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A series of polyoxometalate compounds by tunning N sites and numbers of ligands: syntheses, characterization and electrochemical sensing, photocatalytic and supercapacitor properties

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Table S1. Selected bond distances (Å) and angles (°) for compounds **1**–**7**.

Compound **1**			
Ag(1)–O(14)^2	2.591(2)	Ag(2)–O(19)^4	2.559(2)
Ag(1)–O(2)	2.445(2)	Ag(2)–O(13)	2.574(2)
Ag(1)–O(1)	2.502(3)	Ag(2)–O(14)	2.248(2)
Ag(1)–O(7)^1	2.528(3)	Ag(2)–N(3)	2.176(3)
Ag(1)–O(23)^3	2.485(2)	O(2) –Ag(1) –O(23)^3	72.73(8)
Ag(1)–N(1)	2.294(3)	O(7)^1 –Ag(1) –O(14)^2	70.32(8)
O(2) –Ag(1) –O(14)^2	95.57(8)	O(14) –Ag(2) –O(19)^4	86.43(8)
O(2) –Ag(1) –O(1)	86.37(8)	O(14) –Ag(2) –O(13)	89.05(8)
O(1) –Ag(1) –O(14)^2	177.02(9)	N(3) –Ag(2) –O(19)^4	116.81(10)
O(1) –Ag(1) –O(7)^1	112.37(9)	N(3) –Ag(2) –O(13)	96.72(11)

Symmetry codes**:** ^{1}1-X,1-Y,1-Z; ^{2}-1/2+X,3/2-Y,-1/2+Z; ^{3}3/2-X,1/2+Y,3/2-Z; ^{4}2-X,1-Y,2-Z; ^{5}-X,1-Y,1-Z; ^{6}3-X,1-Y,2-Z; ^{7}1/2+X,3/2-Y,1/2+Z; ^{8}3/2-X,-1/2+Y,3/2-Z

Compound **2**			
Ag(1)–O(1)^1	2.566(3)	Ag(1)–O(23)^3	2.477(3)
Ag(1)–O(4)^1	2.470(3)	Ag(1)–O(20)^3	2.565(3)
Ag(1)–O(25)	2.533(3)	Ag(1)–O(24)	2.496(3)
Ag(1)–O(2)^2	2.542(3)	O(4)^2 –Ag(1) –O(25)	134.76(10)
O(2)^1 –Ag(1) –O(1)^2	161.61(9)	O(20)^3 –Ag(1) –O(1)^2	126.15(9)
O(4)^2 –Ag(1) –O(1)^2	83.38(9)	O(2)^1 –Ag(1) –O(20)^3	68.29(10)
O(4)^2 –Ag(1) –O(2)^1	113.36(9)	O(23)^3 –Ag(1) –O(1)^2	73.30(10)
O(4)^2 –Ag(1) –O(20)^3	74.59(11)	O(23)^3 –Ag(1) –O(2)^1	101.64(10)
O(4)^2 –Ag(1) –O(23)^3	122.86(10)	O(23)^3 –Ag(1) –O(20)^3	78.72(9)
O(4)^2 –Ag(1) –O(24)	68.72(9)	O(23)^3 –Ag(1) –O(24)	168.41(10)

Symmetry codes**:** ^{1}1/2-X,-1/2+Y,3/2-Z; ^{2}1-X,1-Y,2-Z; ^{3}1/2+X,1/2-Y,1/2+Z; ^{4}1/2-X,1/2+Y,3/2-Z; ^{5}-1/2+X,1/2-Y,-1/2+Z

Compound **3**			
Co(1)–O(3)	2.137(18)	Co(1)–O(4)	2.135(18)
Co(1)–N(1)	2.12(2)	Co(1)–N(6)	2.14(2)

Co(1)–N(9)[1]	2.14(2)	Co(1)–O(1W)	2.057(19)
O(3) –Co(1)–N(6)	90.4(8)	O(3) –Co(1)–N(9)[1]	88.8(8)
O(4) –Co(1) –O(3)	92.5(7)	O(4) –Co(1) –N(6)	84.8(8)
O(4) –Co(1) –N(9)[1]	88.2(8)	N(1) –Co(1)–O(3)	175.5(8)
N(1) –Co(1)–O(4)	90.7(8)	N(1) –Co(1)–N(6)	93.2(9)
N(1) –Co(1)–N(9)[1]	88.0(9)	N(9)[1] –Co(1)–N(6)	172.9(9)
O(1W) –Co(1) –O(3)	86.8(8)	O(1W) –Co(1) –O(4)	177.1(8)
O(1W) –Co(1) –N(1)	90.2(9)	O(1W) –Co(1) –N(6)	92.5(9)

Symmetry codes: [1]1/2+X,3/2-Y,1/2+Z; [2]-1/2+X,3/2-Y,-1/2+Z

Compound **4**

Ni(1)–O(15)	2.032(3)	Ni(1)–O(1W)	2.103(4)
Ni(1)–N(3)[3]	2.037(4)	Ni(1)–O(25)	2.019(3)
Ni(1)–N(2)	2.044(4)	Ni(1)–N(1)	2.083(4)
O(15)–Ni(1)–N(3)[3]	84.94(15)	O(15)–Ni(1)–O(1W)	172.17(15)
O(15)–Ni(1)–N(2)	87.23(14)	O(15)–Ni(1)–N(1)	97.84(15)
O(25)–Ni(1)–O(15)	86.01(13)	O(25)–Ni(1)–N(3)[3]	90.06(14)
O(25)–Ni(1)–O(1W)	87.81(14)	O(25)–Ni(1)–N(2)	169.53(14)
O(25)–Ni(1)–N(1)	94.67(14)	N(3)[3]–Ni(1)–O(1W)	90.26(15)
N(3)[3]–Ni(1)–N(2)	97.30(14)	N(3)[3]–Ni(1)–N(1)	174.66(16)
N(2)–Ni(1)–O(1W)	99.54(15)	N(2)–Ni(1)–N(1)	78.34(15)

Symmetry codes: [1]1-X,2-Y,2-Z; [2]1-X,1-Y,2-Z; [3]-X,1-Y,1-Z

Compound **5**

Co(1)–O(13)	2.059(4)	Co(1)–O(12)	2.039(4)
Co(1)–N(2)	2.083(4)	Co(1)–N(1)[3]	2.080(5)
Co(1)–O(1W)	2.122(4)	Co(1)–N(3)	2.144(4)
O(13) –Co(1)–N(2)	85.79(16)	O(13) –Co(1)–N(1)[3]	83.33(17)
O(13)–Co(1)–O(1W)	171.31(16)	O(13) –Co(1)–N(3)	99.69(17)
O(12)–Co(1)–O(13)	85.96(16)	O(12)–Co(1)–N(2)	167.93(16)
O(12)–Co(1)–N(1)[3]	89.69(16)	O(12)–Co(1)–O(1W)	88.16(16)
O(12) –Co(1)–N(3)	95.61(17)	N(2)–Co(1)–O(1W)	100.96(16)
N(2)–Co(1)–N(3)	77.13(17)	N(1)[3]–Co(1)–O(1W)	90.25(18)
N(2)–Co(1)–N(1)[3]	98.08(16)	N(1)[3]–Co(1)–N(3)	174.06(17)

Symmetry codes: [1]1-X,-Y,2-Z; [2]1-X,1-Y,2-Z; [3]1-X,1-Y,1-Z

Compound **6**

Ag(1)–N(1)[1]	2.309(4)	Ag(1)–N(2)[2]	2.254(3)
Ag(1)–N(7)	2.253(3)	Ag(1)–O(6)	2.713(3)
N(1)[1]–Ag(1)–O(6)	78.35(12)	N(2)[2]–Ag(1)–O(6)	105.41(13)
C(6)–N(1)–Ag(1)[1]	129.8(3)	N(7)–Ag(1)–O(6)	97.70(13)
N(7)–N(1)–Ag(1)[1]	122.8(3)	N(7)–Ag(1)–N(2)[2]	130.38(13)

N(7)–Ag(1)–N(1)[1]	108.44(12)	N(2)[2]–Ag(1)–N(1)[1]	118.82(13)
Mo(2)–O(6)–Ag(1)	131.3(2)	C(2)–N(2)–Ag(1)[4]	120.0(3)
C(1)–N(2)–Ag(1)[4]	121.2(3)	N(1)–N(7)–Ag(1)	124.3(3)
C(7)–N(7)–Ag(1)	125.0(3)	O(8)–Mo(2)–O(10)	72.44(11)
C(6)–N(3)–C(8)	129.5(3)	C(7)–N(3)–C(6)	105.0(3)

Symmetry codes: [1]2-X,1-Y,-Z; [2]1+X,+Y,+Z; [3]2-X,-Y,1-Z; [4]-1+X,+Y,+Z

Compound **7**

Co(1)–O(1W)	2.0664(19)	Co(1)–O(1W)[2]	2.0664(19)
Co(1)–N(5)[3]	2.252(2)	Co(1)–N(5)[4]	2.252(2)
Co(1)–N(3)	2.160(2)	Co(1)–N(3)[2]	2.160(2)
O(1W)–Co(1)–O(1W)[2]	180.0	O(1W)–Co(1)–N(5)[3]	90.56(8)
O(1W)[2]–Co(1)–N(5)[3]	89.44(8)	O(1W)–Co(1)–N(5)[4]	89.44(8)
O(1W)[2]–Co(1)–N(5)[4]	90.56(8)	O(1W)–Co(1)–N(3)[2]	92.66(8)
O(1W)[2]–Co(1)–N(3)[2]	87.34(8)	O(1W)[2]–Co(1)–N(3)	92.66(8)
O(1W)–Co(1)–N(3)	87.35(8)	N(5)[4]–Co(1)–N(5)[3]	180.0
N(3)–Co(1)–N(5)[4]	92.47(8)	N(3)–Co(1)–N(5)[3]	87.53(8)
N(3)[2]–Co(1)–N(5)[3]	92.47(8)	N(3)[2]–Co(1)–N(5)[4]	87.53(8)

Symmetry codes: [1]2-X,1-Y,1-Z; [2]-X,1-Y,-Z; [3]-1+X,+Y,+Z; [4]1-X,1-Y,-Z; [5]1+X,+Y,+Z

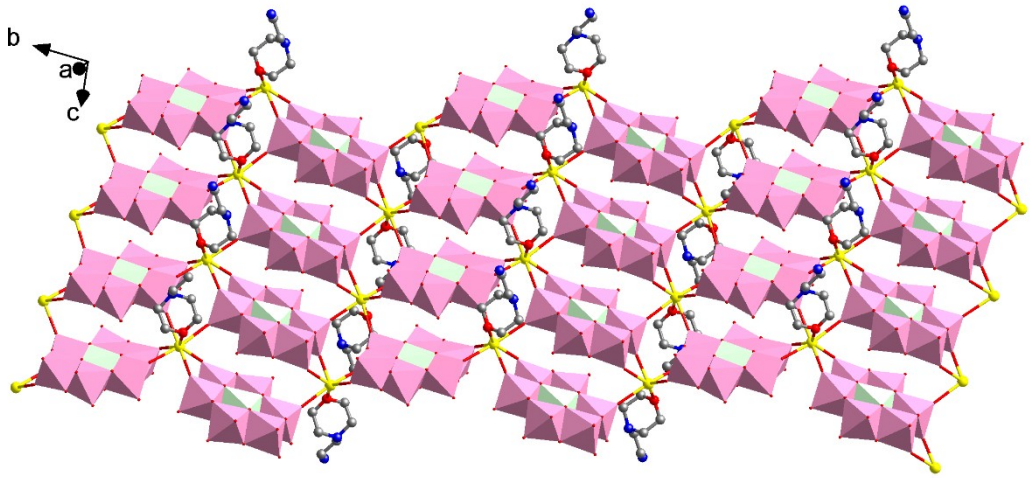

Fig. S1. The 2D layer of compound **2**.

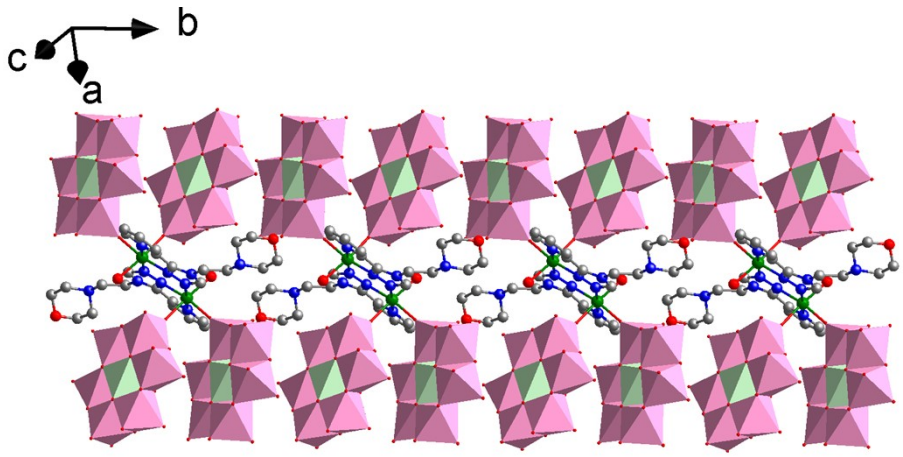

Fig. S2. The 1D sandwich-type chain of compound **4**.

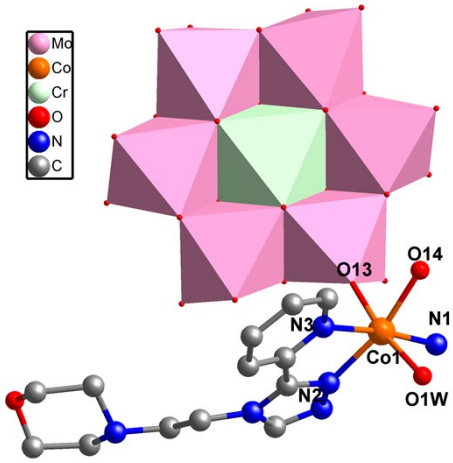

Fig. S3. The unit cell diagram of compound **5** (asymmetric unit). For the sake of clarity, crystal water molecules and hydrogen atoms are omitted here.

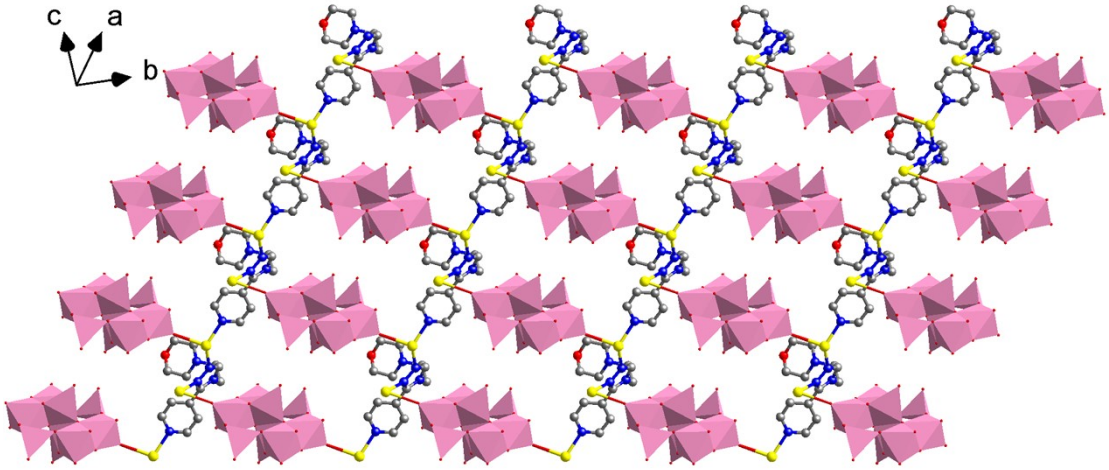

Fig. S4. The 2D layer of compound **6**.

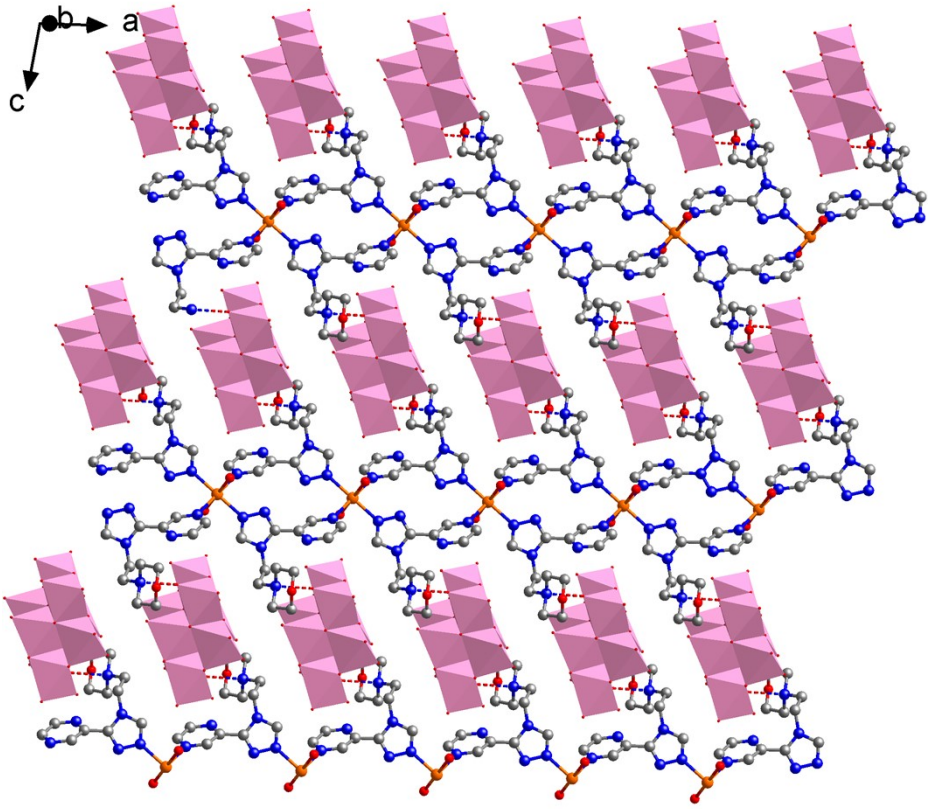

Fig. S5. The 2D layer of compound **7**.

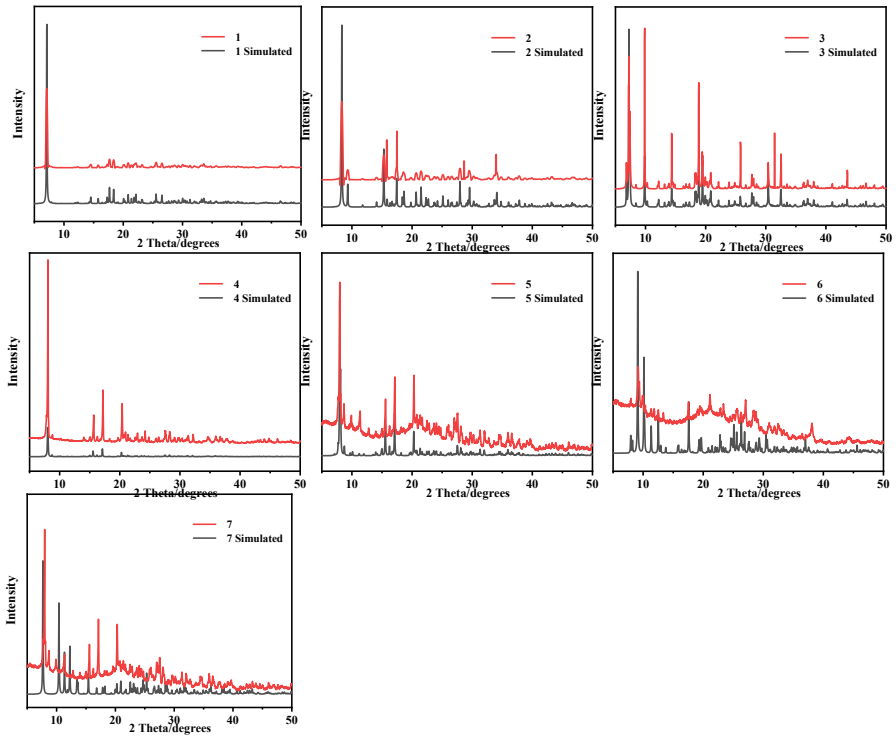

Fig. S6. The PXRD patterns of compounds **1**–**7**.

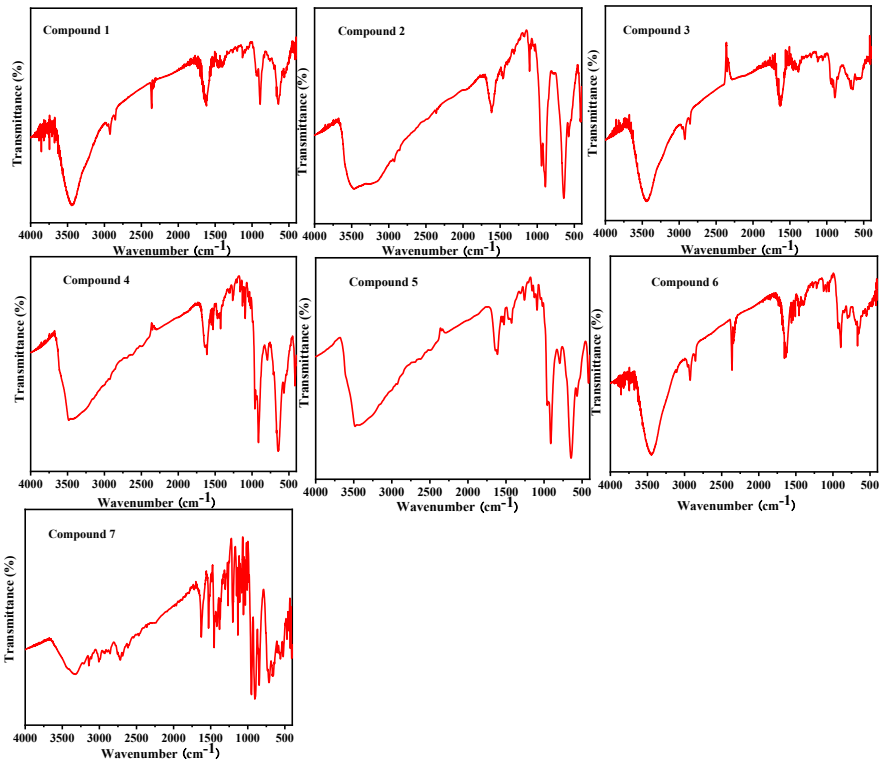

Fig. S7. The IR spectra of compounds **1**–**7**.

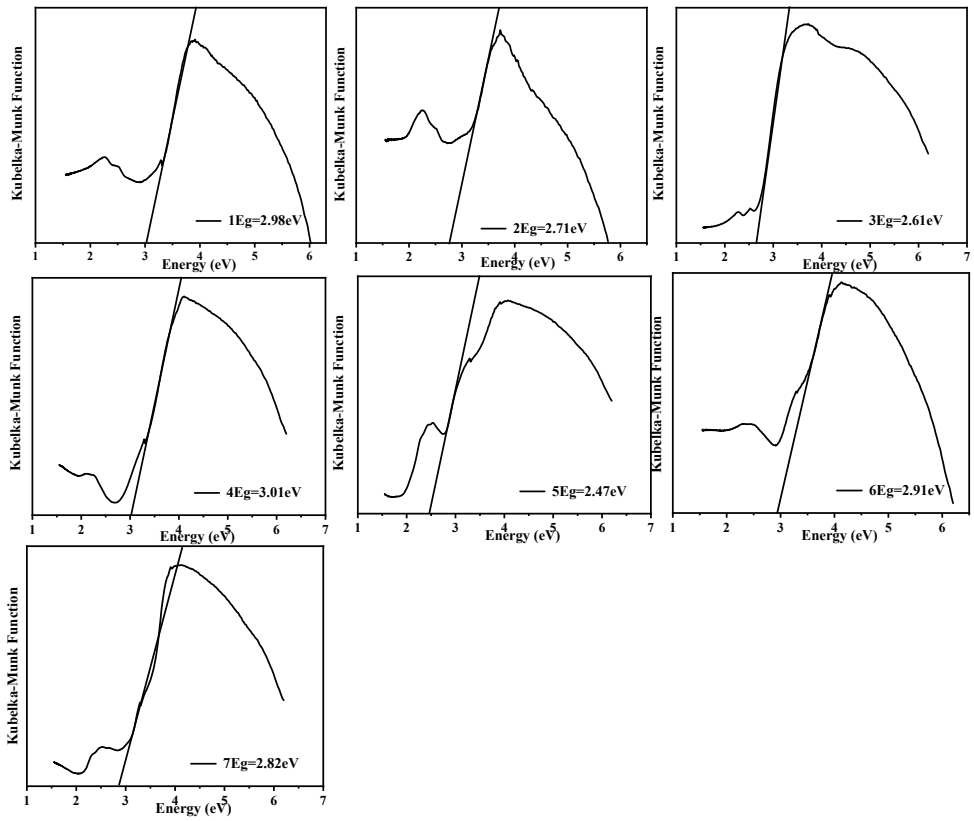

Fig. S8. The Diffuse reflection spectra of compounds **1**–**7**.

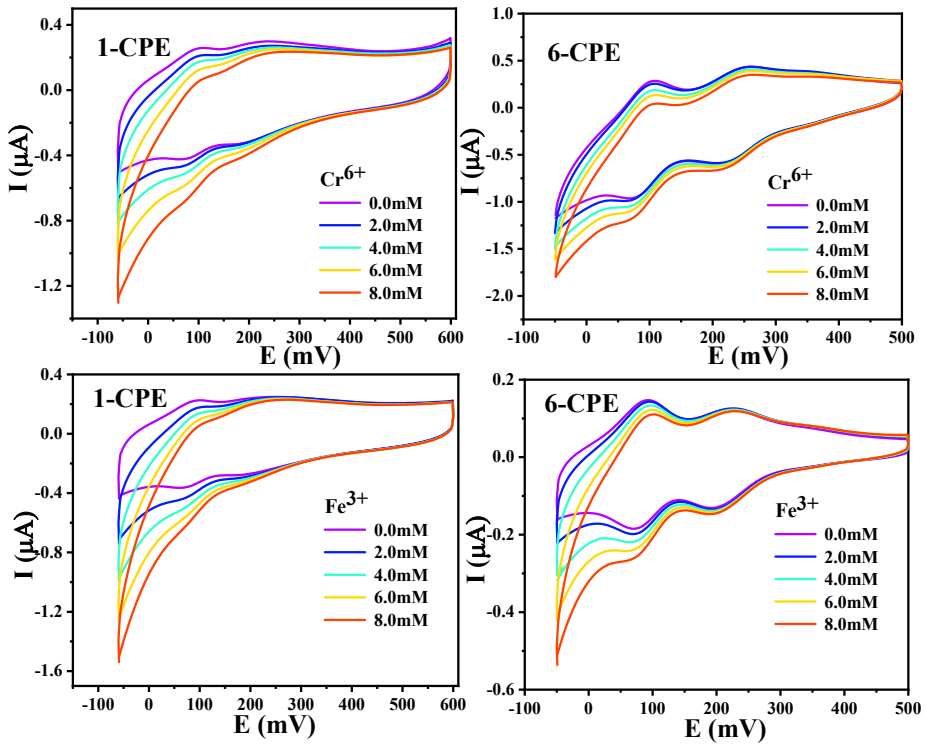

Fig. S9. Cyclic voltammograms of the **1**–, **6**–CPEs in 0.1 M H_2SO_4 + 0.5 M Na_2SO_4 aqueous solution containing 0; 2; 4; 6 and 8 mM Cr(VI) and Fe(III) (Scan rate: 200 mV·s^{-1}).

Table S2. Experimental data for detecting Cr(VI), Fe(III), and KNO_2 using **1**–, **6**–CPEs as amperometric sensors.

CPE	Test substance	Response time(s)	Concentration range(M)	Sensitivity (μA mM^{-1})	Correlation coefficient	Detection limit(M)
1–CPE	Cr(VI)	2.16	2×10^{-3}–4.6×10^{-2}	0.50898	0.99155	4.3×10^{-3}
6–CPE	Cr(VI)	5.13	4×10^{-3}–4.6×10^{-2}	0.17742	0.99524	5.9×10^{-3}
1–CPE	Fe(III)	1.44	2×10^{-3}–4.6×10^{-2}	1.40824	0.99945	3.9×10^{-3}
6–CPE	Fe(III)	1.26	2×10^{-3}–4.6×10^{-2}	0.15909	0.99993	5.7×10^{-4}
1–CPE	KNO_2	2.07	2×10^{-3}–3.2×10^{-2}	2.78635	0.99829	1.24×10^{-2}
6–CPE	KNO_2	3.42	6×10^{-3}–4.6×10^{-2}	0.50389	0.99940	2.9×10^{-3}

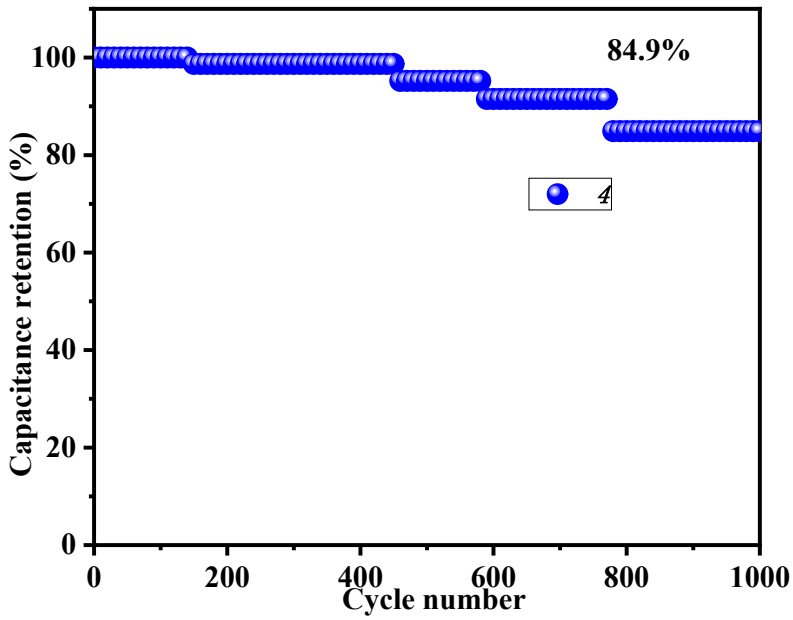

Fig. S10. The Cycling performance of **4**–GCE during 1000 cycles at the current densitites of 5 A g^{-1}.

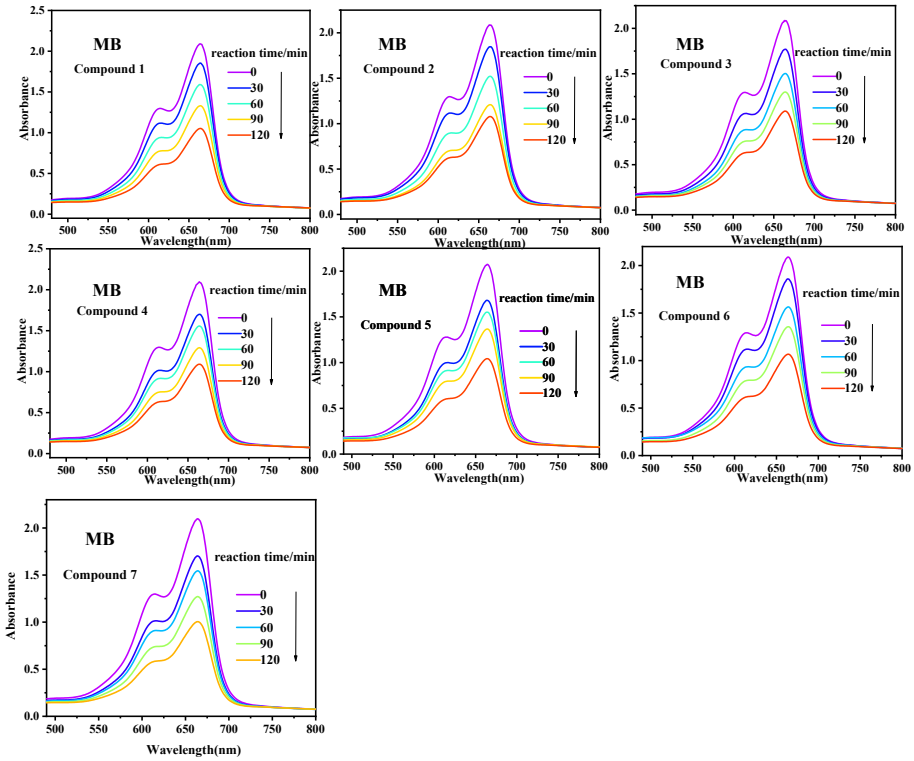

Fig. S11. The UV-vis absorption spectra of aqueous MB under UV light irradiation in the present of compounds **1**–**7**.

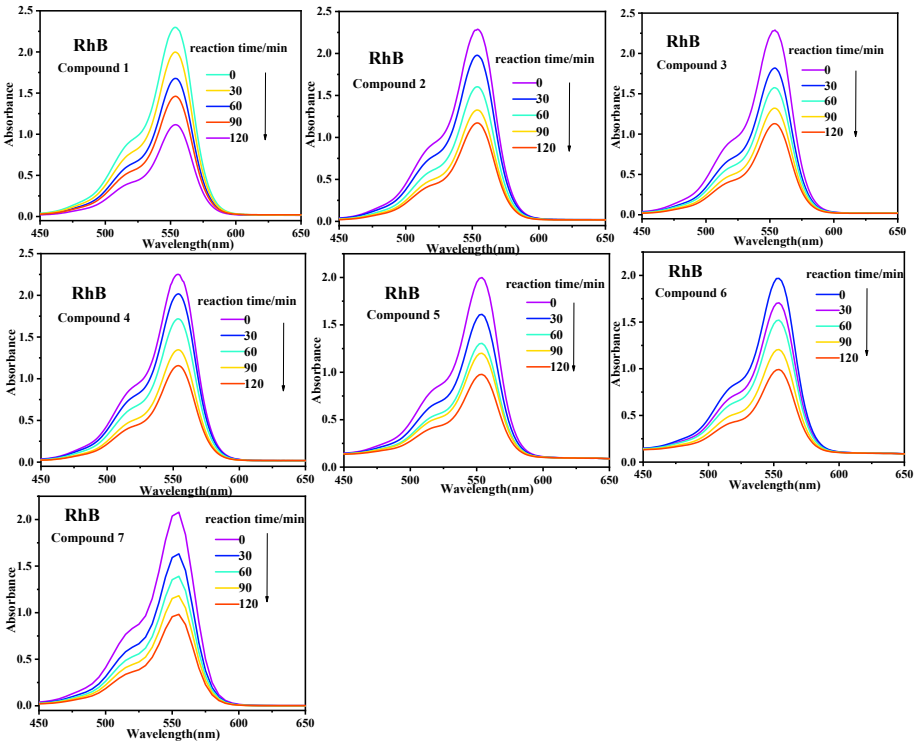

Fig. S12. The UV-vis absorption spectra of aqueous RhB under UV light irradiation in the present of compounds **1**–**7**.

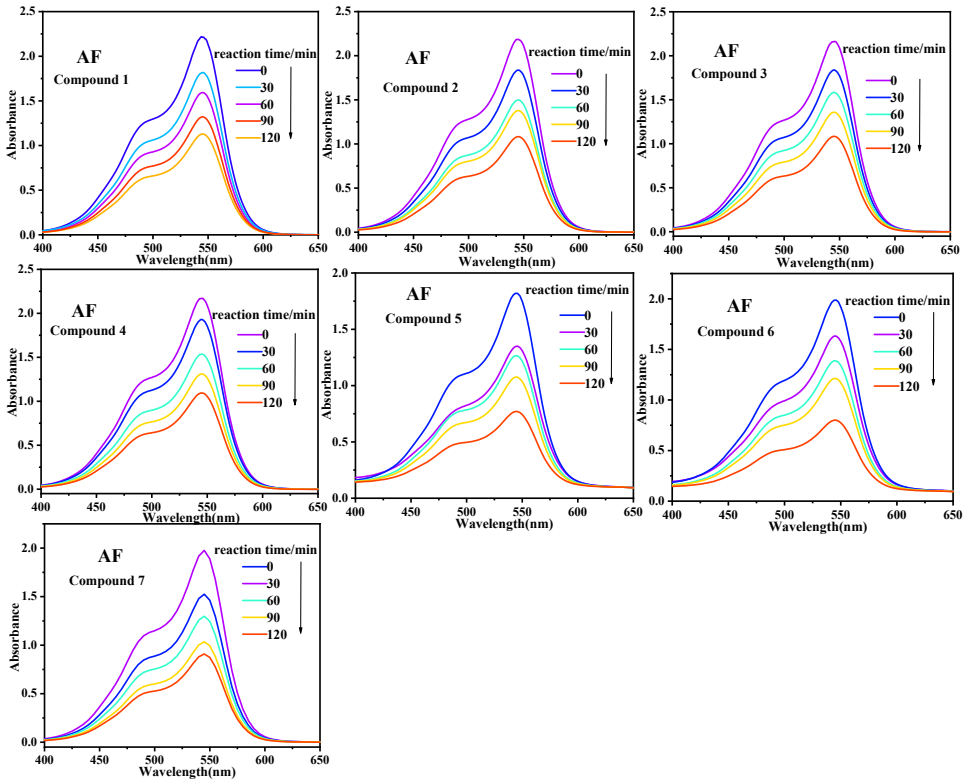

Fig. S13. The UV-vis absorption spectra of aqueous AF under UV light irradiation in the present of compounds **1**–**7**.

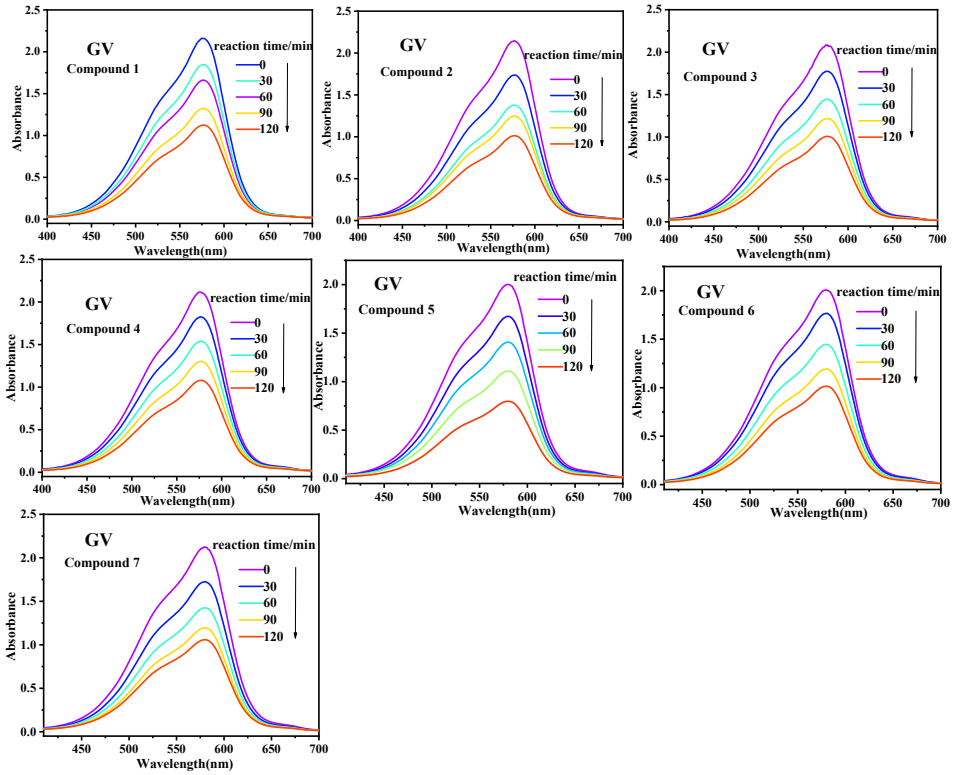

Fig. S14. The UV-vis absorption spectra of aqueous GV under UV light irradiation in the present of complounds **1**–**7**.

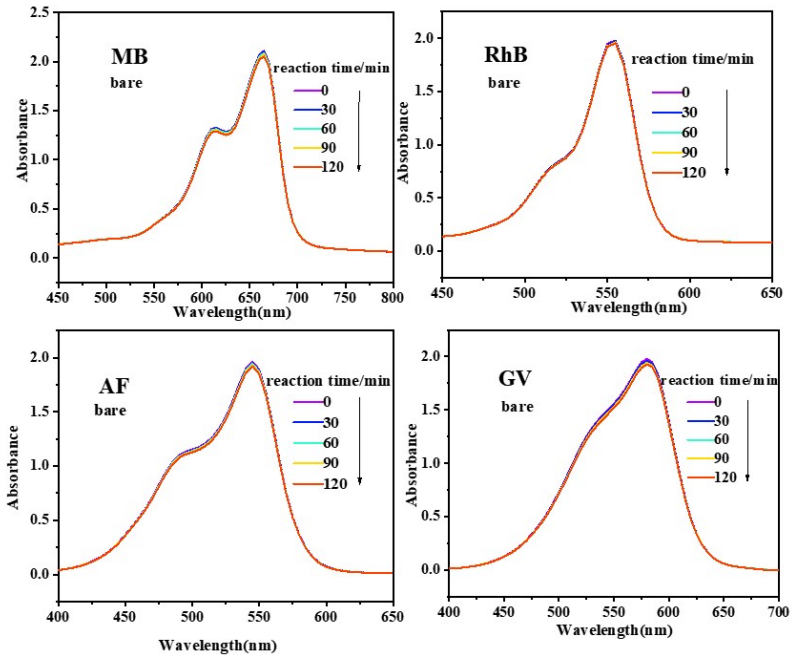

Fig. S15. Absorption spectra of the MB, RhB, AF and GV solution during the decomposition reaction under UV irradiation without the coordination polymers.

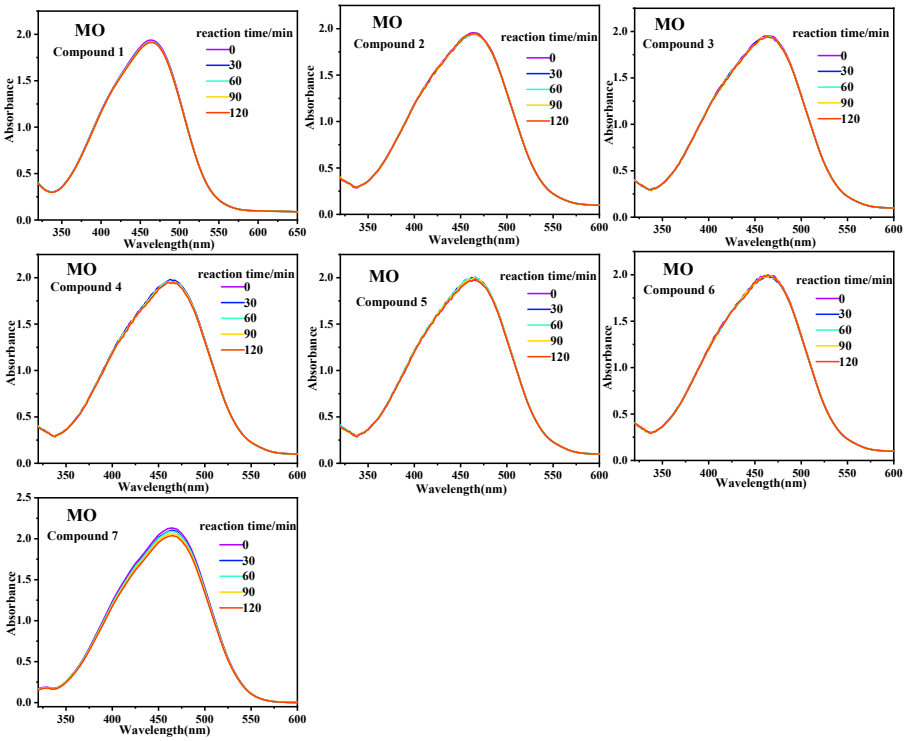

Fig. S16. The UV-vis absorption spectra of aqueous MO under UV light irradiation in the present of complounds **1**–**7**.

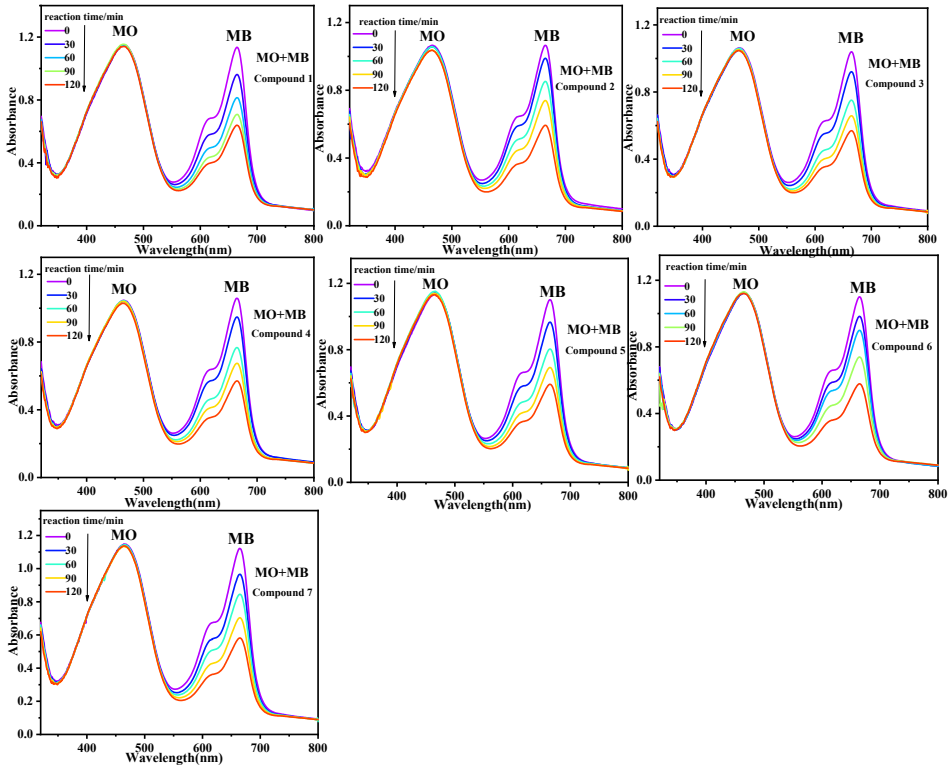

Fig. S17. The UV-vis absorption spectra of aqueous MO and MB under UV light irradiation in the present of compounds **1**–**7**.

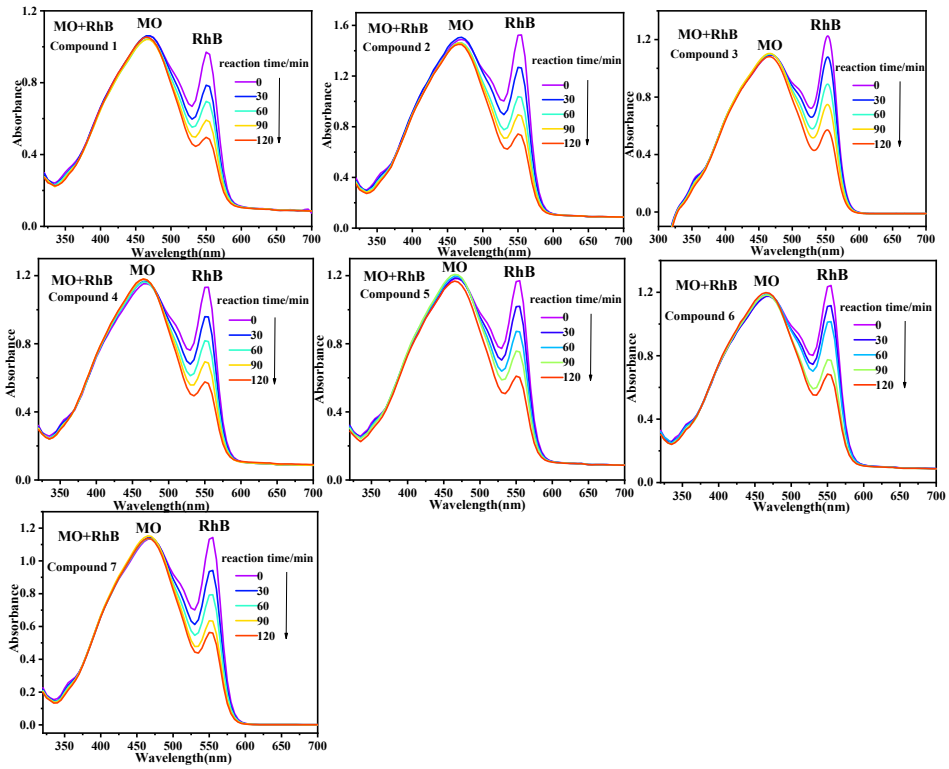

Fig. S18. The UV-vis absorption spectra of aqueous MO and RhB under UV light irradiation in the present of compounds **1**–**7**.

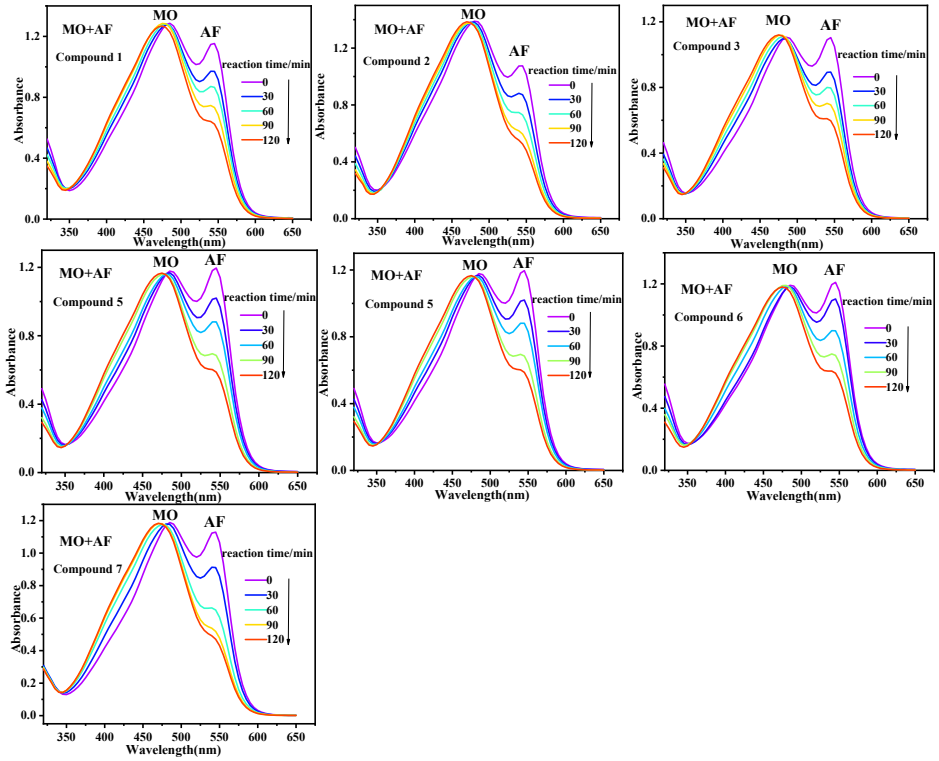

Fig. S19. The UV-vis absorption spectra of aqueous MO and AF under UV light irradiation in the present of compounds **1**–**7**.

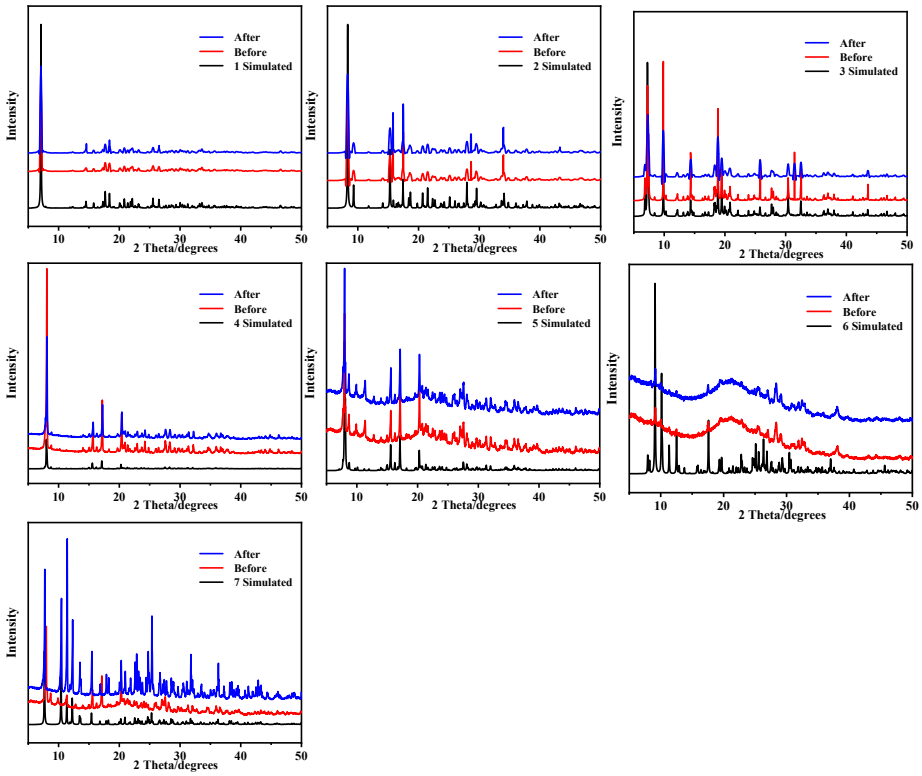

Fig. S20. The PXRD patterns of compounds **1**–**7** (before and after photocatalysis).