

Supplementary Material

Structural Diversity and Properties of Six Zn^{II}/Cd^{II} Coordination Polymers Based on a O–Bridged Semi-rigid Bis-pyridyl-bis-amide and Different Dicarboxylates

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Table S1. (a) Selected bond distances (\AA) and angles ($^\circ$) for complex **1**

$\text{C}_{40}\text{H}_{42}\text{N}_4\text{O}_{13}\text{Zn}_2$			
Zn(1)-O(1)	1.928(5)	Zn(1)-O(4)A	1.937(4)
Zn(1)-O(8)	1.946(5)	Zn(1)-N(4)B	2.010(5)
Zn(2)A-O(3)A	1.894(5)	Zn(2)A-O(7)A	1.948(5)
Zn(2)A-O(5)A	1.962(5)	Zn(2)A-O(6)A	2.438(5)
Zn(2)A-N(1)A	2.052(5)	O(1)-Zn(1)-O(8)	100.7(2)
O(1)-Zn(1)-O(4)A	111.4(2)	O(1)-Zn(1)-N(4)B	128.1(2)
O(4)A-Zn(1)-O(8)	121.1(2)	O(8)-Zn(1)-N(4)B	95.7(2)
O(4)A-Zn(1)-N(4)B	100.7(2)	O(3)A-Zn(2)A-O(5)A	134.0(2)
O(3)A-Zn(2)A-O(7)A	111.5(2)	O(3)A-Zn(2)A-N(1)A	104.0(2)
O(7)A-Zn(2)A-O(5)A	100.1(2)	O(5)A-Zn(2)A-N(1)A	105.6(2)
O(7)A-Zn(2)A-N(1)A	95.0(2)	O(7)A-Zn(2)A-O(6)A	157.17(19)
O(3)A-Zn(2)A-O(6)A	89.44(19)	N(1)A-Zn(2)A-O(6)A	88.3(2)
O(5)A-Zn(2)A-O(6)A	57.44(17)		

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(b) Selected bond distances (Å) and angles (°) for complex 2

C ₃₃ H ₃₀ N ₄ O ₁₀ Zn			
Zn(1)-O(3)A	1.992(4)	Zn(1)-O(1)	1.987(4)
Zn(1)-O(2)	2.613(5)	Zn(1)-O(4)A	2.612(5)
Zn(1)-N(1)	2.025(4)	Zn(1)-N(4)B	2.038(4)
O(3)A-Zn(1)-O(1)	93.11(14)	O(3)A-Zn(1)-N(1)	109.30(16)
O(1)-Zn(1)-N(1)	107.55(17)	O(3)A-Zn(1)-N(4)B	111.09(16)
O(1)-Zn(1)-N(4)B	112.83(17)	N(1)-Zn(1)-N(4)B	111.09(16)

(c) Selected bond distances (Å) and angles (°) for complex 3

C ₃₂ H ₂₄ N ₄ O ₈ Zn			
Zn(1)-O(1)	1.9014(15)	Zn(1)-O(3)A	1.9386(14)
Zn(1)-N(1)	2.0660(18)	Zn(1)-N(4)B	2.1219(19)
O(1)-Zn(1)-O(3)A	133.35(7)	O(1)-Zn(1)-N(1)	118.80(7)
O(3)A-Zn(1)-N(1)	98.05(7)	O(1)-Zn(1)-N(4)B	103.52(7)
O(3)A-Zn(1)-N(4)B	95.45(7)	N(1)-Zn(1)-N(4)B	101.25(7)

(d) Selected bond distances (Å) and angles (°) for complex 4

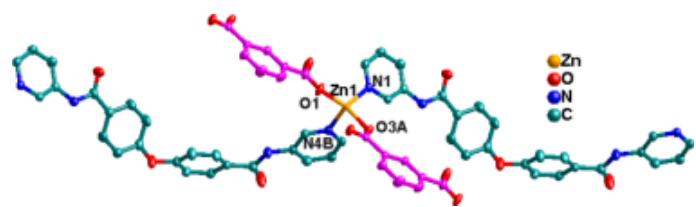
C ₄₀ H ₄₂ N ₄ O ₁₃ Cd ₂			
Cd(1)-O(1)	2.229(6)	Cd(1)-O(7)A	2.242(6)
Cd(1)-O(5)	2.303(6)	Cd(1)-N(1)	2.340(7)
Cd(1)-O(4)	2.389(6)	Cd(1)-O(6)	2.497(6)
Cd(2)-O(8)A	1.999(7)	Cd(2)-O(2)	2.033(6)
Cd(2)-N(4)B	2.099(7)	Cd(2)-O(3)	2.112(6)
Cd(2)-O(4)	2.483(8)	O(1)-Cd(1)-O(7)A	114.2(3)
O(1)-Cd(1)-O(5)	151.2(2)	O(7)A-Cd(1)-O(5)	94.1(2)
O(1)-Cd(1)-N(1)	93.6(2)	O(7)A-Cd(1)-N(1)	87.3(2)
O(5)-Cd(1)-N(1)	93.0(2)	O(1)-Cd(1)-O(4)	89.1(2)
O(7)A-Cd(1)-O(4)	89.3(2)	O(5)-Cd(1)-O(4)	85.8(2)
N(1)-Cd(1)-O(4)	176.3(2)	O(1)-Cd(1)-O(6)	96.9(2)
O(7)A-Cd(1)-O(6)	148.9(2)	O(5)-Cd(1)-O(6)	54.9(2)
N(1)-Cd(1)-O(6)	91.0(3)	O(4)-Cd(1)-O(6)	91.3(3)
O(8)A-Cd(2)-O(2)	118.6(3)	O(8)A-Cd(2)-N(4)B	98.3(3)
O(2)-Cd(2)-N(4)B	100.8(3)	O(8)A-Cd(2)-O(3)	127.5(3)
O(2)-Cd(2)-O(3)	107.6(3)	N(4)B-Cd(2)-O(3)	96.2(3)
O(8)A-Cd(2)-O(4)	94.2(3)	O(2)-Cd(2)-O(4)	95.8(2)
N(4)B-Cd(2)-O(4)	151.1(2)	O(3)-Cd(2)-O(4)	55.9(2)

(e) Selected bond distances (Å) and angles (°) for complex 5

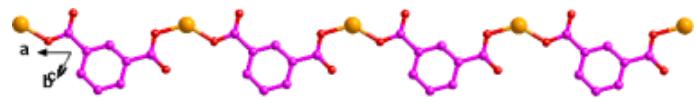
C ₃₃ H ₂₈ N ₄ O ₉ Cd			
Cd(1)-O(1)	2.253(2)	Cd(1)-O(3)A	2.282(2)
Cd(1)-O(7)B	2.496(2)	Cd(1)-O(2)	2.549(2)
Cd(1)-N(4)C	2.338(3)	Cd(1)-N(1)	2.352(3)
O(1)-Cd(1)-O(3)A	88.61(8)	O(1)-Cd(1)-N(4)C	135.72(9)
O(3)ACd(1)-N(4)C	131.64(8)	O(1)-Cd(1)-N(1)	96.13(9)
O(3)A-Cd(1)-N(1)	92.63(8)	N(4)C-Cd(1)-N(1)	98.94(9)
O(1)-Cd(1)-O(7)B	87.63(9)	O(3)A-Cd(1)-O(7)B	82.73(8)
N(4)C-Cd(1)-O(7)B	81.46(8)	N(1)-Cd(1)-O(7)B	173.97(8)
O(1)-Cd(1)-O(2)	53.77(8)	O(3)A-Cd(1)-O(2)	142.32(8)
N(4)C-Cd(1)-O(2)	83.82(8)	N(1)-Cd(1)-O(2)	93.55(9)
O(7)B-Cd(1)-O(2)	92.47(8)		

(f) Selected bond distances (Å) and angles (°) for complex 6

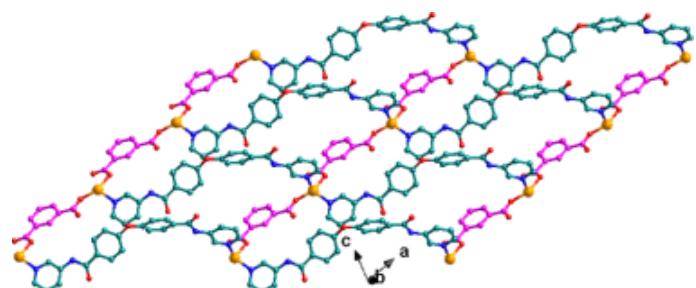
C ₃₂ H ₂₆ N ₄ O ₉ Cd			
Cd(1)-O(1)	2.1962(18)	Cd(1)-N(4)	2.311(2)
Cd(1)-O(3)A	2.3189(19)	Cd(1)-N(1)	2.352(2)
Cd(1)-O(9)	2.4912(19)	Cd(1)-O(4)A	2.5208(19)
O(1)-Cd(1)-N(4)	130.91(7)	O(1)-Cd(1)-O(3)A	92.36(7)
N(4)-Cd(1)-O(3)A	132.80(7)	O(1)-Cd(1)-N(1)	95.50(8)
N(4)-Cd(1)-N(1)	92.07(7)	O(3)A-Cd(1)-N(1)	102.84(7)
O(1)-Cd(1)-O(9)	87.35(7)	N(4)-Cd(1)-O(9)	82.69(7)
O(3)A-Cd(1)-O(9)	81.46(7)	N(1)-Cd(1)-O(9)	174.69(7)
O(1)-Cd(1)-O(4)A	144.79(7)	N(4)-Cd(1)-O(4)A	84.10(7)
O(3)A-Cd(1)-O(4)A	53.59(7)	N(1)-Cd(1)-O(4)A	85.26(7)
O(9)-Cd(1)-O(4)A	95.00(7)		



(a)



(b)



(c)



(d)

Fig.S1 (a) The coordination environment of Zn^{II} ion in complex **3**. The hydrogen atoms and the crystalline water molecules are omitted for clarity (A: $1 + x, y, z$; B: $-2 + x, y, 1 + z$); (b) View of the 1D $[Zn(bdc)]_n$ linear chain and the 1D $[Zn(L)]_n$

left-handed helix chain; (c) 2D layer of complex **3**; (d) Simplification of the 4-connected network.

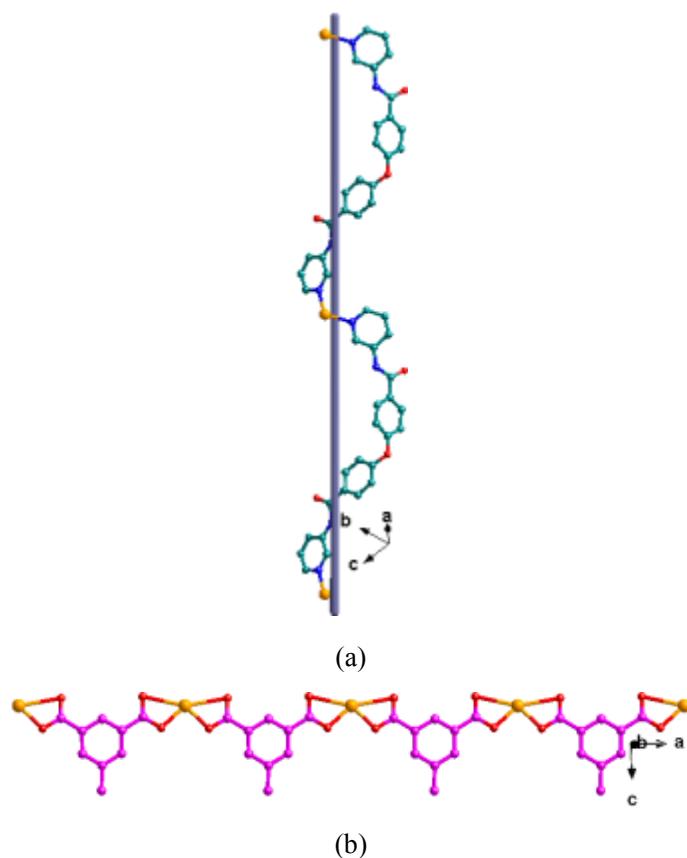
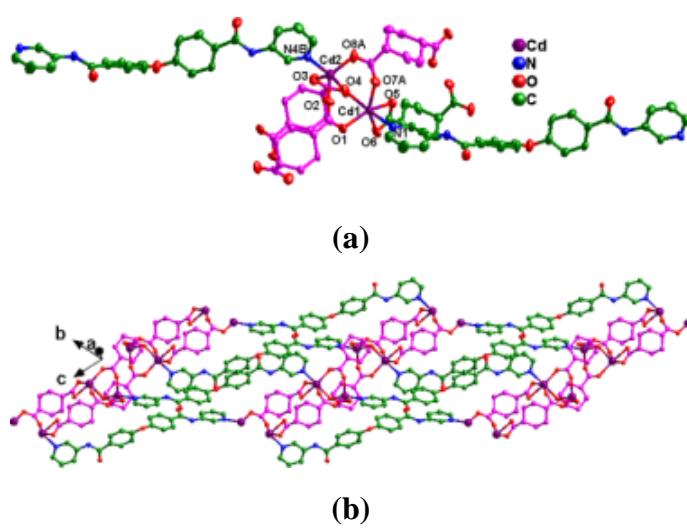
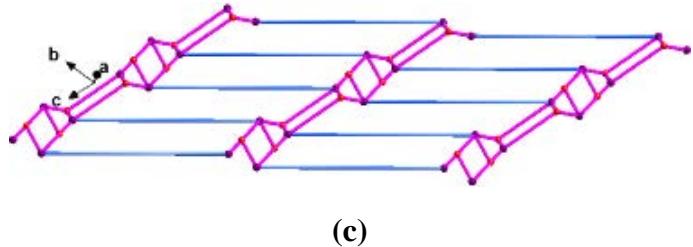


Fig.S2 View of the 1D $[Zn(L)]_n$ left-handed helix chain and $[Zn(mip)]_n$ linear chain in 2.





(c)

Fig.S3 (a) The coordination environment of Cd^{II} ion in complex **4**. The hydrogen atoms and the crystalline water molecules are omitted for clarity (A: $-x, -y, -z$; B: $x, -1 + y, -1 + z$); (b) 2D layer of complex **4**. (c) Simplification of the structure to a 3,4-connected network.

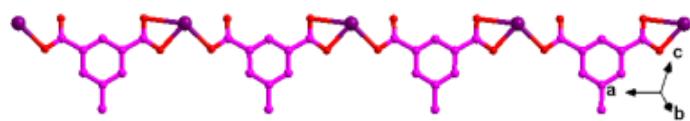
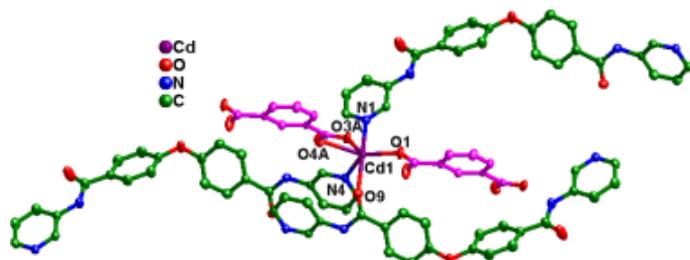
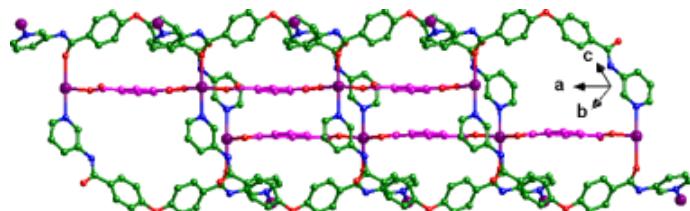


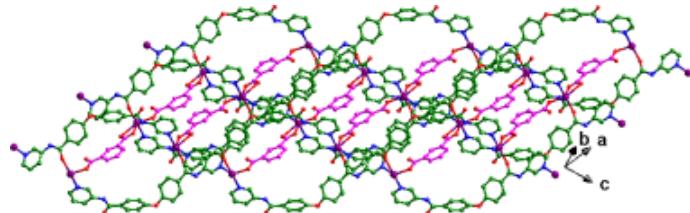
Fig.S4 View of the 1D $[\text{Cd}(\text{mip})]_n$ linear chain in **5**.



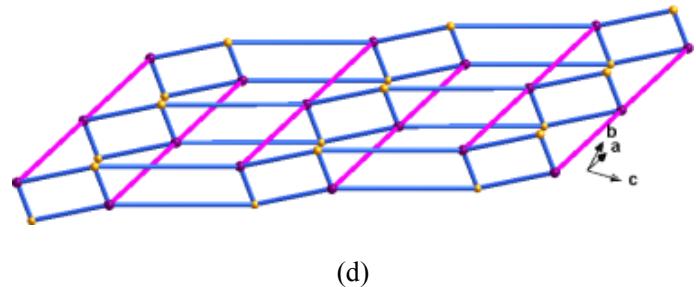
(a)



(b)

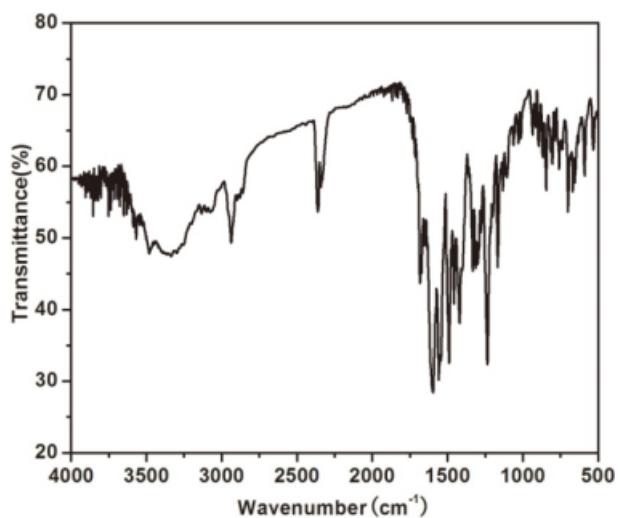


(c)

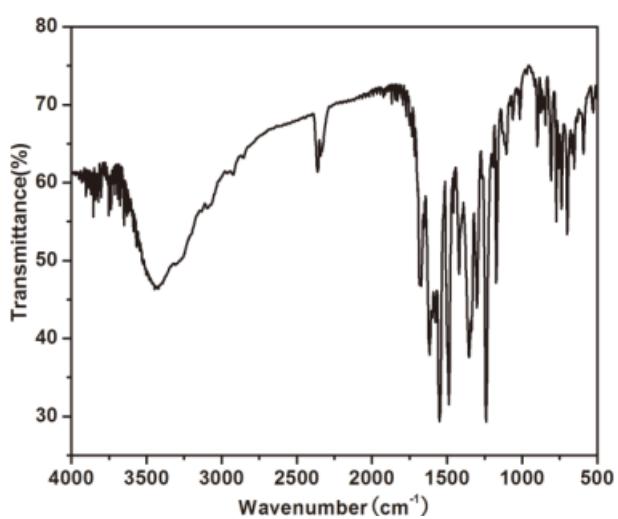


(d)

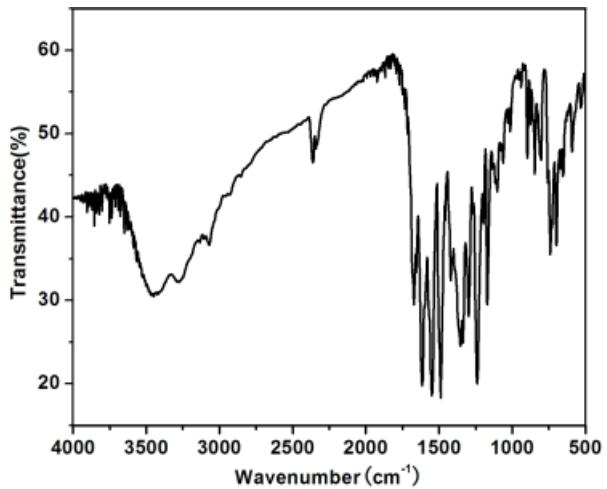
Fig.S5 (a) Coordination environment of Cd^{II} ion in **6**. The hydrogen atoms and the crystalline water molecules are omitted for clarity (A: 1 + x, y, z); (b) The 1D channel-like chain of **6**; (c) 2D layer of complex **6**; (d) Simplification of the 3,5-connected network.



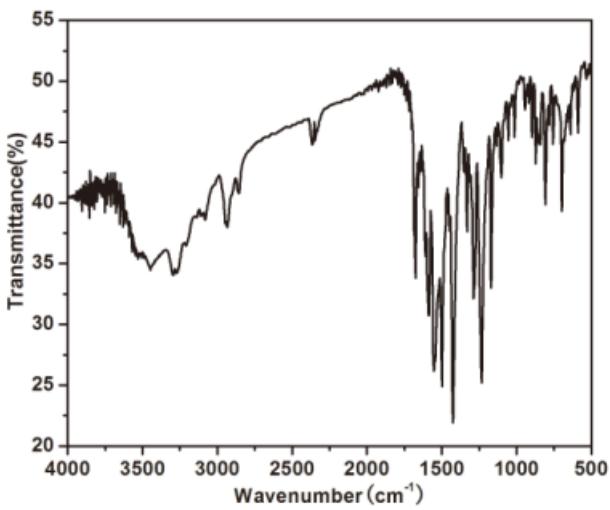
(a)



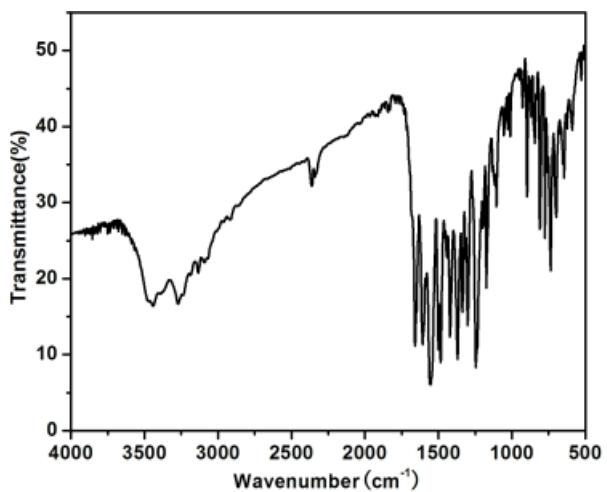
(b)



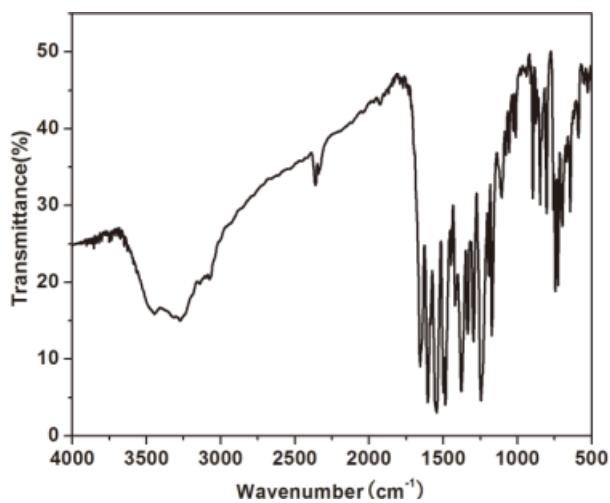
(c)



(d)

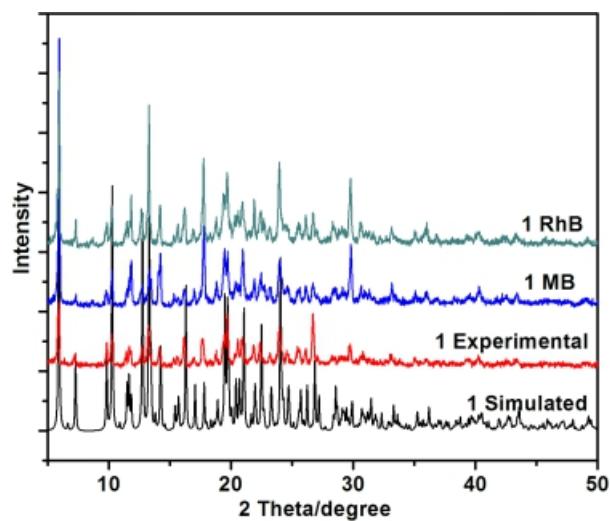


(e)

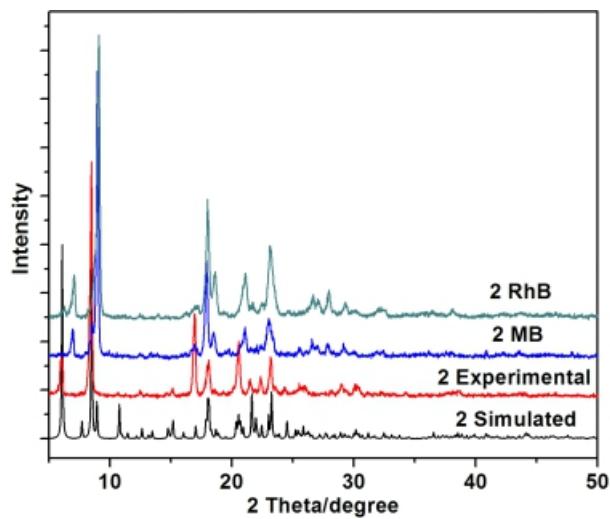


(f)

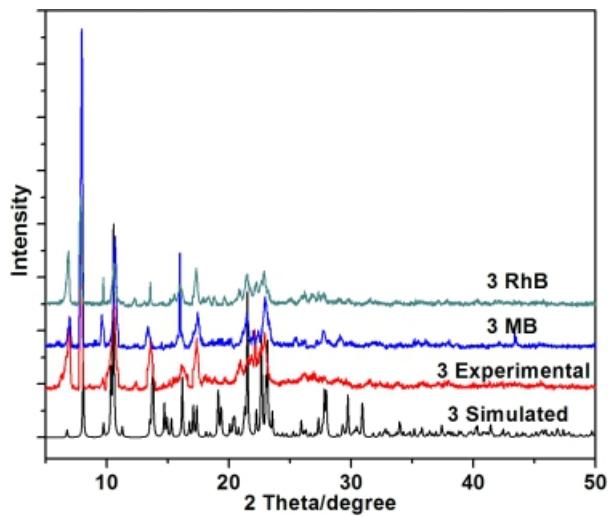
Fig.S6 IR spectra for complexes **1-6**.



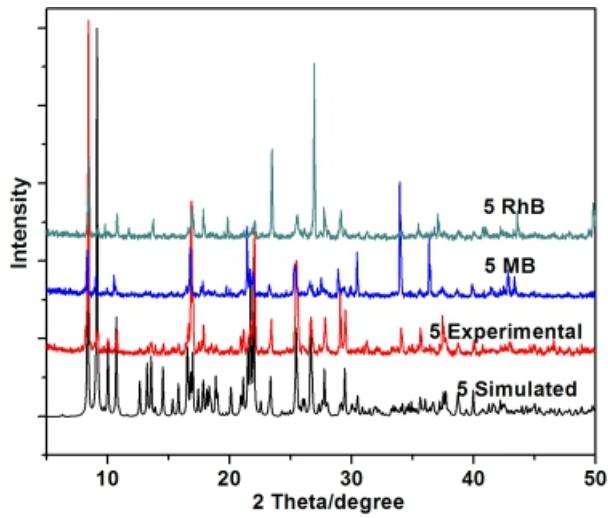
(a)



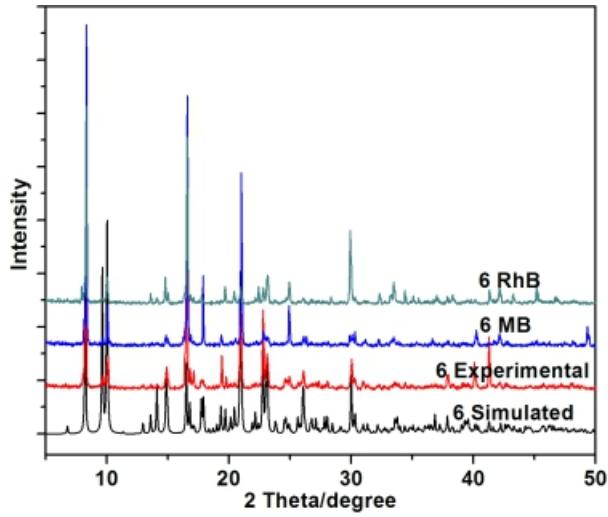
(b)



(c)



(d)



(e)

Fig. S7 The simulated (black) and experimental (red) and after photocatalytic

processes (blue and dark cyan) PXRD patterns for complexes **1–6** (except **4** due to its low yield).

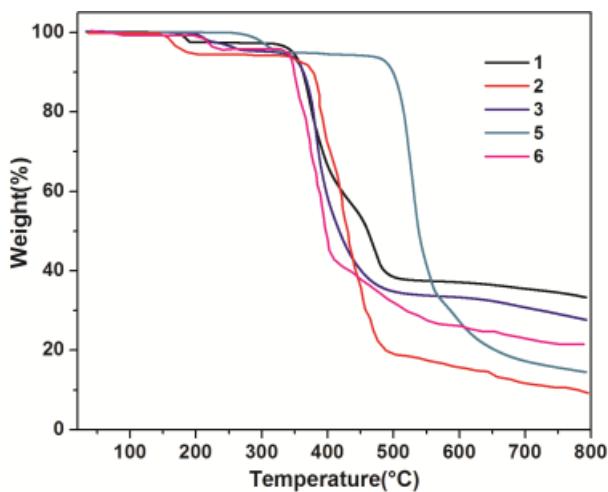
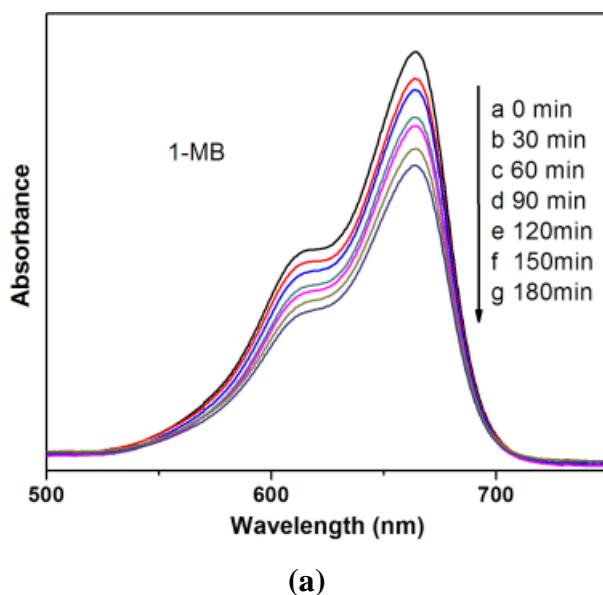
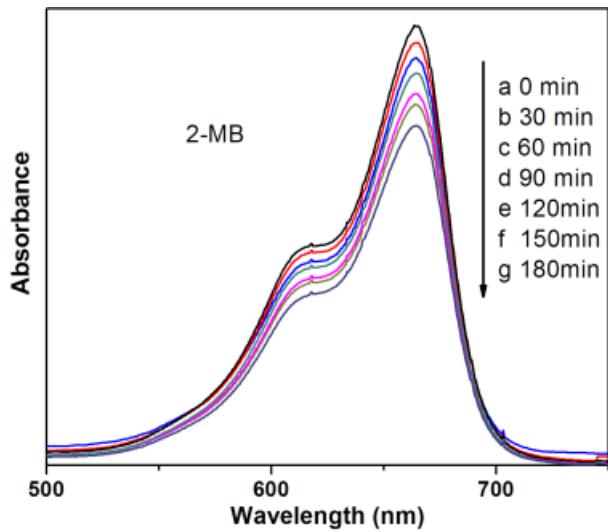


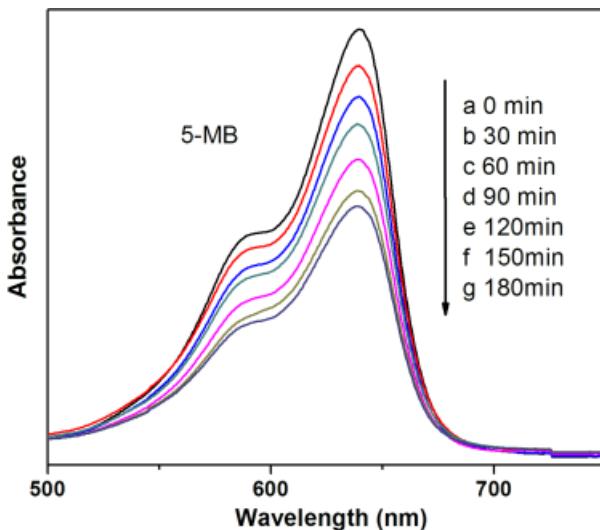
Fig. S8 TG curves for complexes **1–6** (except **4** due to its low yield).



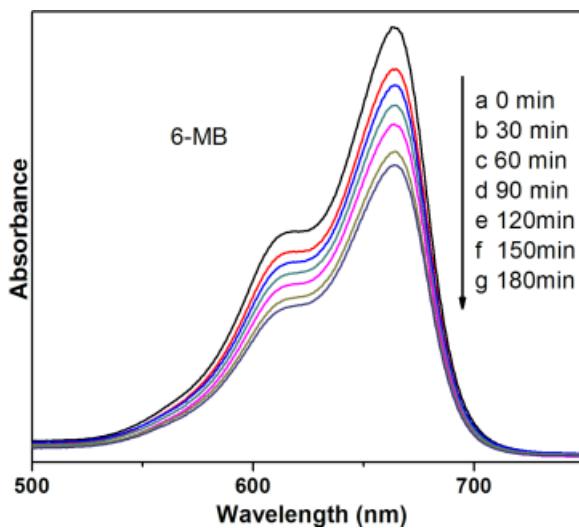
(a)



(b)



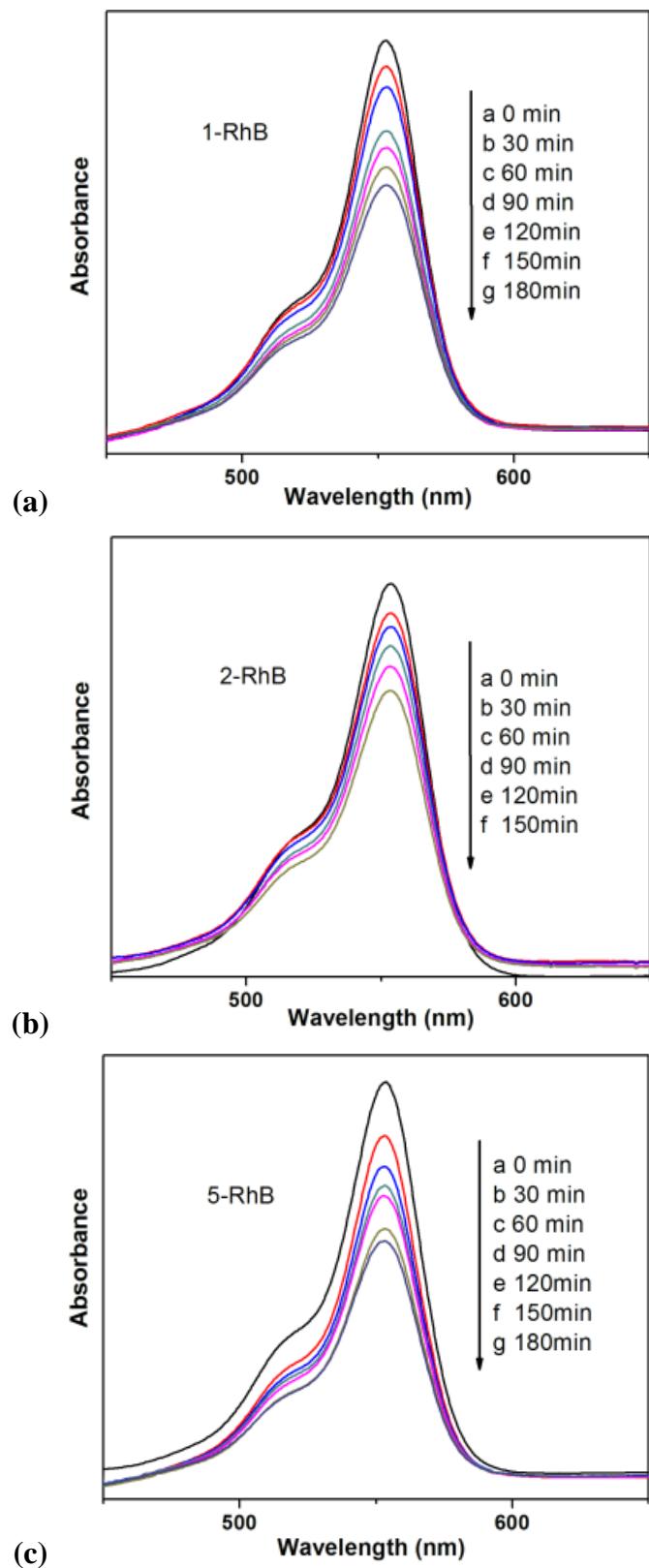
(c)



(d)

Fig. S9 Absorption spectra of the MB solution during the decomposition reaction

under UV light irradiation with the use of complexes **1**, **2**, **5**, and **6**.



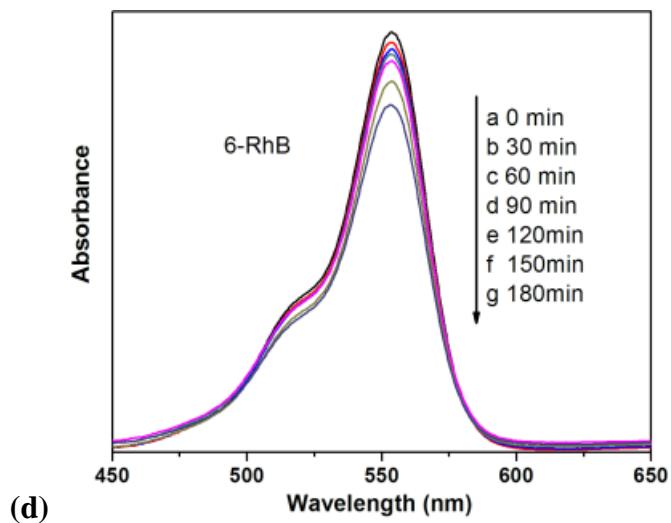


Fig. S10 Absorption spectra of the RhB solution during the decomposition reaction under UV light irradiation with the use of complexes **1**, **2**, **5**, and **6**.