[Supporting information]

Structural diversity of six metal-organic frameworks from a rigid bisimidazole ligand and their adsorption of organic dyes

Siyu Liu, Mingming Guo, Huadong Guo,*[a] Yingying Sun, Xianmin Guo,*[a] Shaowen Sun and Eugeny V. Alexandrov*[b]

[a] *Department of Chemistry, Changchun Normal University, Changchun, 130032, P. R. China. Fax: +86-431-86168210; Tel: +86-431-86168210; E-mail: hdxmguo@163.com*

[b] *Samara Center for Theoretical Materials Science (SCTMS), Samara National Research University, Ac. Pavlov St 1, Samara, Russia 443011; Tel/Fax: +7-846-3356798; E-mail:aleksandrov_ev1@mail.ru (E. Alexandrov)*

PXRD Patterns and Thermal Analyses. The synthesized products of **1-6** have been characterized by powder X-ray diffraction (PXRD). The observed PXRD patterns correspond with the results simulated from the single crystal data, indicating the purity of the bulk samples. The minor discrepancies as to the peak intensity and positions maybe ascribe to the low crystallinity or preferred orientation of crystals. Meanwhile, in order to evaluate the stability of the structures in the adsorption-desorption process, the PXRD patterns of MO-released **1-6** were also measured, and the results of PXRD also show their stability.

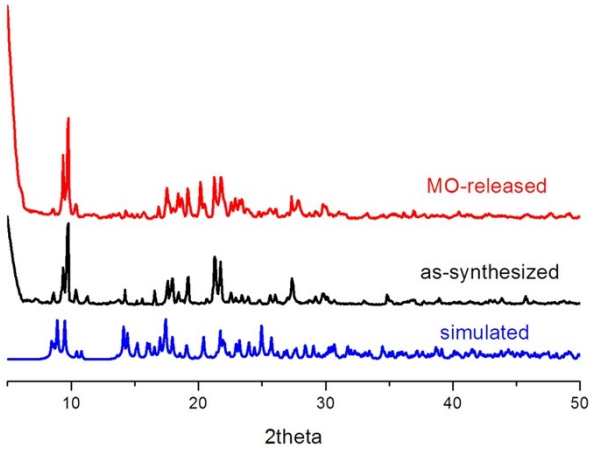

Fig. S1. The simulated (blue) and experimental (black) XRPD patterns for **1**.

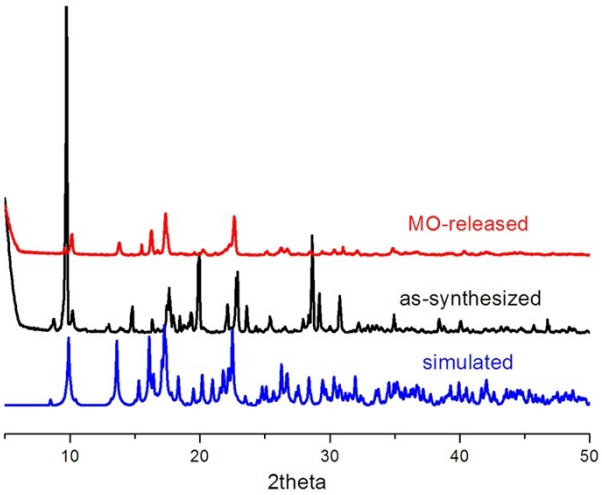

Fig. S2. The simulated (blue) and experimental (black) XRPD patterns for **2**.

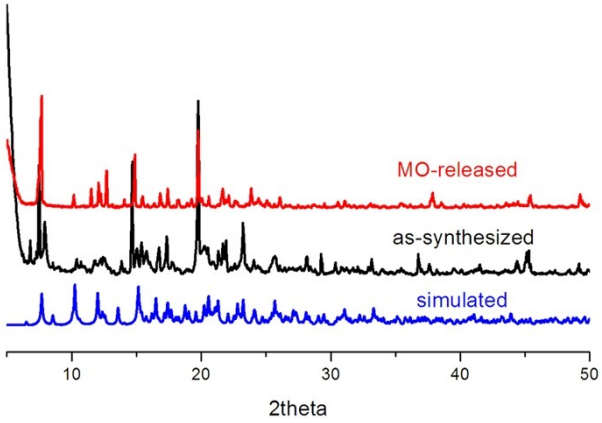

Fig. S3. The simulated (blue) and experimental (black) XRPD patterns for **3**.

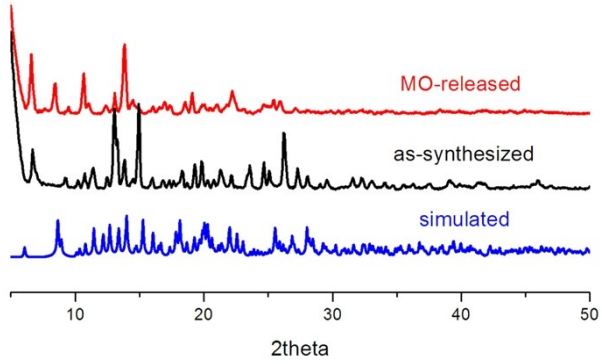

Fig. S4. The simulated (blue) and experimental (black) XRPD patterns for **4**.

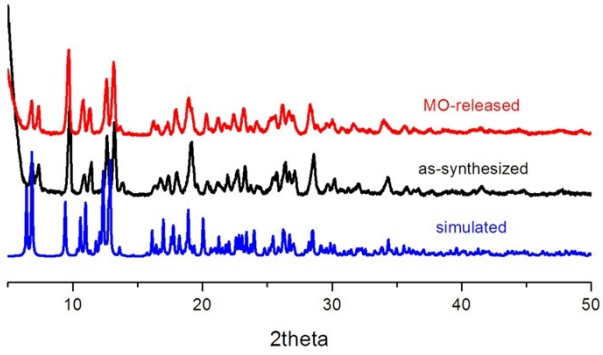

Fig. S5. The simulated (blue) and experimental (black) XRPD patterns for **5**.

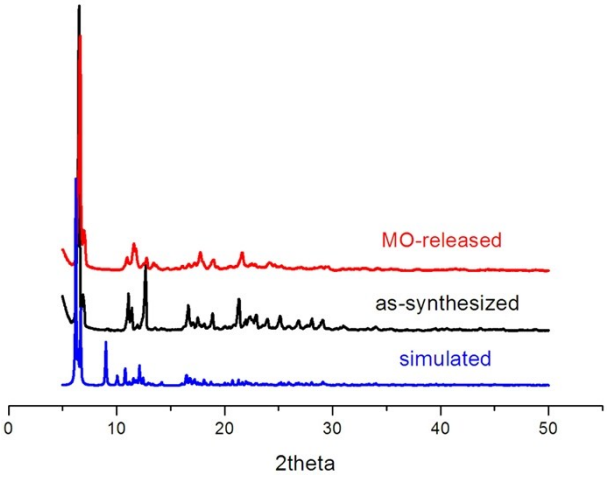

Fig. S6. The simulated (blue) and experimental (black) XRPD patterns for **6**.

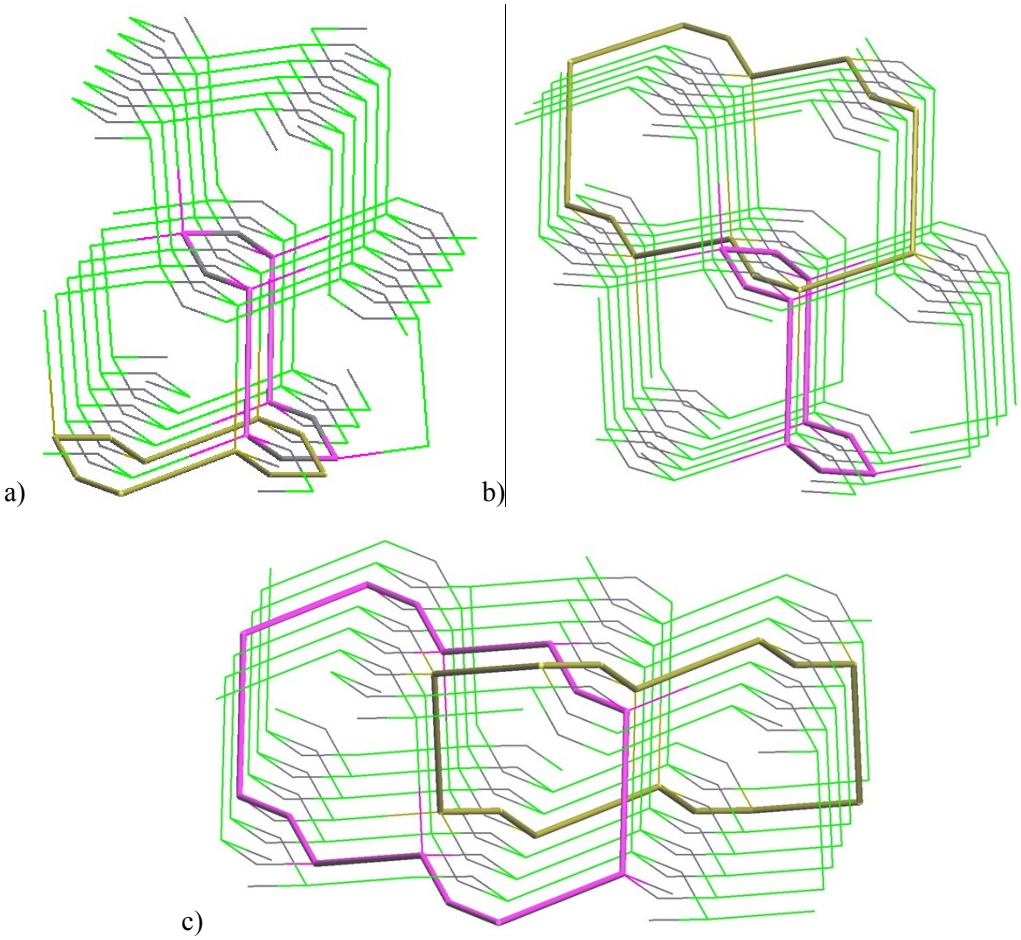

Fig. S7. The catenation of strong rings in the **4T25** underlying net of compound **1**: 10-ring (in magenta) with 10-ring (in yellow), 10-ring (in magenta) with 14-ring (in yellow), 14-ring (in magenta) with 14-ring (in yellow). The odc^{2-} ligand is presented by 2-coordinated nodes (in grey) to avoid edge-crossings in the net.

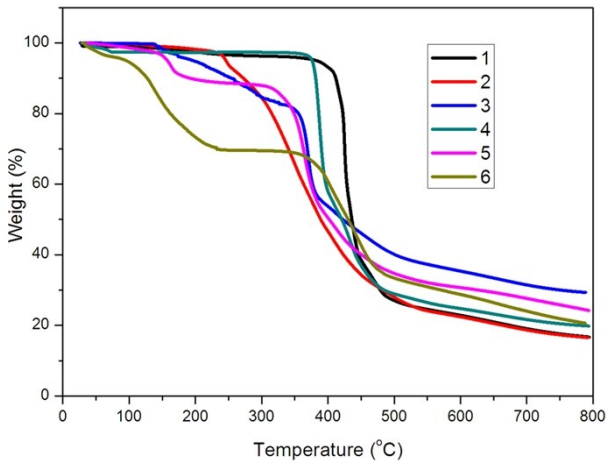

Fig. S8. TGA curves of **1-6**.

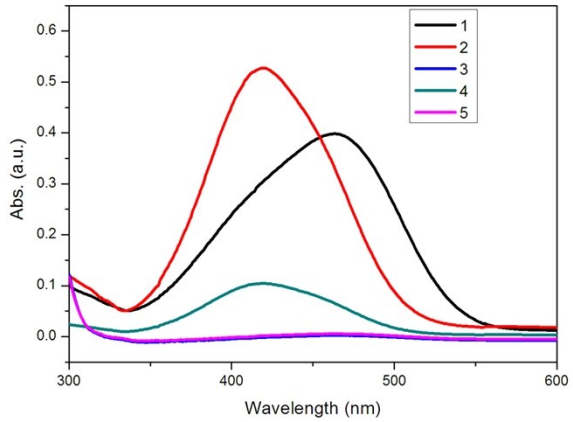

Fig. S9. UV-vis spectroscopic analyses of MO solution with compound **1**：(1) 4×10^{-5} mol/L MO water solution. (2) 4×10^{-5} mol/L MO methanol solution. (3) The water solution after adsorption by as-synthesized **1**. (4) The combined 50 mL methanol solution after desorption. (5) The water solution after adsorption by MO-released **1**.

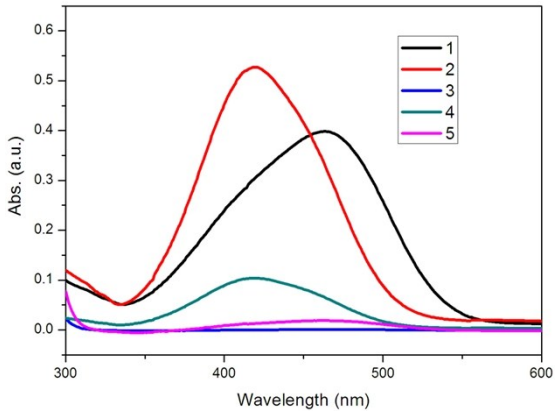

Fig. S10. UV-vis spectroscopic analyses of MO solution with compound **2**：(1) 4×10^{-5} mol/L MO water solution. (2) 4×10^{-5} mol/L MO methanol solution. (3) The water solution after adsorption by as-synthesized **2**. (4) The combined 50 mL methanol solution after desorption. (5) The water solution after adsorption by MO-released **2**.

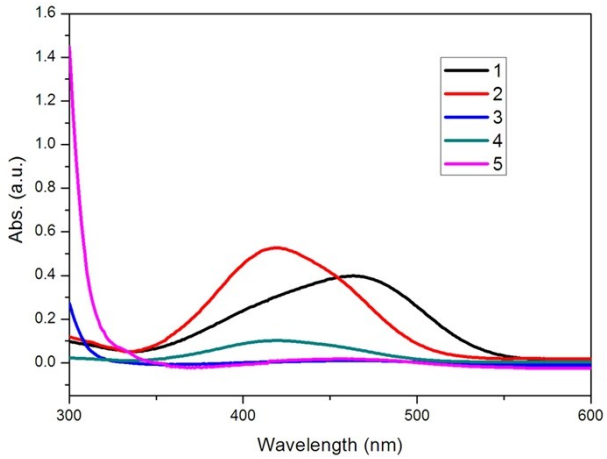

Fig. S11. UV-vis spectroscopic analyses of MO solution with compound **3**: (1) 4×10^{-5} mol/L MO water solution. (2) 4×10^{-5} mol/L MO methanol solution. (3) The water solution after adsorption by as-synthesized **3**. (4) The combined 50 mL methanol solution after desorption. (5) The water solution after adsorption by MO-released **3**.

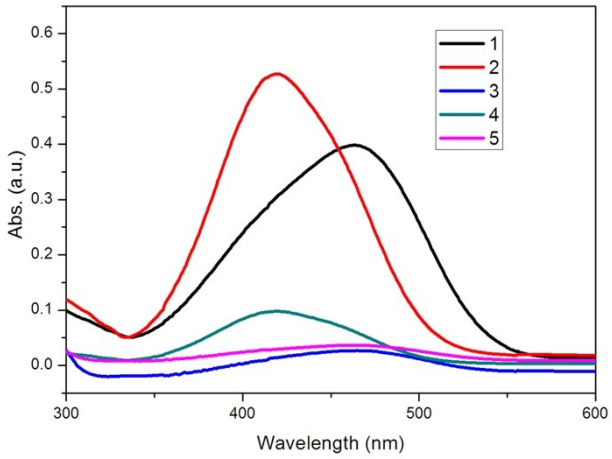

Fig. S12. UV-vis spectroscopic analyses of MO solution with compound **4**: (1) 4×10^{-5} mol/L MO water solution. (2) 4×10^{-5} mol/L MO methanol solution. (3) The water solution after adsorption by as-synthesized **4**. (4) The combined 50 mL methanol solution after desorption. (5) The water solution after adsorption by MO-released **4**.

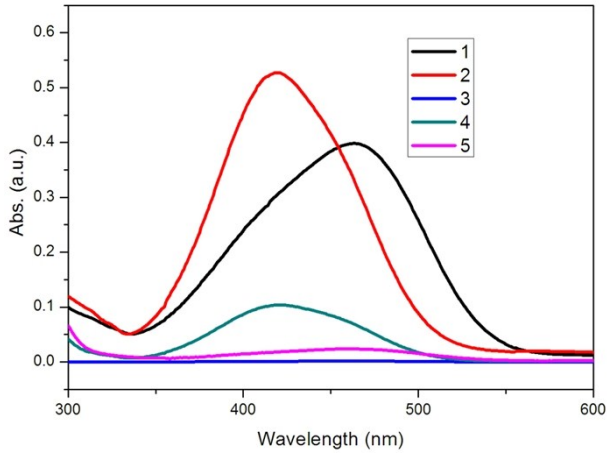

Fig. S13. UV-vis spectroscopic analyses of MO solution with compound **5**: (1) 4×10^{-5} mol/L MO water solution. (2) 4×10^{-5} mol/L MO methanol solution. (3) The water solution after adsorption by as-synthesized **5**. (4) The combined 50 mL methanol solution after desorption. (5) The water solution after adsorption by MO-released **5**.

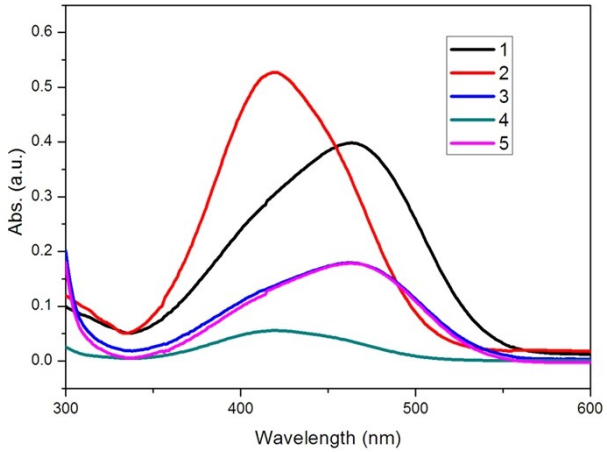

Fig. S14. UV-vis spectroscopic analyses of MO solution with compound **6**: (1) 4×10^{-5} mol/L MO water solution. (2) 4×10^{-5} mol/L MO methanol solution. (3) The water solution after adsorption by as-synthesized **6**. (4) The combined 50 mL methanol solution after desorption. (5) The water solution after adsorption by MO-released **6**.

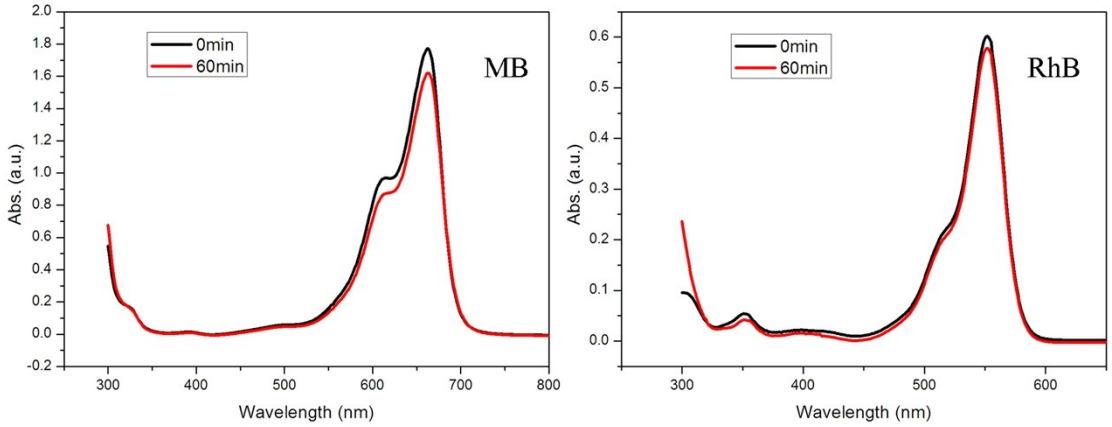

Fig. S15. UV-vis spectra of MB and RhB with **1** at given intervals, respectively.

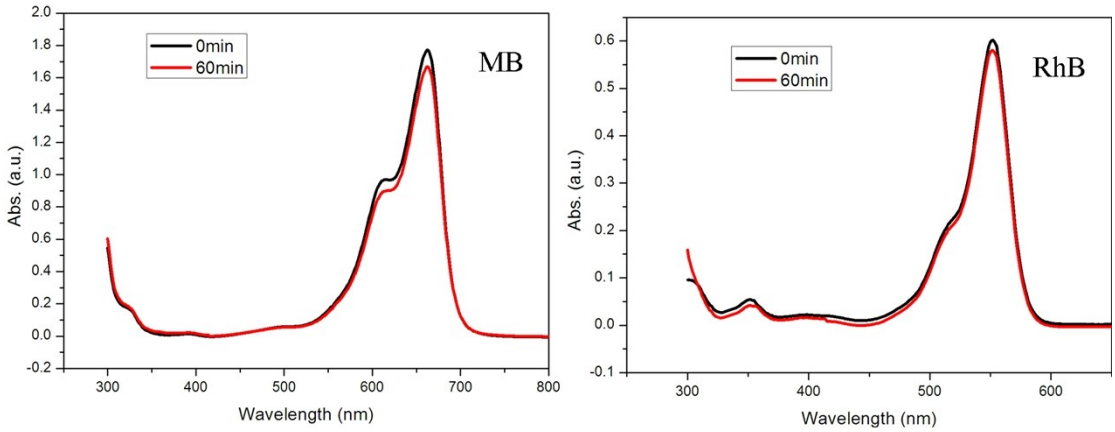

Fig. S16. UV-vis spectra of MB and RhB with **2** at given intervals, respectively.

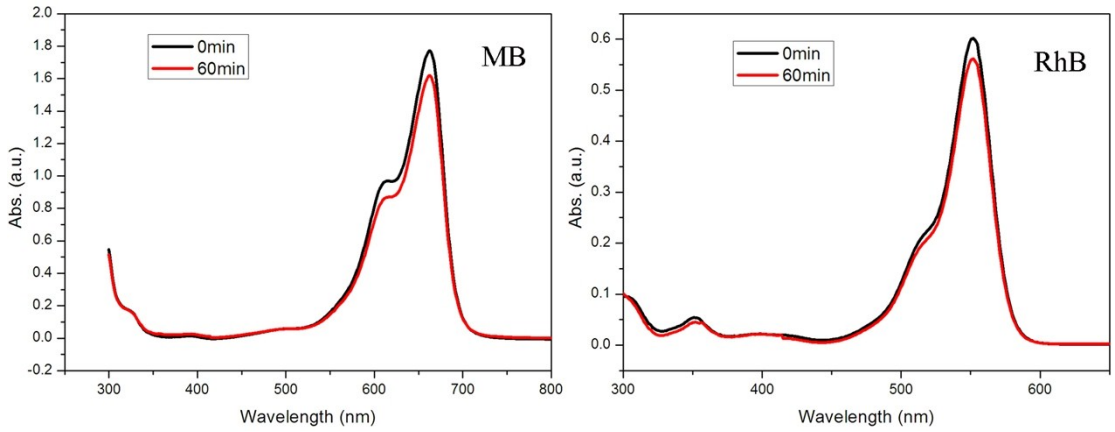

Fig. S17. UV-vis spectra of MB and RhB with **3** at given intervals, respectively.

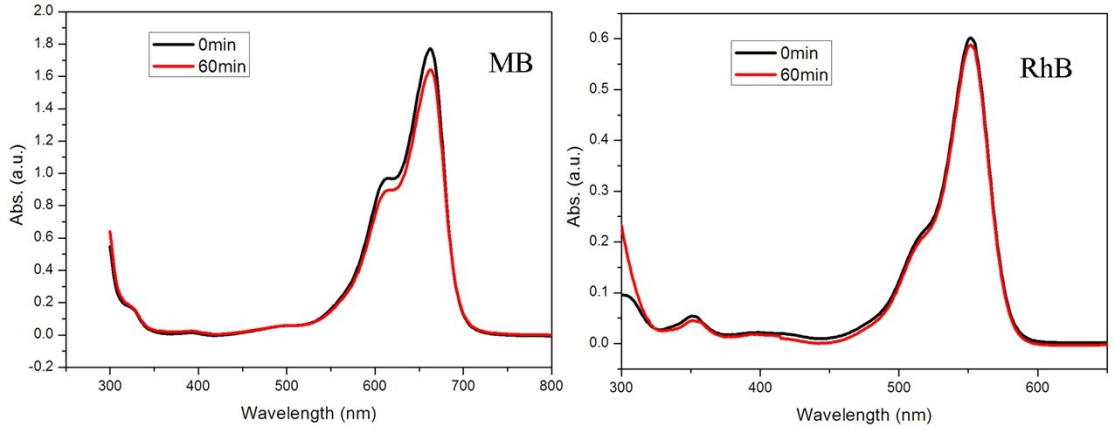

Fig. S18. UV-vis spectra of MB and RhB with **4** at given intervals, respectively.

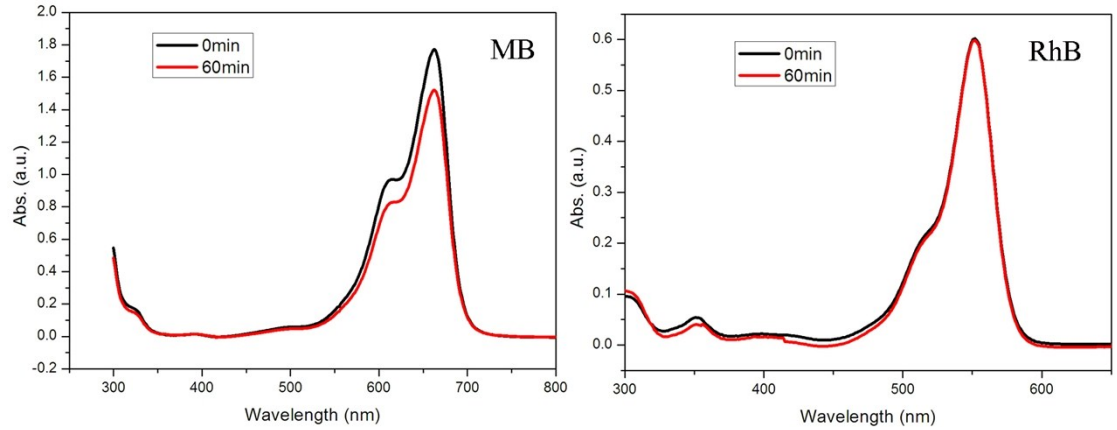

Fig. S19. UV-vis spectra of MB and RhB with **5** at given intervals, respectively.

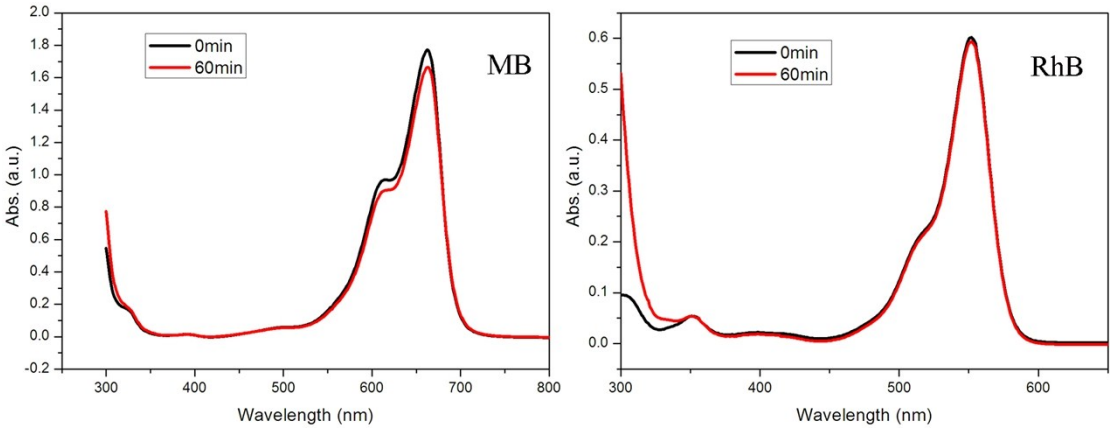

Fig. S20. UV-vis spectra of MB and RhB with **6** at given intervals, respectively.

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

Cd(1)-N(1)	2.2370(17)
Cd(1)-N(3)	2.2594(18)
Cd(1)-O(1)	2.4082(15)
Cd(1)-O(2)	2.3052(16)
Cd(1)-O(3)#1	2.2854(16)
Cd(1)-O(4)#1	2.5380(16)
N(1)-Cd(1)-N(3)	105.44(6)
N(1)-Cd(1)-O(3)#1	98.81(6)
N(3)-Cd(1)-O(3)#1	128.63(7)
N(1)-Cd(1)-O(2)	144.81(6)
N(3)-Cd(1)-O(2)	87.92(6)
O(3)#1-Cd(1)-O(2)	97.49(6)
N(1)-Cd(1)-O(1)	92.32(6)
N(3)-Cd(1)-O(1)	129.41(6)
O(3)#1-Cd(1)-O(1)	93.22(6)
O(2)-Cd(1)-O(1)	55.74(5)
N(1)-Cd(1)-O(4)#1	85.19(6)
N(3)-Cd(1)-O(4)#1	83.36(6)

O(3)#1-Cd(1)-O(4)#1	54.12(6)
O(2)-Cd(1)-O(4)#1	129.24(6)
O(1)-Cd(1)-O(4)#1	146.14(5)

Symmetry transformations used to generate equivalent atoms: #1 -x,y-1,-z+3/2.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Cd(1)-N(1)	2.274(3)
Cd(1)-N(3)	2.276(3)
Cd(1)-O(1)	2.247(2)
Cd(1)-OW1	2.333(2)
Cd(1)-O(3)#1	2.256(3)
O(1)-Cd(1)-O(3)#1	144.26(9)
O(1)-Cd(1)-N(1)	86.04(10)
O(3)#1-Cd(1)-N(1)	103.90(11)
O(1)-Cd(1)-N(3)	119.46(10)
O(3)#1-Cd(1)-N(3)	94.86(10)
N(1)-Cd(1)-N(3)	91.47(11)
O(1)-Cd(1)-OW1	84.78(9)
O(3)#1-Cd(1)-OW1	85.85(9)
N(1)-Cd(1)-OW1	170.05(10)
N(3)-Cd(1)-OW1	89.69(10)

Symmetry transformations used to generate equivalent atoms: #1 x+1,-y+1/2,z+1/2.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Cd(1)-N(1)	2.256(2)
Cd(1)-N(3)	2.238(2)
Cd(1)-O(1)	2.3840(18)

Cd(1)-O(2)	2.3215(19)
Cd(1)-O(4)#1	2.2787(18)
Cd(1)-O(3)#1	2.4132(18)
N(3)-Cd(1)-N(1)	99.33(8)
N(3)-Cd(1)-O(4)#1	142.34(7)
N(1)-Cd(1)-O(4)#1	97.16(7)
N(3)-Cd(1)-O(2)	93.05(8)
N(1)-Cd(1)-O(2)	140.44(7)
O(4)#1-Cd(1)-O(2)	95.40(7)
N(3)-Cd(1)-O(1)	98.52(7)
N(1)-Cd(1)-O(1)	84.92(7)
O(4)#1-Cd(1)-O(1)	116.53(6)
O(2)-Cd(1)-O(1)	56.02(6)
N(3)-Cd(1)-O(3)#1	87.32(7)
N(1)-Cd(1)-O(3)#1	102.44(7)
O(4)#1-Cd(1)-O(3)#1	56.05(6)
O(2)-Cd(1)-O(3)#1	115.62(6)
O(1)-Cd(1)-O(3)#1	169.82(6)

Symmetry transformations used to generate equivalent atoms: #1 x-1,y,z-1.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Cd(1)-N(1)	2.235(2)
Cd(1)-N(3)	2.245(2)
Cd(1)-O(1)	2.2175(17)
Cd(1)-O(2)	2.6164(17)
Cd(1)-O(4)#1	2.355(3)
Cd(1)-O(3)#1	2.403(3)
O(1)-Cd(1)-N(1)	107.80(7)

O(1)-Cd(1)-N(3)	112.79(8)
N(1)-Cd(1)-N(3)	113.77(8)
O(1)-Cd(1)-O(4)#1	99.97(9)
N(1)-Cd(1)-O(4)#1	84.33(9)
N(3)-Cd(1)-O(4)#1	133.54(9)
O(1)-Cd(1)-O(3)#1	104.12(8)
N(1)-Cd(1)-O(3)#1	131.81(9)
N(3)-Cd(1)-O(3)#1	84.72(8)
O(4)#1-Cd(1)-O(3)#1	55.00(10)
O(1)-Cd(1)-O(2)	54.06(6)
N(1)-Cd(1)-O(2)	80.22(7)
N(3)-Cd(1)-O(2)	83.86(7)
O(4)#1-Cd(1)-O(2)	142.56(8)
O(3)#1-Cd(1)-O(2)	147.80(9)

Symmetry transformations used to generate equivalent atoms: #1 x,y,z-1.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Cd(1)-N(1)	2.262(3)
Cd(2)-N(5)	2.271(3)
Cd(1)-O(2)	2.272(3)
Cd(1)-N(4)#2	2.299(3)
Cd(1)-O(3)#3	2.320(3)
Cd(1)-O(3)#1	2.448(3)
Cd(2)-O(5)	2.285(3)
Cd(1)-OW1	2.376(3)
Cd(2)-OW2	2.318(3)
Cd(2)-N(5)#4	2.271(3)
Cd(2)-O(5)#4	2.285(3)

Cd(2)-OW2#4	2.318(3)
N(1)-Cd(1)-O(2)	90.85(12)
N(1)-Cd(1)-N(4)#2	175.02(12)
O(2)-Cd(1)-N(4)#2	85.10(12)
N(1)-Cd(1)-O(3)#3	96.59(11)
O(2)-Cd(1)-O(3)#3	164.08(10)
N(4)#2-Cd(1)-O(3)#3	88.05(11)
N(1)-Cd(1)-OW1	87.50(12)
O(2)-Cd(1)-OW1	88.02(10)
N(4)#2-Cd(1)-OW1	89.45(12)
O(3)#3-Cd(1)-OW1	106.30(10)
N(1)-Cd(1)-O(3)#1	96.73(11)
O(2)-Cd(1)-O(3)#1	84.85(10)
N(4)#2-Cd(1)-O(3)#1	85.82(11)
O(3)#3-Cd(1)-O(3)#1	80.32(10)
OW1-Cd(1)-O(3)#1	171.76(9)
N(5)#4-Cd(2)-N(5)	180.00(8)
N(5)#4-Cd(2)-O(5)#4	89.04(11)
N(5)-Cd(2)-O(5)#4	90.96(11)
N(5)#4-Cd(2)-O(5)	90.96(11)
N(5)-Cd(2)-O(5)	89.04(11)
O(5)#4-Cd(2)-O(5)	180.00(16)
N(5)#4-Cd(2)-OW2#4	94.10(11)
N(5)-Cd(2)-OW2#4	85.90(11)
O(5)#4-Cd(2)-OW2#4	88.91(10)
O(5)-Cd(2)-OW2#4	91.09(10)
N(5)#4-Cd(2)-OW2	85.90(11)
N(5)-Cd(2)-OW2	94.10(11)
O(5)#4-Cd(2)-OW2	91.09(10)
O(5)-Cd(2)-OW2	88.91(10)

OW2#4-Cd(2)-OW2	180.00(7)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z; #2 x,y,z+1; #3 x+1,y-1,z; #4 -x-1,-y,-z+1.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Zn(1)-O(2)	2.067(2)
Zn(1)-O(4)#2	2.100(2)
Zn(1)-O(6)#4	2.1019(19)
Zn(2) - N(1)	2.005(2)
Zn(2) - O(1)	1.930(2)
Zn(2)-O(5)#4	1.908(2)
Zn(2)-O(3)#3	1.962(2)
O(2)-Zn(1)-O(2)#1	180.00(11)
O(2)-Zn(1)-O(4)#2	86.26(8)
O(2)#1-Zn(1)-O(4)#2	93.74(8)
O(2)-Zn(1)-O(4)#7	93.74(8)
O(2)#1-Zn(1)-O(4)#3	86.26(8)
O(4)#2-Zn(1)-O(4)#3	180.00(11)
O(2)-Zn(1)-O(6)#4	88.88(8)
O(2)#1-Zn(1)-O(6)#4	91.12(8)
O(4)#2-Zn(1)-O(6)#4	82.33(8)
O(4)#3-Zn(1)-O(6)#4	97.67(8)
O(2)-Zn(1)-O(6)#5	91.12(8)
O(2)#1-Zn(1)-O(6)#5	88.88(8)
O(4)#2-Zn(1)-O(6)#5	97.67(8)
O(4)#3-Zn(1)-O(6)#5	82.33(8)
O(6)#4-Zn(1)-O(6)#5	180.000(1)
O(5)#4-Zn(2)-O(1)	121.07(10)
O(5)#4-Zn(2)-O(3)#3	110.08(10)

O(1)-Zn(2)-O(3)#3	117.67(9)
O(5)#4-Zn(2)-N(1)	100.55(9)
O(1)-Zn(2)-N(1)	102.94(9)
O(3)#3-Zn(2)-N(1)	100.03(9)

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