

Supplementary Material (ESI) for Dalton Transactions
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A series of Keggin-based compounds constructed by conjugate ring-rich pyrazine and quinoxaline derivatives

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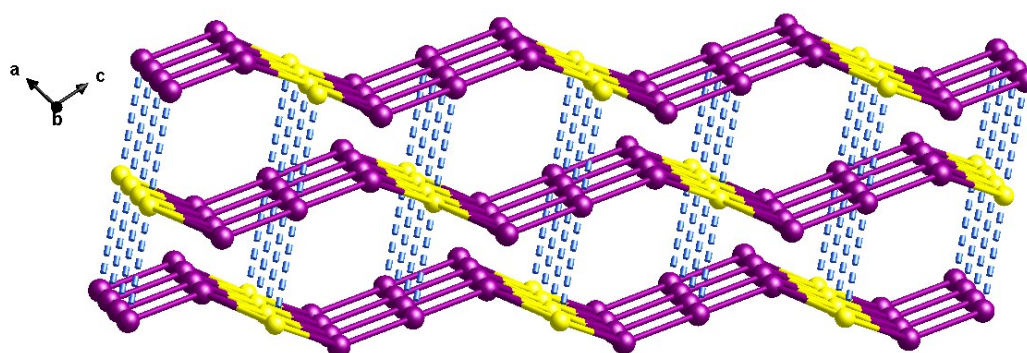


Fig. S1. The supramolecular 3D network of **1** linked by intermolecular weak interactions between layers.

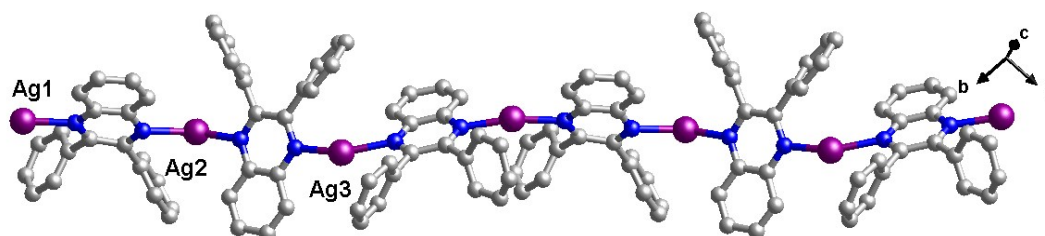


Fig. S2. View of 1D Ag-L² line in **3**.

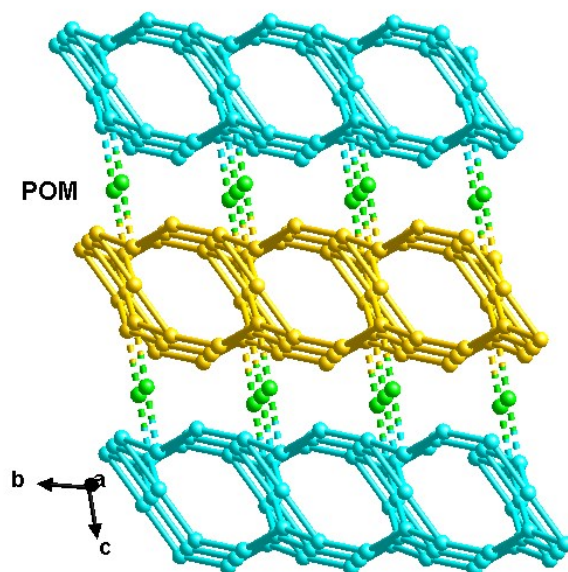


Fig. S3. The 3D supramolecular structure of **3** connected by intermolecular force.

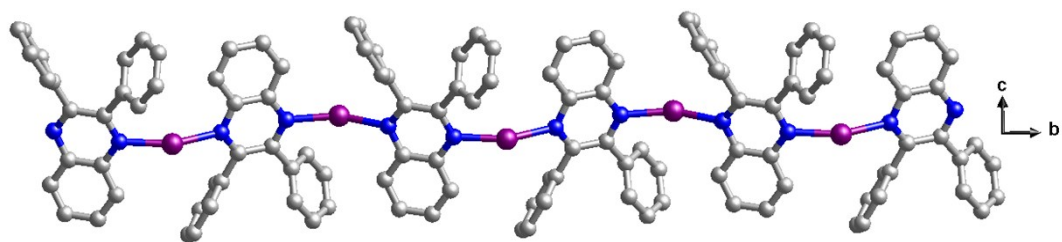


Fig. S4. The 1D wave-like Ag- L^2 chain of compound **4**.

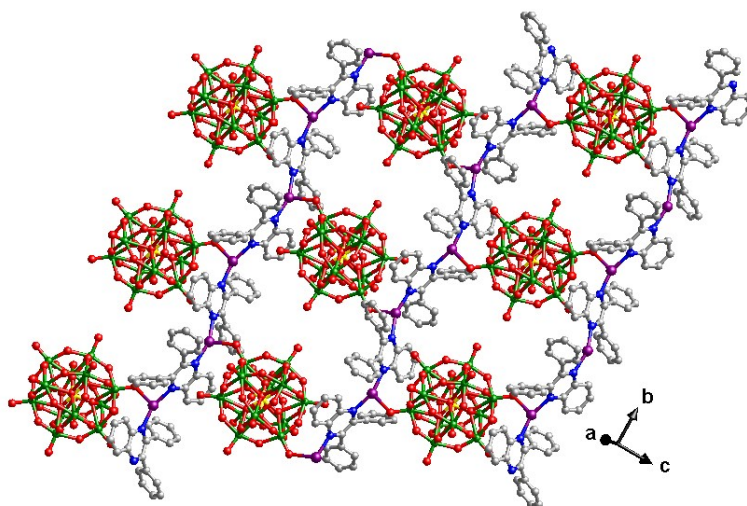


Fig. S5. The 2D grid-like metal-organic layer of compound **4**.

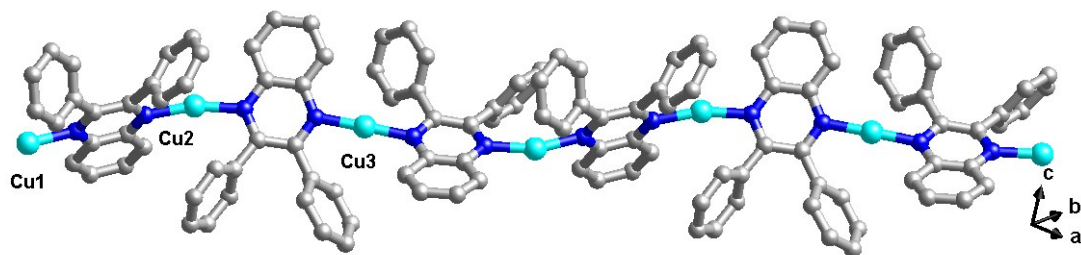


Fig. S6. The 1D wave-like Cu-L² line of compound 5.

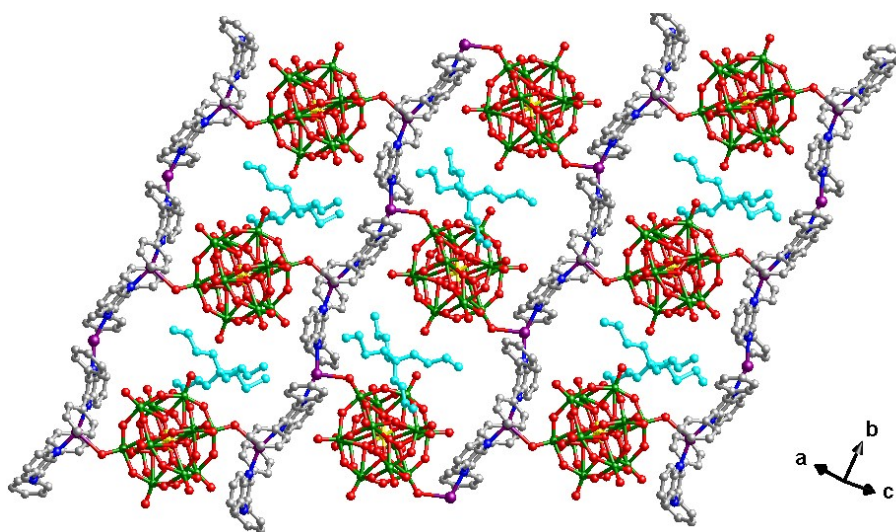


Fig. S7. The tetrabutyl ammonium ions accommodated in the grid of the layer for compound 4.

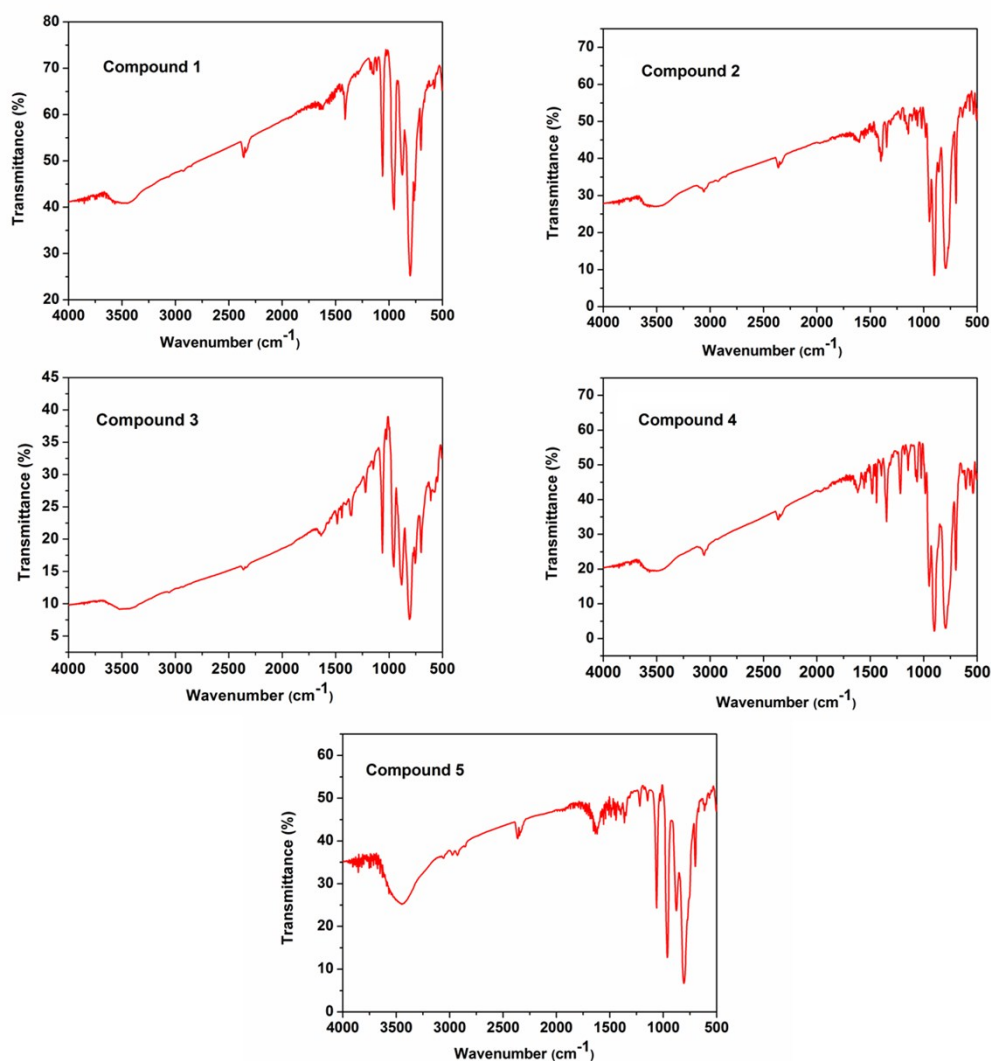


Fig. S8. The IR spectra of compounds **1–5**.

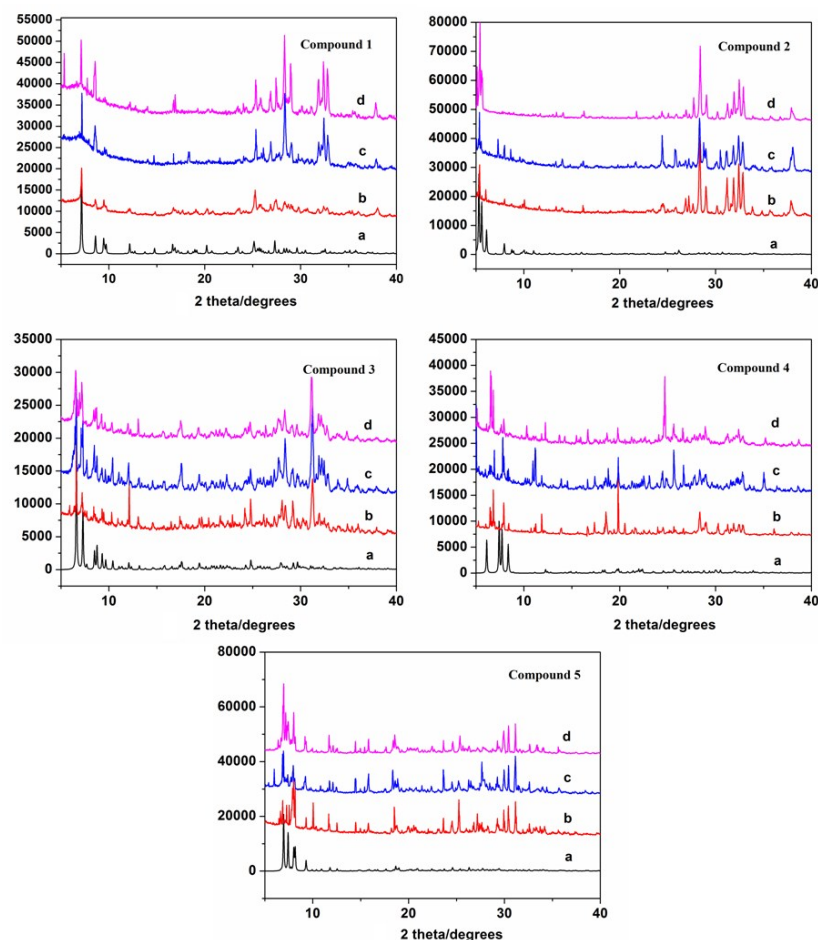


Fig. S9. The simulative (a), experimental (b) and recycled after photocatalysis (c for MB and d for RhB) powder X-ray diffraction patterns for compounds 1–5.

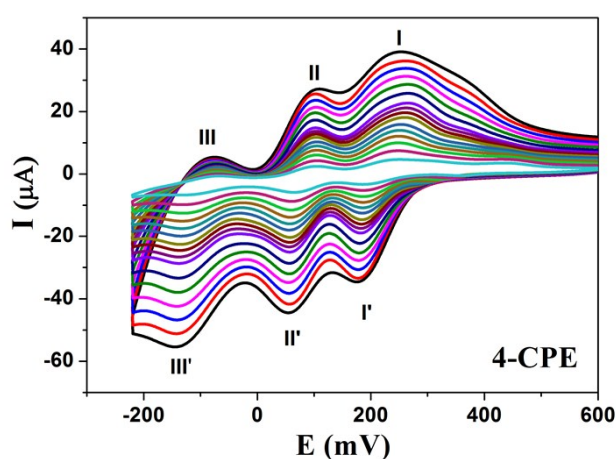


Fig. S10. The cyclic voltammograms of the 4–CPE in 0.1M H₂SO₄ + 0.5M Na₂SO₄ aqueous solution at different scan rates (from inner to outer: 20, 40, 60, 80, 100, 120, 140, 160, 180, 200, 250, 300, 350, 400, 450 and 500 mV·s⁻¹, respectively.).

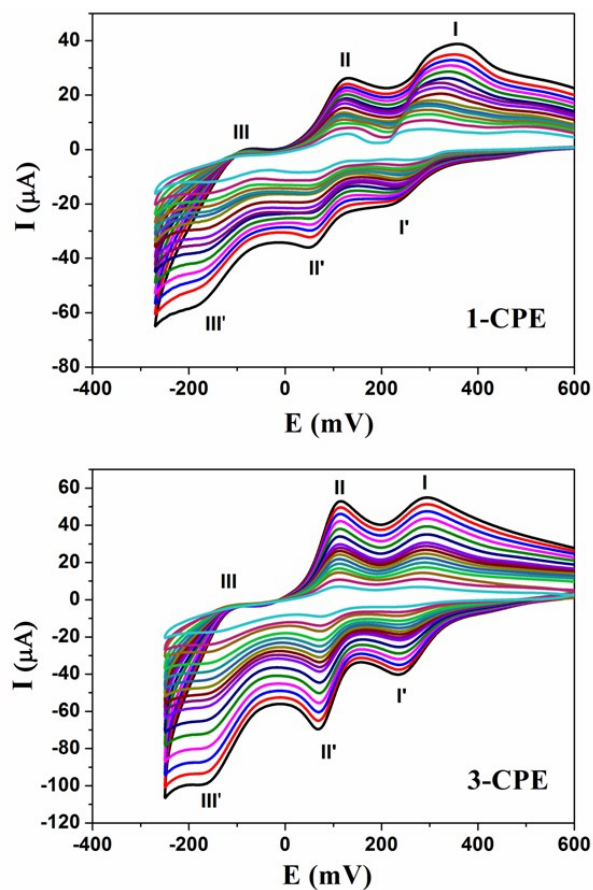


Fig. S11. The cyclic voltammograms of the 1-CPE and 3-CPE in 0.1M H_2SO_4 + 0.5M Na_2SO_4 aqueous solution at different scan rates (from inner to outer: 20, 40, 60, 80, 100, 120, 140, 160, 180, 200, 250, 300, 350, 400, 450 and 500 $\text{mV}\cdot\text{s}^{-1}$, respectively.).

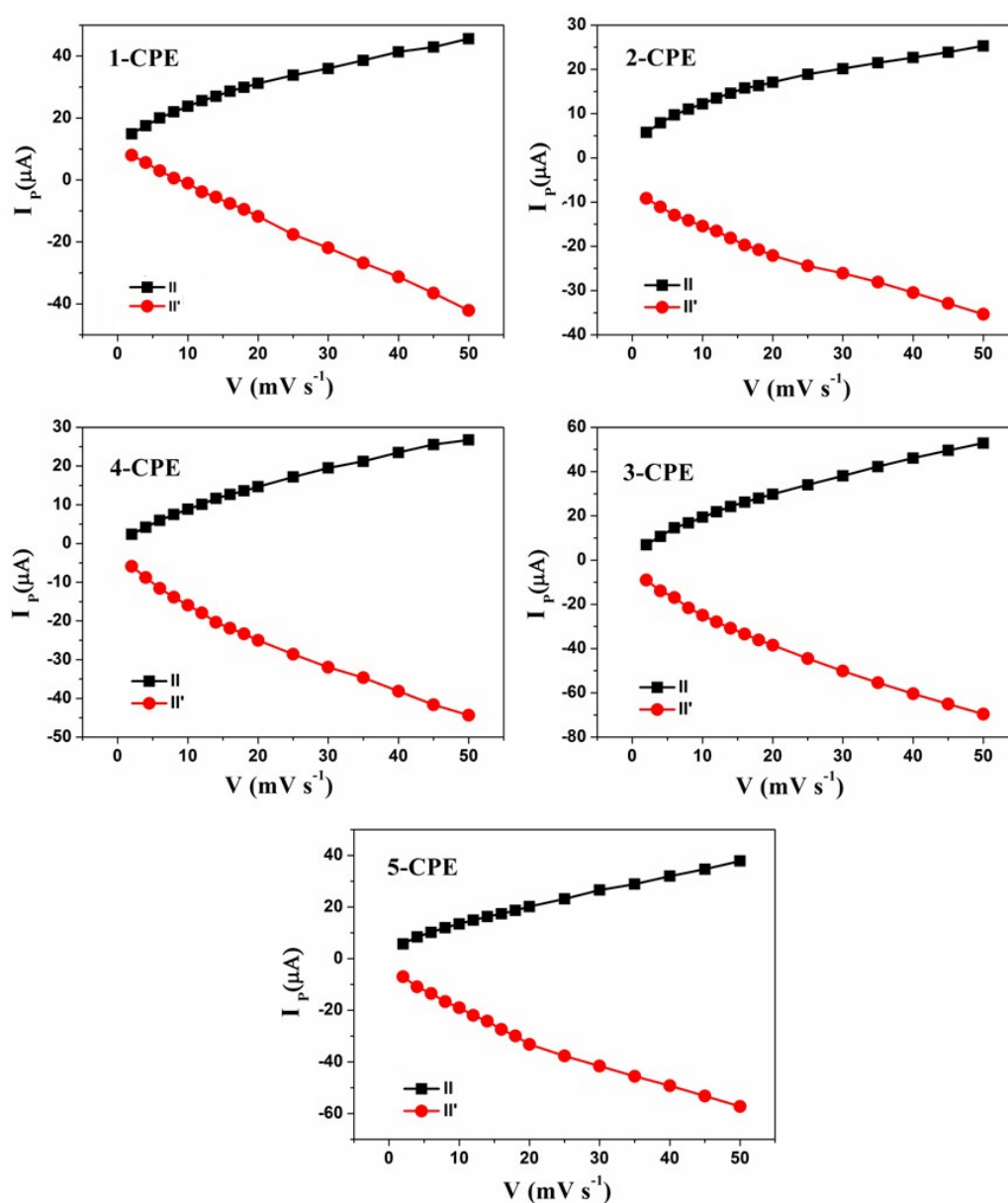


Fig. S12. The dependence of anodic peak (II) and cathodic peak (II') currents of 1–5–CPE on scan rates.

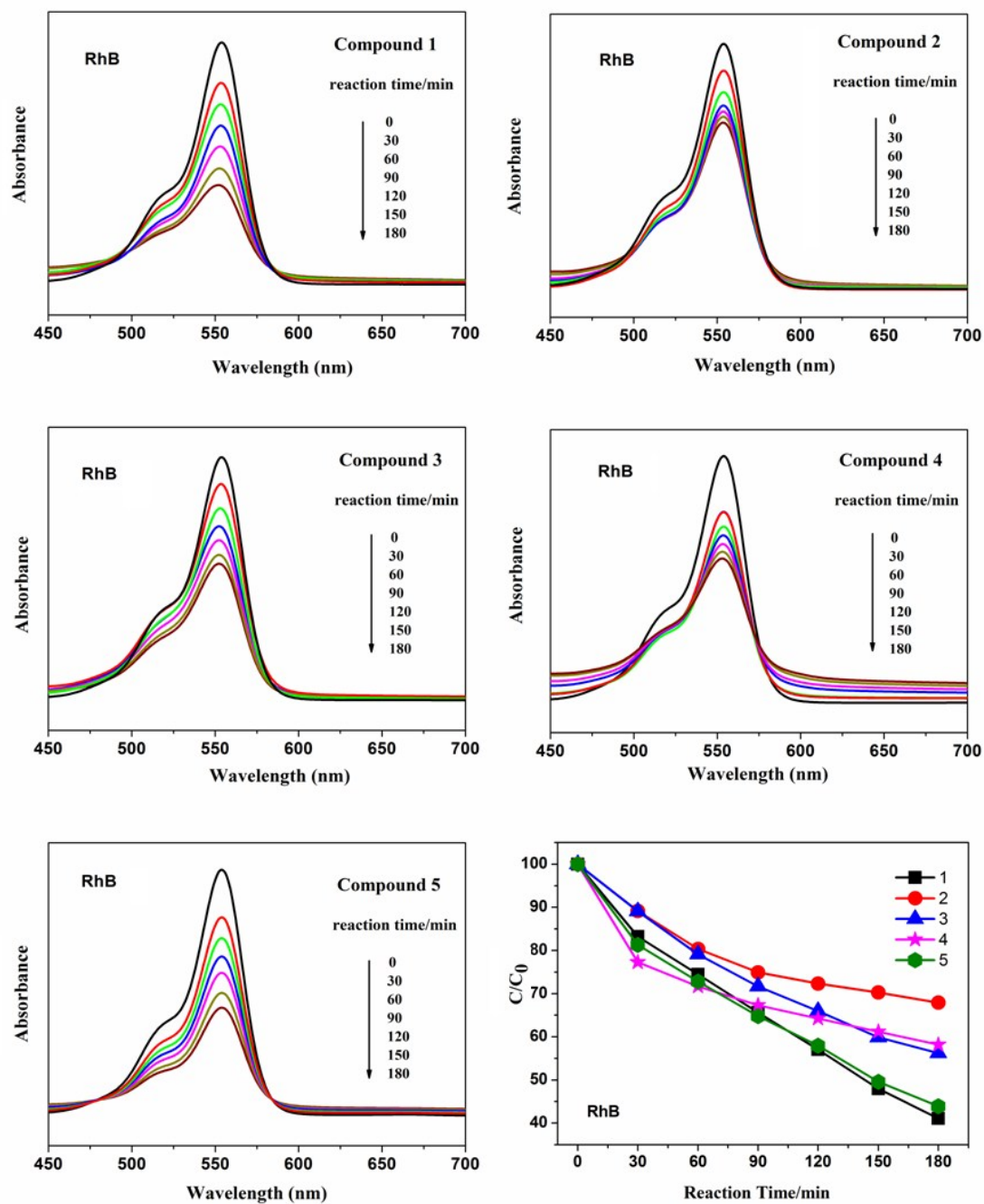


Fig. S13. Absorption spectra of the RhB solution during the decomposition reaction under UV irradiation with the compounds 1–5 as the catalysts.

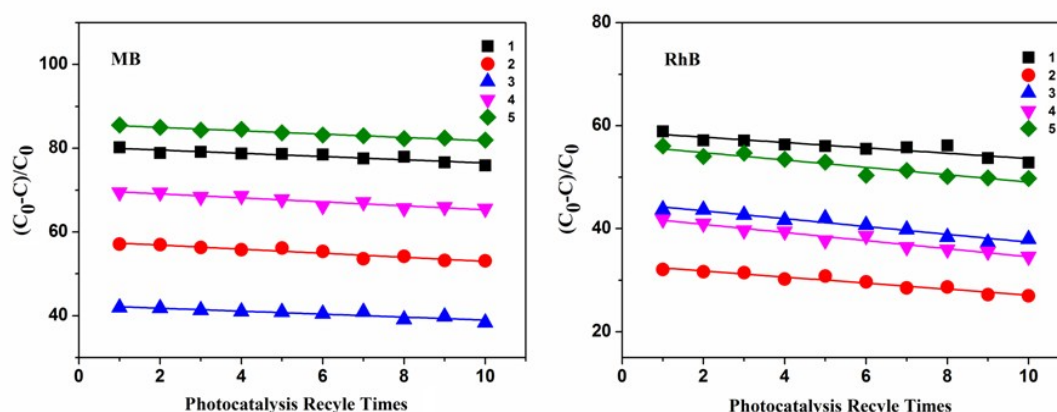


Fig. S14. The recycle test of catalysts 1–5.

Table S1. Selected bond distances (Å) and angles (deg) for compounds 1–5.

compound 1			
O(4)-Ag(1)	2.475(8)	Ag(1)-N(1)	2.286(9)
Ag(1)-O(1W)	2.33(2)	Ag(1)-O(1W')	2.33(3)
Ag(2)-N(2)	2.173(9)	Ag(2)-N(2)#2	2.173(9)
Mo(6)-O(4)-Ag(1)	134.4(5)	N(1)-Ag(1)-O(1W)	124.7(7)
N(1)-Ag(1)-O(1W')	145.9(7)	O(1W)-Ag(1)-O(1W')	35.7(10)
N(1)-Ag(1)-O(4)	98.2(3)	O(1W)-Ag(1)-O(4)	136.8(7)
O(1W')-Ag(1)-O(4)	104.8(9)	N(2)-Ag(2)-N(2)#2	179.999(1)
C(2)-N(1)-Ag(1)	122.1(7)	C(4)-N(1)-Ag(1)	118.9(8)
C(1)-N(2)-Ag(2)	119.5(8)	C(3)-N(2)-Ag(2)	120.9(7)
O(1W')-O(1W)-Ag(1)	72.4(17)	O(1W')#3-O(1W')-Ag(1)	138(4)
O(1W)-O(1W')-Ag(1)	72.0(14)		
Symmetry transformations used to generate equivalent atoms for 1: #1 -x+1,-y+1,-z-2; #2 -x,-y+1,-z-1; #3 -x,-y+2,-z-2			
compound 2			
Ag(1)-N(1)	2.187(9)	Ag(1)-N(3)	2.265(9)
Ag(1)-O(15)	2.511(8)	Ag(2)-N(5)	2.311(10)
Ag(2)-N(4)	2.311(10)	N(2)-Ag(4)#1	2.228(9)
Ag(3)-N(6)	2.265(10)	Ag(3)-N(7)	2.307(10)
Ag(4)-N(2)#2	2.228(9)	Ag(4)-N(8)	2.257(9)
Ag(4)-N(9)	2.496(12)	N(1)-Ag(1)-N(3)	142.9(3)
N(1)-Ag(1)-O(15)	104.1(3)	N(3)-Ag(1)-O(15)	97.4(3)
C(4)-N(1)-Ag(1)	123.7(7)	C(1)-N(1)-Ag(1)	117.5(7)
N(5)-Ag(2)-N(4)	130.8(3)	C(3)-N(2)-Ag(4)#1	118.8(8)
C(2)-N(2)-Ag(4)#1	123.1(8)	N(6)-Ag(3)-N(7)	139.6(4)
C(20)-N(3)-Ag(1)	124.5(8)	C(17)-N(3)-Ag(1)	113.9(7)
N(2)#2-Ag(4)-N(8)	152.9(4)	N(2)#2-Ag(4)-N(9)	91.8(4)
N(8)-Ag(4)-N(9)	112.6(4)	C(18)-N(4)-Ag(2)	116.0(8)
C(19)-N(4)-Ag(2)	124.0(8)	C(33)-N(5)-Ag(2)	119.1(8)

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C(36)-N(5)-Ag(2)	123.2(8)	C(35)-N(6)-Ag(3)	122.2(8)
C(34)-N(6)-Ag(3)	117.5(8)	C(52)-N(7)-Ag(3)	122.5(8)
C(49)-N(7)-Ag(3)	114.1(8)	C(51)-N(8)-Ag(4)	122.6(8)
C(50)-N(8)-Ag(4)	119.1(8)	C(65)-N(9)-Ag(4)	115.8(9)
C(68)-N(9)-Ag(4)	123.8(11)	Mo(5)-O(15)-Ag(1)	113.7(4)
Symmetry transformations used to generate equivalent atoms for 2 : #1 $x+1, y, z+1$; #2 $x-1, y, z-1$			
compound 3			
Ag(1)-N(1)	2.139(3)	Ag(1)-N(6)#1	2.151(3)
Ag(2)-N(3)	2.194(3)	Ag(2)-N(2)	2.204(3)
Ag(3)-N(4)	2.223(3)	Ag(3)-N(5)	2.228(3)
N(6)-Ag(1)#4	2.151(3)	N(1)-Ag(1)-N(6)#1	168.1(13)
C(8)-N(1)-Ag(1)	127.4(3)	C(1)-N(1)-Ag(1)	114.2(3)
N(3)-Ag(2)-N(2)	138.3(11)	C(2)-N(2)-Ag(2)	116.6(3)
C(3)-N(2)-Ag(2)	121.3(3)	N(4)-Ag(3)-N(5)	147.5(11)
C(21)-N(3)-Ag(2)	119.3(3)	C(28)-N(3)-Ag(2)	120.8(2)
C(22)-N(4)-Ag(3)	118.1(3)	C(23)-N(4)-Ag(3)	122.6(3)
C(41)-N(5)-Ag(3)	118.3(2)	C(48)-N(5)-Ag(3)	121.9(2)
C(42)-N(6)-Ag(1)#4	117.3(3)	C(43)-N(6)-Ag(1)#4	122.1(2)
Symmetry transformations used to generate equivalent atoms for 3 : #1 $x-1, y+1, z$; #2 $-x, -y+2, -z+1$; #3 $-x+1, -y+2, -z+2$; #4 $x+1, y-1, z$			
Compound 4			
Ag(1)-N(1)	2.167(4)	Ag(1)-N(2)#1	2.173(4)
Ag(1)-O(3)	2.505(4)	N(2)-Ag(1)#3	2.173(4)
N(1)-Ag(1)-N(2)#1	154.65(17)	N(1)-Ag(1)-O(3)	94.99(16)
N(2)#1-Ag(1)-O(3)	110.33(16)	C(1)-N(1)-Ag(1)	122.0(3)
C(8)-N(1)-Ag(1)	119.3(3)	C(2)-N(2)-Ag(1)#3	119.7(3)
C(3)-N(2)-Ag(1)#3	120.3(4)	Mo(4)-O(3)-Ag(1)	123.4(2)
Symmetry transformations used to generate equivalent atoms for 4 : #1 $-x+1/2, y+1/2, -z+3/2$; #2 $-x, -y+2, -z+2$; #3 $-x+1/2, y-1/2, -z+3/2$			
Compound 5			
Cu(1)-N(1)	1.918(2)	Cu(1)-N(3)	1.932(2)
Cu(2)-N(5)	1.908(3)	Cu(2)-N(4)	1.920(2)
N(2)-Cu(3)	1.889(3)	Cu(3)-N(6)#3	1.908(3)
N(6)-Cu(3)#4	1.908(3)	N(1)-Cu(1)-N(3)	160.3(12)
C(2)-N(1)-Cu(1)	114.1(2)	C(1)-N(1)-Cu(1)	126.6(2)
N(5)-Cu(2)-N(4)	165.4(14)	C(3)-N(2)-Cu(3)	117.3(2)
C(4)-N(2)-Cu(3)	122.5(2)	C(22)-N(3)-Cu(1)	117.5(2)
C(21)-N(3)-Cu(1)	121.9(2)	N(2)-Cu(3)-N(6)#3	177.9(12)
C(23)-N(4)-Cu(2)	116.3(2)	C(24)-N(4)-Cu(2)	123.1(2)
C(42)-N(5)-Cu(2)	116.4(2)	C(41)-N(5)-Cu(2)	123.4(3)
C(43)-N(6)-Cu(3)#4	115.2(2)	C(44)-N(6)-Cu(3)#4	122.8(2)
Symmetry transformations used to generate equivalent atoms for 5 : #1 $-x+1, -y+1, -z+1$; #2 $-x+2, -y, -z$; #3 $x+1, y+1, z$; #4 $x-1, y-1, z$			

