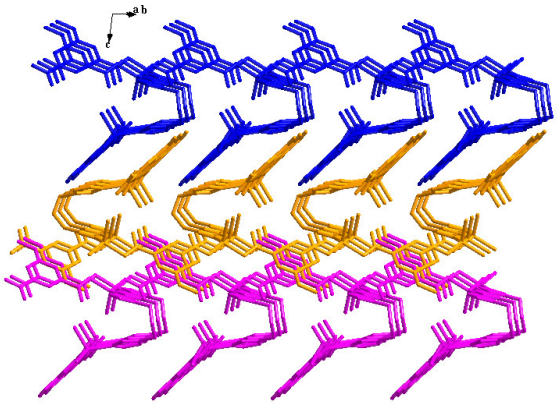
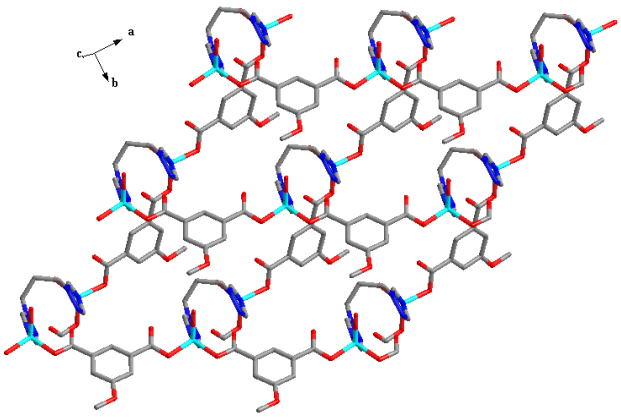
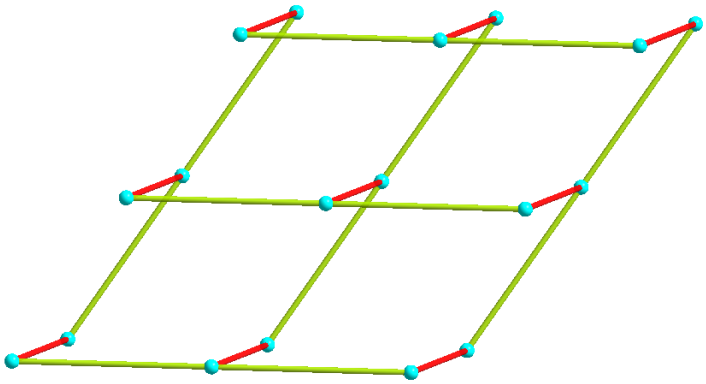


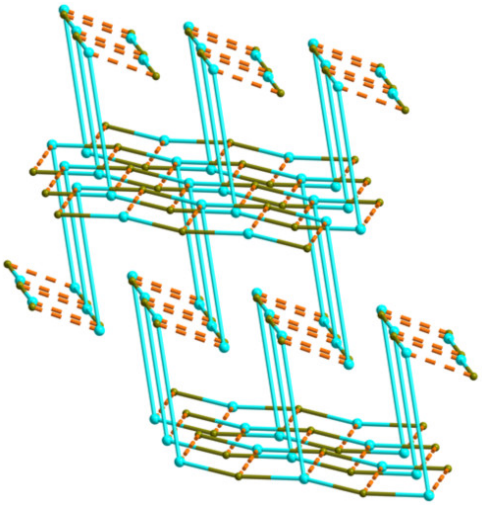
Fig. S2. View of 3D framework in **4**: different colors for different layers



(a)



(b)



(c)

Fig. S3. (a) View of the 2D layer. (b) Schematic view of 2D layer. Turquiose blue spheres represent Zn atoms. Red bonds represent btp bridges and lime bonds represent moip bridges. (c) Schematic view of 3D net of **5**. Turquiose blue spheres represent Zn atoms. Dark yellow spheres represent μ_3-moip ligands. Orange dash line represent hydrogen bonds.

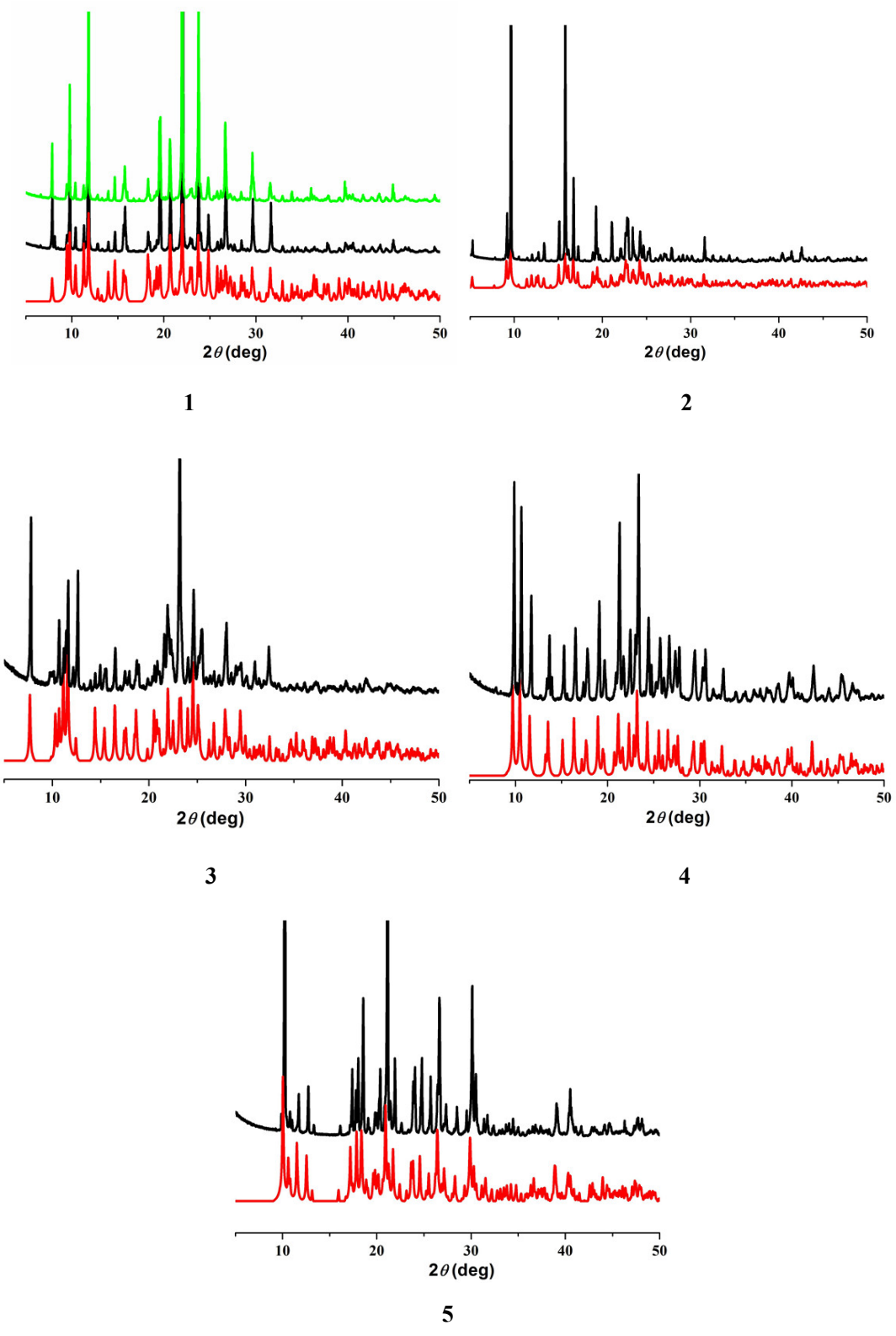


Fig. S4. PXRD patterns of the single crystals of complexes **1**-**5**: observed PXRD patterns (red), as-synthesized (black) for **1**-**5** and dehydrated sample for **1** (green).

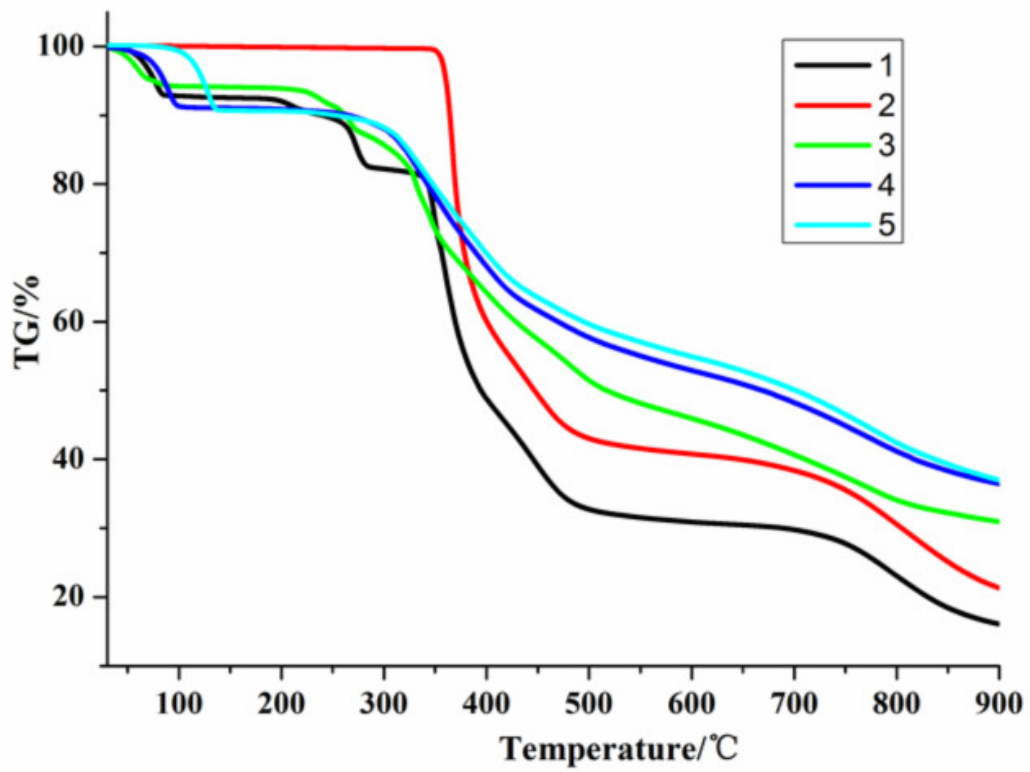


Fig. S5. TGA plots of complexes **1**-**5**.