

Electronic Supplementary Information (ESI) for

Structural Diversity, Luminescence, and Photocatalytic Properties of Six Coordination Polymers Based on Designed Bifunctional 2-(1-imidazol-yl)terephthalic Acid

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ESI

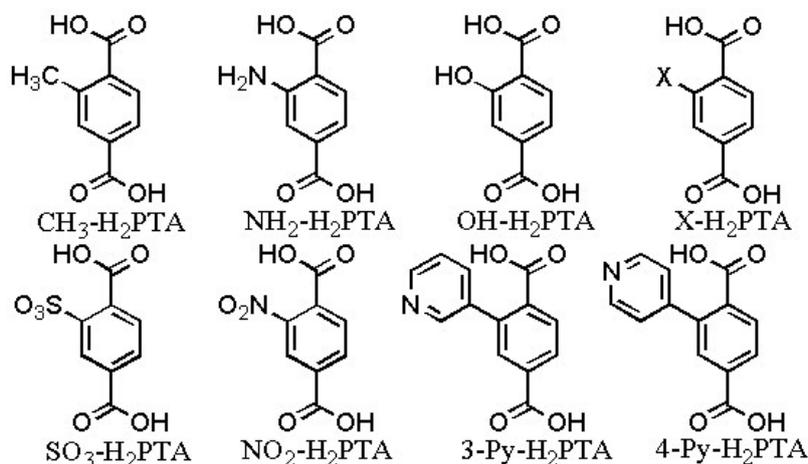


Figure S1. Various 2-position modified H₂TPA derivatives.

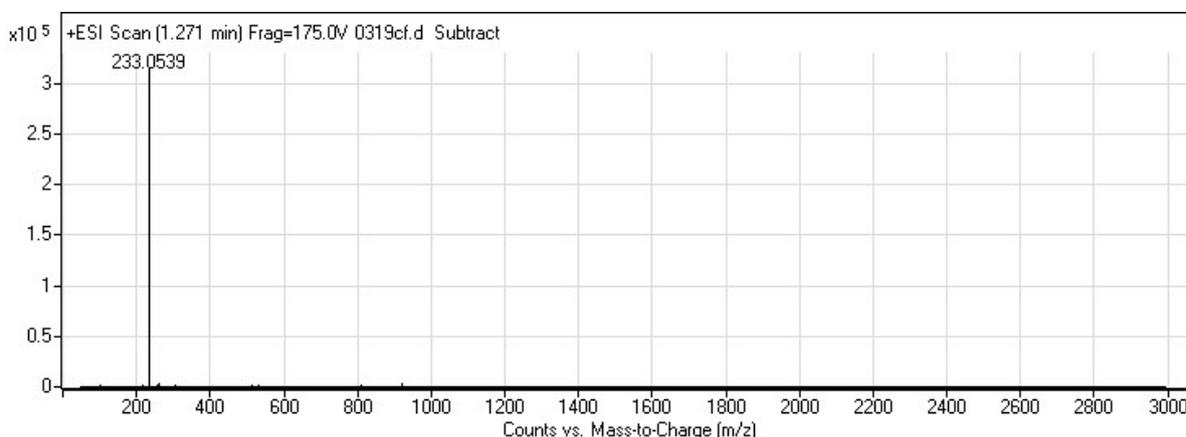
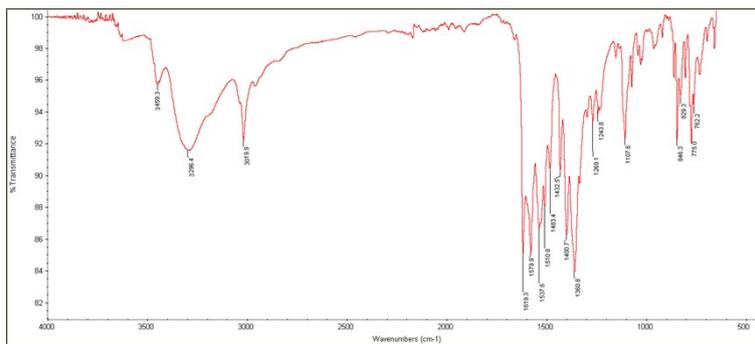
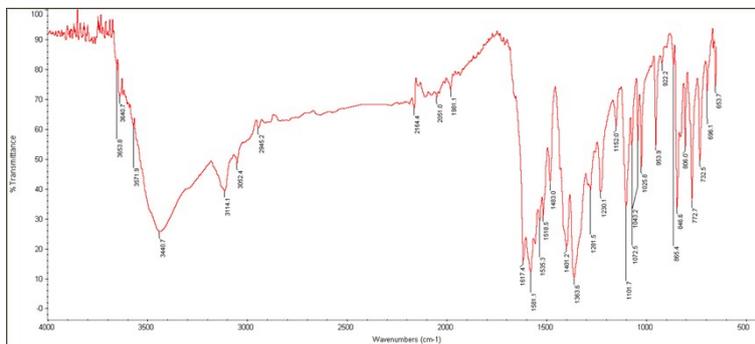


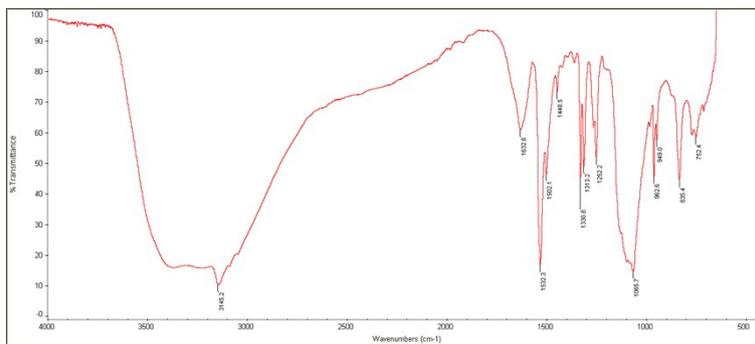
Figure S2. The MS data of the obtained H₂TPA.



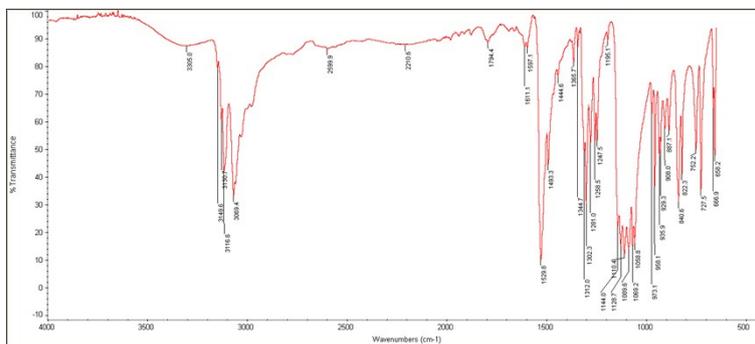
(1)



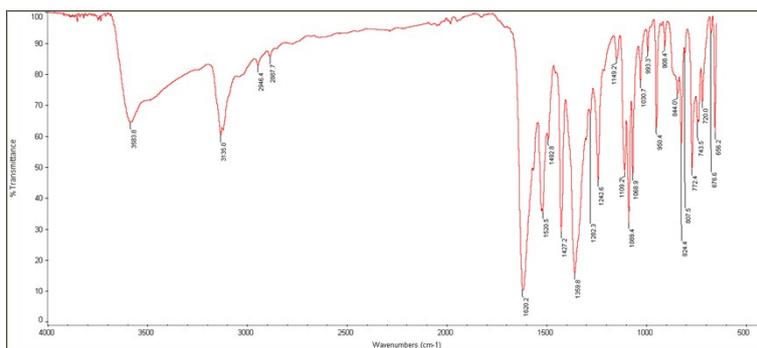
(2)



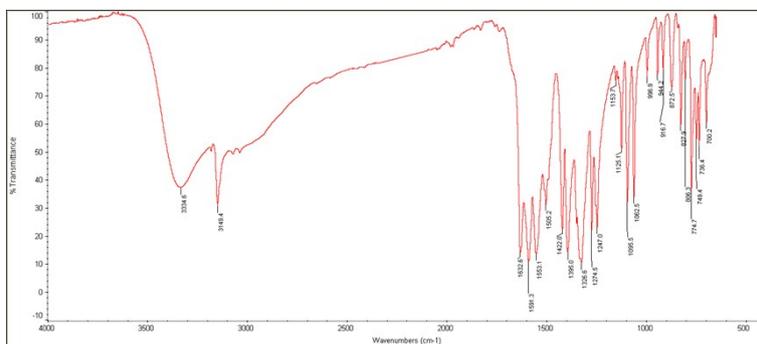
(3)



(4)



(5)



(6)

Figure S3. The IR spectra of complexes 1-6.

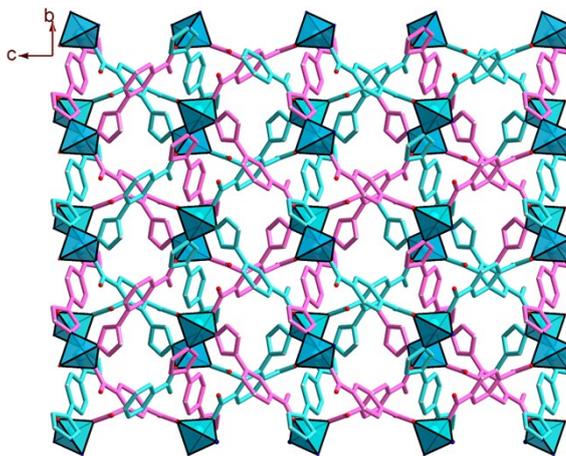


Figure S4. The 2-fold interpenetrated framework of 1.

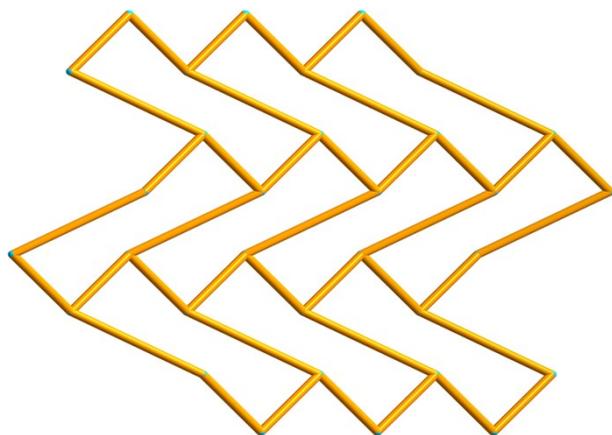


Figure S5. The 2D $\{6^3\}$ -hcb sheet of **4**.

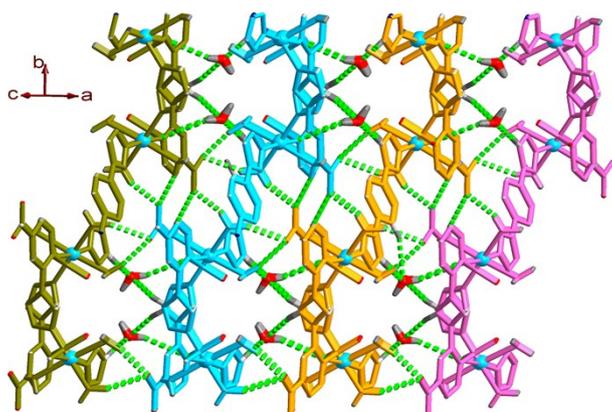
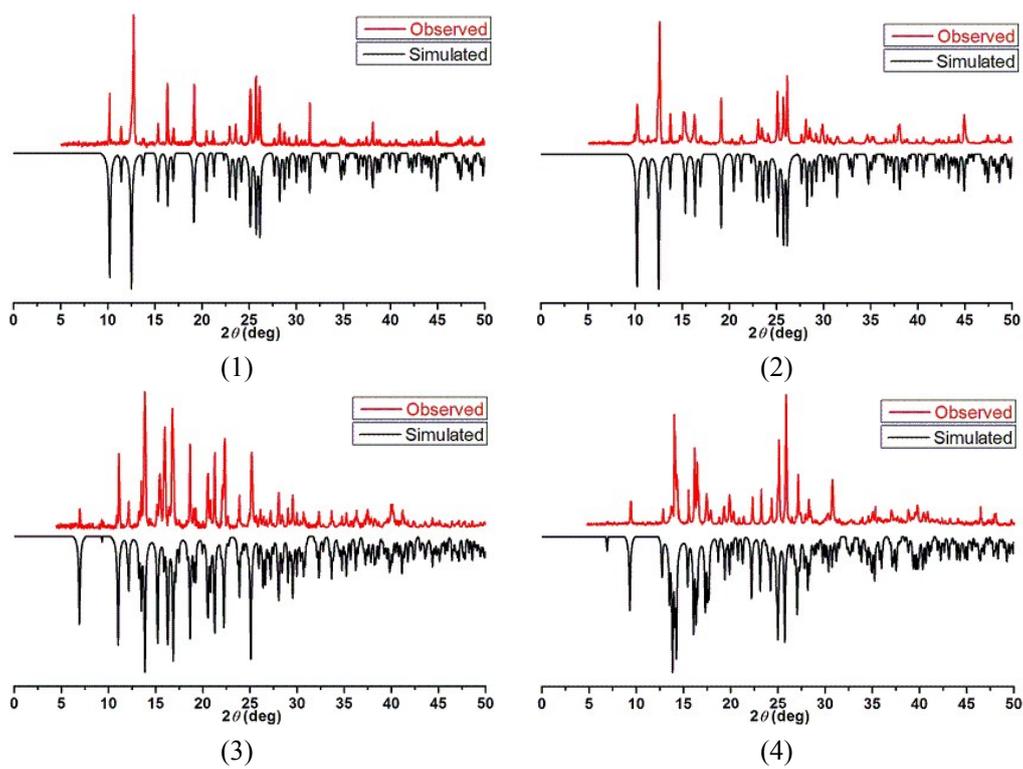


Figure S6. The 3D supramolecular structure of **4**.



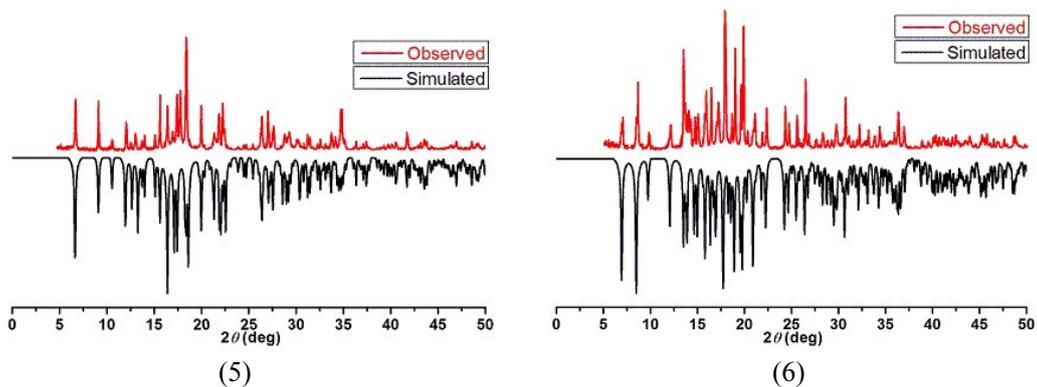


Figure S7. PXRD patterns of **1-6**. Dark: calculated from the X-ray single-crystal data; Red: observed for the as-synthesized solids.

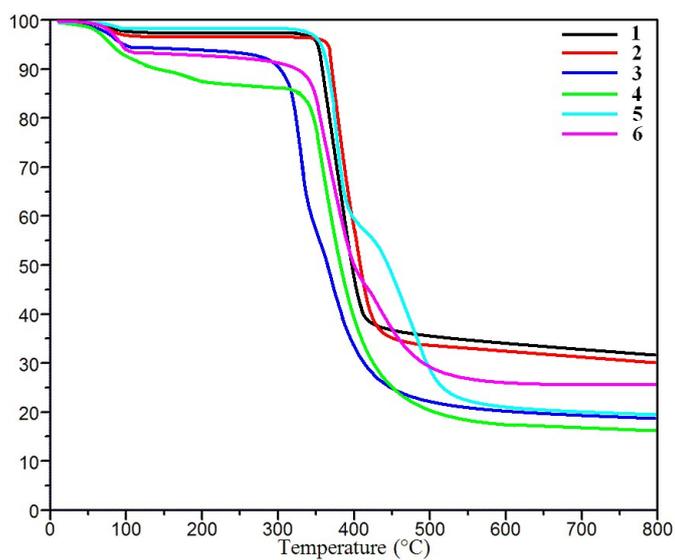
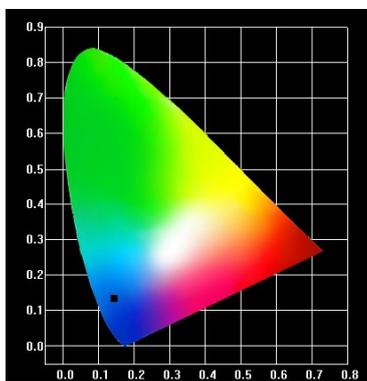
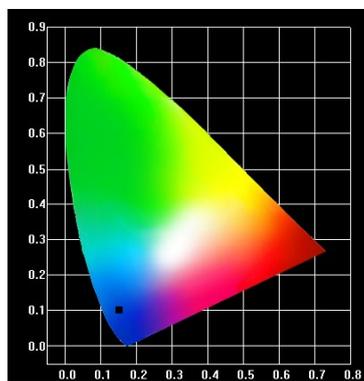


Figure S8. TGA curves for complexes **1-6**.



(a)



(b)

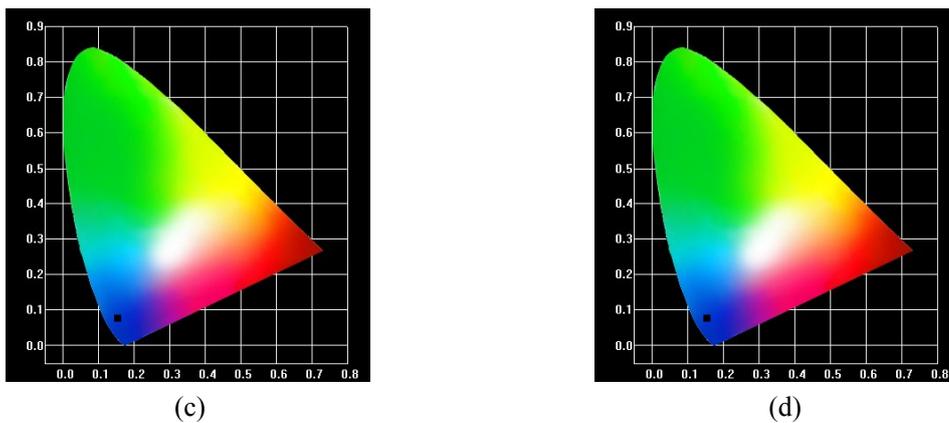


Figure S9. The CIE PXRD patterns of **1** (a), **3** (b), **5** (c), and **6** (d).

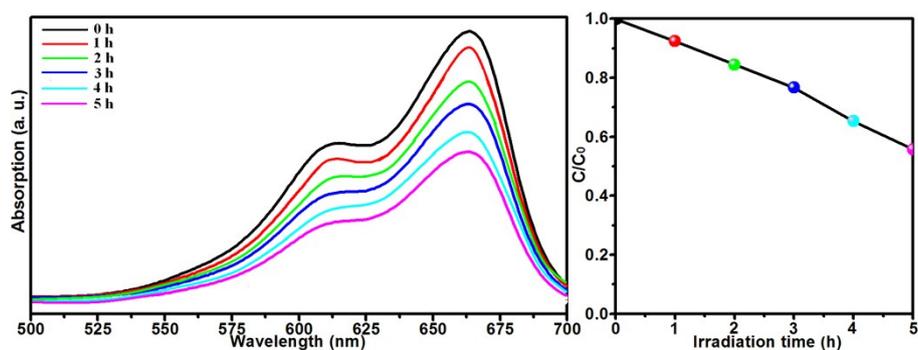


Figure S10. UV-Vis absorption spectra of the MB solutions degraded without catalyst under UV irradiation at different time intervals.

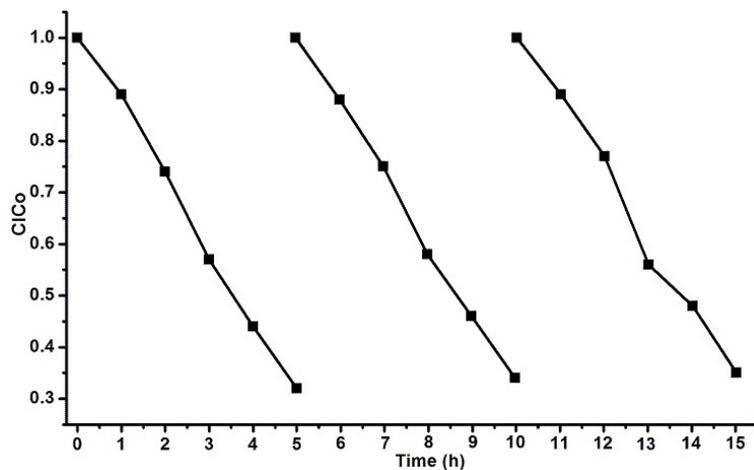


Figure S11. Recycling test on complex **1** for MB photodegradation.

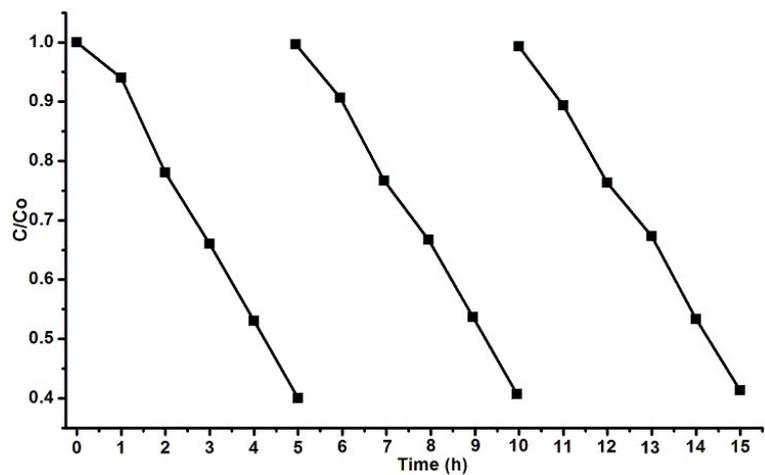


Figure S12. Recycling test on complex 3 for MB photodegradation.

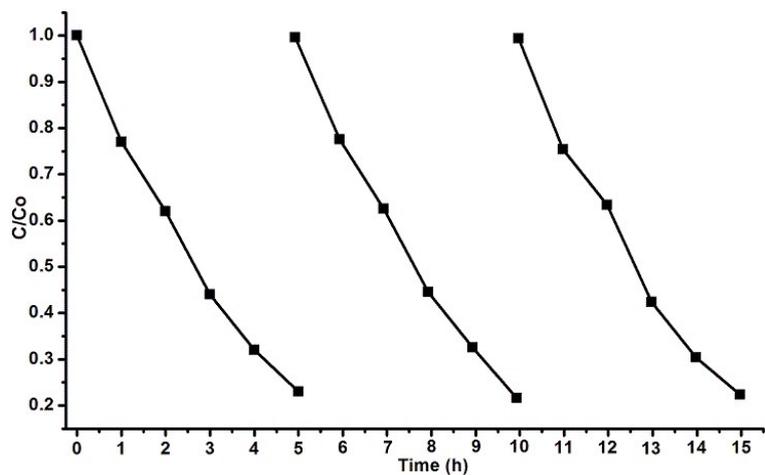


Figure S13. Recycling test on complex 5 for MB photodegradation.

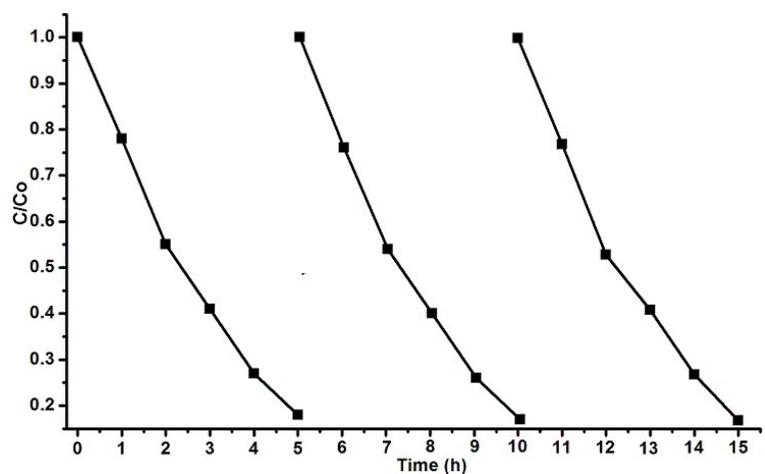


Figure S14. Recycling test on complex 6 for MB photodegradation.

Table S1 Selected bond lengths (Å) and angles (°) for **1**, and **3–6**.

Complex 1							
O(2B)-Zn(1)	2.01(7)	Zn(1)-N(2) ^{#4}	1.9923(18)	Zn(1)-O(3) ^{#5}	2.0845(16)	Zn(1)-O(4) ^{#5}	2.4328(16)
Zn(1)-O(2A)	1.90(8)	Zn(1)-O(4) ^{#3}	2.0423(16)	N(2) ^{#4} -Zn(1)-O(3) ^{#5}	113.49(7)	N(2) ^{#4} -Zn(1)-O(4) ^{#5}	91.14(7)
O(2A)-Zn(1)-N(2) ^{#4}	140.9(17)	N(2) ^{#4} -Zn(1)-O(4) ^{#3}	93.69(7)	O(2B)-Zn(1)-O(3) ^{#5}	93(2)	O(2B)-Zn(1)-O(4) ^{#5}	89(2)
N(2) ^{#4} -Zn(1)-O(2B)	147.8(17)	O(2B)-Zn(1)-O(4) ^{#3}	101(2)	O(4) ^{#3} -Zn(1)-O(3) ^{#5}	96.80(6)	O(4) ^{#3} -Zn(1)-O(4) ^{#5}	153.07(5)
O(2A)-Zn(1)-O(4) ^{#3}	105(2)	O(2A)-Zn(1)-O(3) ^{#5}	98(2)	O(2A)-Zn(1)-O(4) ^{#5}	87(2)	O(3) ^{#5} -Zn(1)-O(4) ^{#5}	57.24(5)
Symmetry codes: #3 -x+2, -y+2, -z+1; #4 x+1/2, y+1/2, -z+3/2; #5 x+1/2, -y+3/2, -z+1.							
Complex 3							
N(1)-Zn(1)	2.038(3)	N(3)-Zn(1)	2.012(3)	Zn(1)-O(2) ^{#4}	1.922(3)	Zn(1)-O(3) ^{#3}	1.930(3)
O(2) ^{#4} -Zn(1)-O(3) ^{#3}	130.90(15)	O(3) ^{#3} -Zn(1)-N(3)	110.32(13)	O(3) ^{#3} -Zn(1)-N(1)	100.72(13)	N(3)-Zn(1)-N(1)	104.49(13)
O(2) ^{#4} -Zn(1)-N(3)	100.33(13)	O(2) ^{#4} -Zn(1)-N(1)	107.72(13)				
Symmetry codes: #3 -x+2, -y+2, -z+1; #4 -x+3/2, y+1, -z+1/2.							
Complex 4							
N(1)-Ni(1)	2.0382(17)	Ni(1)-O(3) ^{#2}	2.0389(15)	Ni(1)-O(7)	2.1051(16)	Ni(1)-O(6)	2.1228(18)
N(3)-Ni(1)	2.0726(17)	Ni(1)-O(5)	2.0746(15)	O(3) ^{#2} -Ni(1)-O(7)	84.48(6)	O(3) ^{#2} -Ni(1)-O(6)	84.02(8)
N(1)-Ni(1)-O(3) ^{#2}	91.14(7)	O(3) ^{#2} -Ni(1)-O(5)	93.04(6)	N(3)-Ni(1)-O(7)	91.22(7)	N(3)-Ni(1)-O(6)	92.43(9)
N(1)-Ni(1)-N(3)	92.58(7)	N(3)-Ni(1)-O(5)	90.98(7)	O(5)-Ni(1)-O(7)	175.03(6)	O(5)-Ni(1)-O(6)	87.76(7)
O(3) ^{#2} -Ni(1)-N(3)	174.52(7)	N(1)-Ni(1)-O(7)	94.45(7)	N(1)-Ni(1)-O(6)	174.50(8)	O(7)-Ni(1)-O(6)	87.69(7)
N(1)-Ni(1)-O(5)	89.89(7)						
Symmetry code: #2 x-1/2, -y+3/2, z-1/2.							
Complex 5							
Zn(1)-O(1)	1.917(2)	Zn(1)-O(3) ^{#1}	1.9369(19)	Zn(1)-N(1)	2.006(2)	Zn(1)-N(3) ^{#2}	2.026(2)
O(1)-Zn(1)-O(3) ^{#1}	126.16(11)	O(3) ^{#1} -Zn(1)-N(1)	94.93(9)	O(3) ^{#1} -Zn(1)-N(3) ^{#2}	110.32(10)	N(1)-Zn(1)-N(3) ^{#2}	107.01(10)
O(1)-Zn(1)-N(1)	116.26(10)	O(1)-Zn(1)-N(3) ^{#2}	101.31(9)				
Symmetry codes: #1 x-1/2, -y, z-1/2; #2 -x+1, -y+1, -z+1.							
Complex 6							
Cd(1)-N(1) ^{#2}	2.233(2)	Cd(1)-O(5)	2.417(2)	Cd(1)-O(4)	2.483(2)	Cd(1)-O(1) ^{#3}	2.510(2)
Cd(1)-N(3)	2.245(2)	Cd(1)-O(2) ^{#3}	2.438(2)	Cd(1)-O(6)	2.497(2)	N(1) ^{#2} -Cd(1)-N(3)	168.46(8)
N(1) ^{#2} -Cd(1)-O(5)	90.47(9)	N(1) ^{#2} -Cd(1)-O(4)	86.70(8)	N(3)-Cd(1)-O(6)	83.39(8)	N(3)-Cd(1)-O(1) ^{#3}	97.71(9)
N(3)-Cd(1)-O(5)	95.87(9)	N(3)-Cd(1)-O(4)	85.63(8)	O(5)-Cd(1)-O(6)	150.18(9)	O(5)-Cd(1)-O(1) ^{#3}	74.16(9)
N(1) ^{#2} -Cd(1)-O(2) ^{#3}	86.01(8)	O(5)-Cd(1)-O(4)	75.10(9)	O(2) ^{#3} -Cd(1)-O(6)	83.39(7)	O(2) ^{#3} -Cd(1)-O(1) ^{#3}	52.36(7)
N(3)-Cd(1)-O(2) ^{#3}	97.93(8)	O(2) ^{#3} -Cd(1)-O(4)	157.70(7)	O(4)-Cd(1)-O(6)	75.12(7)	O(4)-Cd(1)-O(1) ^{#3}	149.26(7)
O(5)-Cd(1)-O(2) ^{#3}	125.99(9)	N(1) ^{#2} -Cd(1)-O(6)	86.32(8)	N(1) ^{#2} -Cd(1)-O(1) ^{#3}	93.30(8)	O(6)-Cd(1)-O(1) ^{#3}	135.60(7)
Symmetry codes: #2 -x+2, -y+2, -z+2; #3 x, -y+1, z-1/2.							