Supplementary materials for

Four hybrid compounds based on new type of molybdates and a flexible tripodal ligand: synthesis, structures, photochemical and electrochemical properties

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Table S1. Selected bond distances(Å) and angles(°)for compounds **1-4**

		Compound 1			
Mo(1)-O(1)	1.696(5)	Mo(1)-O(2)	1.706(5)	Mo(1)-O(3)	1.887(5)
Mo(1)-O(7)	2.248(4)	Mo(1)-O(8)	2.197(4)	Mo(1)-N(1)	2.189(6)
Mo(2)-O(3)	1.933(5)	Mo(2)-O(4)	1.694(5)	Mo(2)-O(5)	1.693(5)
Mo(2)-O(6)	2.297(4)	Mo(2)-O(7)	2.392(4)	Mo(2)-O(19)^{1}	1.969(5)
Mo(3)-Mo(6)	2.468(4)	Mo(3)-O(7)	1.835(4)	Mo(3)-O(8)	2.137(4)
Mo(3)-O(9)	1.751(4)	Mo(3)-O(10)	1.680(4)	Mo(3)-O(14)	2.037(4)
Mo(4)-O(8)	1.903(4)	Mo(4)-O(11)	1.696(5)	Mo(4)-O(12)	1.688(5)
Mo(4)-O(13)	1.972(4)	Mo(4)-O(14)	2.290(4)	Mo(4)-Mo(15)^{1}	2.384(4)
Mo(5)-O(6)^{1}	1.872(4)	Mo(5)-O(13)	2.168(4)	Mo(5)-O(14)	1.979(4)
Mo(5)-O(14)^{1}	2.506(4)	Mo(5)-O(15)	1.733(4)	Mo(5)-O(16)	1.679(4)
Mo(6)-O(6)^{1}	2.306(4)	Mo(6)-O(9)^{1}	2.321(4)	Mo(6)-O(13)	2.000(4)
Mo(6)-O(17)	1.696(5)	Mo(6)-O(18)	1.700(5)	Mo(6)-O(19)	1.876(5)
O(6)-Mo(5)^{1}	1.872(4)	O(6)-Mo(6)^{1}	2.306(4)	O(9)-Mo(6)^{1}	2.321(4)
O(14)-Mo(5)^{1}	2.506(4)	O(15)-Mo(4)^{1}	2.384(4)	O(19)-Mo(2)^{1}	1.969(5)
O(1)-Mo(1)-O(2)	105.0(3)	O(1)-Mo(1)-O(3)	103.3(2)	O(1)-Mo(1)-O(7)	161.3(2)
O(1)-Mo(1)-O(8)	91.7(2)	O(1)-Mo(1)-N(1)	94.0(2)	O(2)-Mo(1)-O(3)	101.6(2)
O(2)-Mo(1)-O(7)	93.1(2)	O(2)-Mo(1)-O(8)	158.3(2)	O(2)-Mo(1)- N(1)	86.1(2)
O(3)-Mo(1)-O(7)	76.85(18)	O(3) -Mo(1)-O(8)	87.60(19)	O(3) -Mo(1)-N(1)	158.4(2)
O(8)-Mo(1)-O(7)	69.61(15)	N(1)-Mo(1)-O(7)	82.58(18)	N(1)-Mo(1)-O(8)	78.90(19)
O(3)-Mo(2)-O(6)	83.87(18)	O(3)-Mo(2)-O(7)	72.54(17)	O(3)-Mo(2)-O(19)^{1}	148.92(18)
O(4)-Mo(2)-O(3)	100.9(3)	O(4)-Mo(2)-O(6)	161.9(2)	O(4)-Mo(2)-O(19)^{1}	96.2(3)
O(5)-Mo(2)-O(3)	99.8(2)	O(5)-Mo(2)-O(4)	105.3(3)	O(5)-Mo(2)-O(6)	90.8(2)
O(5)-Mo(2)-O(7)	161.4(2)	O(5)-Mo(2)-O(19)^{1}	100.5(2)	O(6)-Mo(2)-O(7)	71.79(15)
O(19)^{1}-Mo(2)-O(6)	72.51(17)	O(19)^{1}-Mo(2)-O(7)	80.92(17)	O(7)-Mo(3)-O(6)	77.95(17)
O(7)-Mo(3)-O(8)	79.03(18)	O(7)-Mo(3)-O(14)	143.49(18)	O(8)-Mo(3)-O(6)	79.37(15)
O(9)-Mo(3)-O(6)	76.54(17)	O(9)-Mo(3)-O(7)	102.6(2)	O(9)-Mo(3)-O(8)	154.88(19)
O(9)-Mo(3)-O(14)	94.16(18)	O(10)-Mo(3)-O(6)	175.48(19)	O(10)-Mo(3)-O(7)	106.3(2)
O(10)-Mo(3)-O(8)	99.78(19)	O(10)-Mo(3)-O(14)	100.76(19)	O(14)-Mo(3)-O(6)	74.74(14)

O(14)-Mo(3)-O(8)	72.53(16)	O(8)-Mo(4)-O(13)	140.76(17)	O(8)-Mo(4)-O(14)	71.51(16)
O(8)-Mo(4)-O(15)^{1}	82.71(17)	O(11)-Mo(4)-O(8)	99.5(2)	O(11)-Mo(4)-O(13)	95.6(2)
O(11)-Mo(4)-O(14)	102.8(2)	O(11)-Mo(4)-O(15)^{1}	171.6(2)	O(12)-Mo(4)-O(8)	106.8(2)
O(12)-Mo(4)-O(11)	104.0(3)	O(12)-Mo(4)-O(13)	104.2(2)	O(12)-Mo(4)-O(14)	153.1(2)
O(12)-Mo(4)- O(15)^{1}	82.9(2)	O(13)-Mo(4)-O(14)	69.90(15)	O(13)-Mo(4)- O(15)^{1}	77.91(16)
O(14)-Mo(4)- O(15)^{1}	70.16(14)	O(6)^{1}-Mo(5)-O(13)	75.72(17)	O(6)^{1}-Mo(5)-O(14)	141.28(17)
O(6)^{1}-Mo(5)- O(14)^{1}	76.49(15)	O(13)-Mo(5)- O(14)^{1}	78.27(14)	O(14)-Mo(5)- O(13)	72.47(15)
O(14)-Mo(5)- O(14)^{1}	75.93(17)	O(15)-Mo(5)- O(6)^{1}	101.5(2)	O(15)-Mo(5)- O(13)	154.30(18)
O(15)-Mo(5)- O(14)^{1}	76.28(16)	O(15)-Mo(5)- O(14)	97.72(18)	O(16)-Mo(5)- O(6)^{1}	104.9(2)
O(16)-Mo(5)- O(13)	101.6(2)	O(16)-Mo(5)- O(14)	102.6(2)	O(16)-Mo(5)- O(14)^{1}	178.5(2)
O(16)-Mo(5)- O(15)	103.7(2)	O(6)^{1}-Mo(6)- O(9)^{1}	70.56(15)	O(13) -Mo(6)- O(6)^{1}	70.26(16)
O(13)-Mo(6)- O(9)^{1}	78.07(16)	O(17)-Mo(6)- O(6)^{1}	156.4(2)	O(17)-Mo(6)- O(9)^{1}	85.9(2)
O(17)-Mo(6)- O(13)	104.0(2)	O(17)-Mo(6)- O(18)	105.1(3)	O(17)-Mo(6)- O(19)	105.2(3)
O(18)-Mo(6)- O(6)^{1}	98.2(2)	O(18)-Mo(6)- O(9)^{1}	168.2(2)	O(18)-Mo(6)- O(13)	94.8(2)
O(18)-Mo(6)- O(19)	98.9(2)	O(19)-Mo(6)- O(6)^{1}	73.87(18)	O(19)-Mo(6)- O(9)^{1}	81.90(18)
O(19)-Mo(6)- O(13)	143.02(19)				
		Compound 2			
Mo(1)-O(2)	1.926(4)	Mo(1)-O(3)	1.719(4)	Mo(1)-O(4)^{1}	2.205(4)
Mo(1)-O(4)	1.947(4)	Mo(1)-O(5)	1.703(5)	Mo(1)-N(4)^{2}	2.471(5)
Mo(2)-O(1)^{3}	1.841(4)	Mo(2)-O(2)	2.083(4)	Mo(2)-O(4)^{1}	2.014(4)
Mo(2)-O(6)	1.709(5)	Mo(2)-O(7)	1.702(5)	Zn(1)-Zn(1)^{3}	3.1467(14)
Zn(1)-O(1)^{3}	2.048(5)	Zn(1)-O(1)	2.082(4)	Zn(1)-O(2)	2.115(4)
Zn(1)-N(2)	1.999(5)	Zn(1)-N(6)^{3}	1.999(5)	O(1)-Mo(2)^{3}	1.842(4)
O(1)- Zn(1)^{3}	2.048(4)	O(4)- Mo(1)^{1}	2.205(4)	O(4)- Mo(2)^{1}	2.014(4)
N(4)- Mo(1)^{4}	2.471(5)	N(6)- Zn(1)^{3}	1.999(5)		
O(2)-Mo(1)-O(4)^{1}	72.60(17)	O(2)-Mo(1)-O(4)	141.6(2)	O(2)-Mo(1)-N(4)^{2}	79.22(18)
O(3)-Mo(1)-O(2)	103.9(2)	O(3)-Mo(1)-O(4)^{1}	161.64(19)	O(3)-Mo(1)-O(4)	104.04(19)
O(3)-Mo(1)-N(4)^{2}	82.3(2)	O(4)-Mo(1)-O(4)^{1}	72.54(17)	O(4)-Mo(1)-N(4)^{2}	78.98(18)
O(4)^{1}-Mo(1)-N(4)^{2}	79.31(17)	O(5)-Mo(1)-O(2)	98.7(2)	O(5)-Mo(1)-O(3)	102.8(2)
O(5)-Mo(1)-O(4)	100.2(2)	O(5)-Mo(1)- O(4)^{1}	95.60(19)	O(5)-Mo(1)- N(4)^{2}	174.9(2)
O(1)^{3}-Mo(2)-O(2)	76.54(18)	O(1)^{3}-Mo(2)-O(4)^{1}	149.8(2)	O(4)^{1}-Mo(2)-O(2)	73.63(17)
O(6) -Mo(2)-O(1)^{3}	102.0(2)	O(6) -Mo(2)-O(2)	118.2(2)	O(6) -Mo(2)-O(4)^{1}	96.4(2)
O(7) -Mo(2)-O(1)^{3}	101.1(2)	O(7) -Mo(2)-O(2)	133.4(2)	O(7) -Mo(2)-O(4)^{1}	95.7(2)
O(7) -Mo(2)-O(6)	107.9(3)	O(1)^{3}-Zn(1)-Zn(1)^{3}	40.76(12)	O(1)-Zn(1)-Zn(1)^{3}	39.96(12)
O(1)^{3}-Zn(1)-O(1)	80.72(18)	O(1)^{3}-Zn(1)-O(2)	71.69(17)	O(1)-Zn(1)-O(2)	152.38(19)
O(2)-Zn(1)-Zn(1)^{3}	112.44(12)	N(2)-Zn(1)-Zn(1)^{3}	114.36(16)	N(2)-Zn(1)-O(1)	95.2(2)
N(2)-Zn(1)-O(1)^{3}	112.8(2)	N(2)-Zn(1)-O(2)	98.57(19)	N(6)^{3}-Zn(1)-Zn(1)^{3}	112.27(16)
N(6)^{3}-Zn(1)-O(1)	96.9(2)	N(6)^{3}-Zn(1)- O(1)^{3}	117.4(2)	N(6)^{3}-Zn(1)-O(2)	96.8(2)
N(6)^{3}-Zn(1)-N(2)	119.8(2)				
		Compound 3			
Cd(1)-O(14)#1	2.229(4)	Cd(1)-O(14)	2.229(4)	Cd(1)-O(6)#1	2.268(3)
Cd(1)-O(6)	2.268(3)	Cd(1)-O(3)#1	2.317(3)	Cd(1)-O(3)	2.317(3)
Mo(1)-O(4)	1.688(3)	Mo(1)-O(3)	1.741(3)	Mo(1)-O(5)	1.914(3)

Mo(1)-O(2)	1.940(3)	Mo(1)-O(10)#2	2.226(3)	Mo(1)-O(1)	2.485(3)
Mo(2)-O(7)	1.692(3)	Mo(2)-O(6)	1.733(3)	Mo(2)-O(2)	1.893(3)
Mo(2)-O(8)	1.983(3)	Mo(2)-O(11)#2	2.296(3)	Mo(2)-O(1)	2.362(3)
Mo(3)-O(9)	1.694(3)	Mo(3)-O(10)	1.756(3)	Mo(3)-O(8)	1.958(3)
Mo(3)-O(11)	1.969(3)	Mo(3)-O(1)	2.137(3)	Mo(3)-O(1)#2	2.349(3)
Mo(4)-O(13)	1.695(3)	Mo(4)-O(12)	1.716(3)	Mo(4)-O(5)	1.905(3)
Mo(4)-O(11)	2.014(3)	Mo(4)-O(1)	2.319(3)	Mo(4)-O(8)#2	2.334(3)
Mo(5)-O(17)	1.697(3)	Mo(5)-O(18)	1.707(3)	Mo(5)-O(19)	1.913(3)
Mo(5)-O(16)	1.913(3)	Mo(5)-O(15)	2.434(3)	Mo(5)-O(25)#3	2.469(3)
Mo(6)-O(21)	1.705(3)	Mo(6)-O(20)	1.708(3)	Mo(6)-O(19)	1.904(3)
Mo(6)-O(22)	1.916(3)	Mo(6)-O(15)	2.440(3)	Mo(6)-O(27)#3	2.449(3)
Mo(7)-O(24)	1.701(3)	Mo(7)-O(23)	1.707(3)	Mo(7)-O(16)#3	1.914(3)
Mo(7)-O(22)	1.920(3)	Mo(7)-O(25)	2.411(3)	Mo(7)-O(27)#3	2.432(3)
Mo(8)-O(26)	1.709(3)	Mo(8)-O(15)	1.790(3)	Mo(8)-O(27)	1.794(3)
Mo(8)-O(25)	1.791(3)	O(1)-Mo(3)#2	2.349(3)	O(8)-Mo(4)#2	2.334(3)
O(10)-Mo(1)#2	2.226(3)	O(11)-Mo(2)#2	2.296(3)	O(16)-Mo(7)#3	1.914(3)
O(25)-Mo(5)#3	2.469(3)	O(27)-Mo(7)#3	2.432(3)	O(27)-Mo(6)#3	2.449(3)
O(14)#1-Cd(1)-O(14)	180.00(17)	O(14)#1-Cd(1)-O(6)#1	91.65(13)	O(14)-Cd(1)-O(6)#1	88.35(13)
O(14)#1-Cd(1)-O(6)	88.35(13)	O(14)-Cd(1)-O(6)	91.65(13)	O(6)#1-Cd(1)-O(6)	180.000(1)
O(14)#1-Cd(1)-O(3)#1	85.75(13)	O(14)-Cd(1)-O(3)#1	94.25(13)	O(6)#1-Cd(1)-O(3)#1	82.55(11)
O(6)-Cd(1)-O(3)#1	97.45(11)	O(14)#1-Cd(1)-O(3)	94.25(13)	O(14)-Cd(1)-O(3)	85.75(13)
O(6)#1-Cd(1)-O(3)	97.45(11)	O(6)-Cd(1)-O(3)	82.55(11)	O(3)#1-Cd(1)-O(3)	180.000(1)
O(4)-Mo(1)-O(3)	104.93(16)	O(4)-Mo(1)-O(5)	103.50(15)	O(3)-Mo(1)-O(5)	98.94(14)
O(4)-Mo(1)-O(2)	103.78(15)	O(3)-Mo(1)-O(2)	94.97(14)	O(5)-Mo(1)-O(2)	144.88(13)
O(4)-Mo(1)-O(10)#2	93.36(14)	O(3)-Mo(1)-O(10)#2	161.52(13)	O(5)-Mo(1)-O(10)#2	78.92(12)
O(2)-Mo(1)-O(10)#2	77.81(12)	O(4)-Mo(1)-O(1)	162.96(14)	O(3)-Mo(1)-O(1)	92.11(12)
O(5)-Mo(1)-O(1)	73.68(11)	O(2)-Mo(1)-O(1)	73.73(11)	O(10)#2-Mo(1)-O(1)	69.60(10)
O(7)-Mo(2)-O(6)	104.56(16)	O(7)-Mo(2)-O(2)	101.35(15)	O(6)-Mo(2)-O(2)	99.44(14)
O(7)-Mo(2)-O(8)	102.41(14)	O(6)-Mo(2)-O(8)	97.47(14)	O(2)-Mo(2)-O(8)	146.19(13)
O(7)-Mo(2)-O(11)#2	91.82(13)	O(6)-Mo(2)-O(11)#2	162.53(13)	O(2)-Mo(2)-O(11)#2	82.93(12)
O(8)-Mo(2)-O(11)#2	72.64(11)	O(7)-Mo(2)-O(1)	163.99(13)	O(6)-Mo(2)-O(1)	91.32(13)
O(2)-Mo(2)-O(1)	77.57(12)	O(8)-Mo(2)-O(1)	72.96(11)	O(11)#2-Mo(2)-O(1)	72.18(10)
O(9)-Mo(3)-O(10)	105.00(15)	O(9)-Mo(3)-O(8)	101.58(14)	O(10)-Mo(3)-O(8)	96.11(13)
O(9)-Mo(3)-O(11)	100.59(14)	O(10)-Mo(3)-O(11)	96.91(13)	O(8)-Mo(3)-O(11)	150.35(12)
O(9)-Mo(3)-O(1)	98.88(13)	O(10)-Mo(3)-O(1)	156.12(12)	O(8)-Mo(3)-O(1)	78.74(11)
O(11)-Mo(3)-O(1)	78.59(11)	O(9)-Mo(3)-O(1)#2	174.27(13)	O(10)-Mo(3)-O(1)#2	80.73(12)
O(8)-Mo(3)-O(1)#2	77.60(11)	O(11)-Mo(3)-O(1)#2	78.37(11)	O(1)-Mo(3)-O(1)#2	75.39(12)
O(13)-Mo(4)-O(12)	104.75(16)	O(13)-Mo(4)-O(5)	101.17(14)	O(12)-Mo(4)-O(5)	101.09(15)
O(13)-Mo(4)-O(11)	100.60(14)	O(12)-Mo(4)-O(11)	96.22(14)	O(5)-Mo(4)-O(11)	147.59(12)

O(13)-Mo(4)-O(1)	160.39(13)	O(12)-Mo(4)-O(1)	94.57(13)	O(5)-Mo(4)-O(1)	77.97(11)
O(11)-Mo(4)-O(1)	73.50(11)	O(13)-Mo(4)-O(8)#2	88.96(13)	O(12)-Mo(4)-O(8)#2	163.18(13)
O(5)-Mo(4)-O(8)#2	85.40(12)	O(11)-Mo(4)-O(8)#2	71.29(11)	O(1)-Mo(4)-O(8)#2	71.42(10)
O(17)-Mo(5)-O(18)	105.71(17)	O(17)-Mo(5)-O(19)	103.54(16)	O(18)-Mo(5)-O(19)	100.41(15)
O(17)-Mo(5)-O(16)	100.27(16)	O(18)-Mo(5)-O(16)	101.15(16)	O(19)-Mo(5)-O(16)	141.95(14)
O(17)-Mo(5)-O(15)	89.87(14)	O(18)-Mo(5)-O(15)	164.03(15)	O(19)-Mo(5)-O(15)	71.90(12)
O(16)-Mo(5)-O(15)	78.96(12)	O(17)-Mo(5)-O(25)#3	165.66(15)	O(18)-Mo(5)-O(25)#3	87.77(14)
O(19)-Mo(5)-O(25)#3	78.21(12)	O(16)-Mo(5)-O(25)#3	71.73(12)	O(15)-Mo(5)-O(25)#3	77.05(11)
O(21)-Mo(6)-O(20)	105.78(17)	O(21)-Mo(6)-O(19)	100.31(15)	O(20)-Mo(6)-O(19)	102.27(16)
O(21)-Mo(6)-O(22)	102.68(16)	O(20)-Mo(6)-O(22)	100.01(15)	O(19)-Mo(6)-O(22)	142.04(13)
O(21)-Mo(6)-O(15)	165.32(14)	O(20)-Mo(6)-O(15)	88.26(14)	O(19)-Mo(6)-O(15)	71.90(12)
O(22)-Mo(6)-O(15)	78.51(12)	O(21)-Mo(6)-O(27)#3	89.43(15)	O(20)-Mo(6)-O(27)#3	164.28(14)
O(19)-Mo(6)-O(27)#3	78.33(12)	O(22)-Mo(6)-O(27)#3	72.15(12)	O(15)-Mo(6)-O(27)#3	76.93(11)
O(24)-Mo(7)-O(23)	105.35(18)	O(24)-Mo(7)-O(16)#3	102.94(16)	O(23)-Mo(7)-O(16)#3	100.36(15)
O(24)-Mo(7)-O(22)	99.90(16)	O(23)-Mo(7)-O(22)	100.60(15)	O(16)#3-Mo(7)-O(22)	143.47(14)
O(24)-Mo(7)-O(25)	90.40(15)	O(23)-Mo(7)-O(25)	164.05(15)	O(16)#3-Mo(7)-O(25)	73.11(12)
O(22)-Mo(7)-O(25)	78.65(12)	O(24)-Mo(7)-O(27)#3	166.31(15)	O(23)-Mo(7)-O(27)#3	87.47(15)
O(16)#3-Mo(7)-O(27)#3	78.91(12)	O(22)-Mo(7)-O(27)#3	72.50(12)	O(25)-Mo(7)-O(27)#3	77.07(11)
O(26)-Mo(8)-O(15)	109.40(16)	O(26)-Mo(8)-O(27)	109.27(16)	O(15)-Mo(8)-O(27)	109.21(15)
O(26)-Mo(8)-O(25)	109.75(16)	O(15)-Mo(8)-O(25)	109.49(15)	O(27)-Mo(8)-O(25)	109.71(15)
		Compound 4			
Mo(1)- O(1)	1.704(3)	Mo(1)- O(2)	1.691(3)	Mo(1)- O(3)	1.917(3)
Mo(1)- O(6)	2.429(3)	Mo(1)- O(9)[1]	1.906(3)	Mo(1)- O(11)[1]	2.399(3)
Mo(2)- O(3)	1.910(3)	Mo(2)- O(4)	1.711(3)	Mo(2)- O(5)	1.702(3)
Mo(2)- O(6)	2.455(3)	Mo(2)- O(7)	1.895(3)	Mo(2)- O(13)[1]	2.448(3)
Mo(3)- O(7)	1.917(3)	Mo(3)- O(8)	1.702(3)	Mo(3)- O(9)	1.915(3)
Mo(3)- O(10)	1.698(3)	Mo(3)- O(11)	2.464(3)	Mo(3)- O(13)[1]	2.422(3)
Mo(4)- O(6)	1.791(3)	Mo(4)- O(11)	1.793(3)	Mo(4)- O(12)	1.707(3)
Mo(4)- O(13)	1.784(3)	O(9)-Mo(1)[1]	1.906(3)	O(11)-Mo(1)[1]	2.399(3)
O(13)-Mo(2)[1]	2.448(3)	O(13)-Mo(3)[1]	2.422(3)	Mo(5)- O(14)	1.739(3)
Mo(5)- O(15)	1.689(3)	Mo(5)- O(16)	1.911(3)	Mo(5)- O(17)	2.229(3)
Mo(5)- O(19)[2]	2.476(3)	Mo(5)- O(26)	1.932(3)	Mo(6)- Mo(7)	3.2151(5)
Mo(6)- O(17)	1.750(3)	Mo(6)- O(18)	1.694(3)	Mo(6)- O(19)[2]	2.361(3)
Mo(6)- O(19)	2.134(3)	Mo(6)- O(20)	1.963(3)	Mo(6)- O(23)[2]	1.955(3)
Mo(7)- O(16)[2]	1.911(3)	Mo(7)- O(19)	2.300(3)	Mo(7)- O(20)	2.006(3)
Mo(7)- O(21)	1.710(3)	Mo(7)- O(22)	1.695(3)	Mo(7)- O(23)	2.356(3)
Mo(8)- O(19)[2]	2.358(3)	Mo(8)- O(20)	2.318(3)	Mo(8)- O(23)	1.978(3)
Mo(8)- O(24)	1.692(3)	Mo(8)- O(25)	1.734(3)	Mo(8)- O(26)	1.893(3)
Co(1)-O(14)[3]	2.147(3)	Co(1)-O(14)	2.147(3)	Co(1)-O(25)	2.129(3)
Co(1)-O(25)[3]	2.129(3)	Co(1)-O(27)[3]	2.026(3)	Co(1)-O(27)	2.026(3)
O(16)-Mo(7)[2]	1.911(3)	O(19)-Mo(5)[2]	2.476(3)	O(19)-Mo(6)[2]	2.361(3)
O(19)-Mo(8)[2]	2.358(3)	O(23)-Mo(6)[2]	1.955(3)		
O(1)-Mo(1)-O(3)	100.22(14)	O(1)-Mo(1)-O(6)	87.81(14)	O(1)-Mo(1)-O(9)[1]	100.76(14)
O(1)-Mo(1)-O(11)[1]	164.86(14)	O(2)-Mo(1)-O(1)	105.35(17)	O(2)-Mo(1)-O(3)	99.79(14)

O(2)-Mo(1)-O(6)	165.87(14)	O(2)-Mo(1)-O(9)[1]	102.65(14)	O(2)-Mo(1)-O(11)[1]	89.65(14)
O(3)-Mo(1)-O(6)	72.27(11)	O(3)-Mo(1)- O(11)[1]	78.76(11)	O(9)[1]-Mo(1)-O(3)	143.79(13)
O(9)[1]-Mo(1)-O(6)	79.40(11)	O(9)[1]-Mo(1)- O(11)[1]	73.37(12)	O(11)[1]-Mo(1)-O(6)	77.46(11)
O(3)-Mo(2)-O(6)	71.75(11)	O(3)-Mo(2)-O(13)[1]	78.14(12)	O(4)-Mo(2)-O(3)	100.48(14)
O(4)-Mo(2)-O(6)	164.28(14)	O(4)-Mo(2)-O(7)	102.36(15)	O(4)-Mo(2)-O(13) [1]	88.18(14)
O(5)-Mo(2)-O(3)	102.93(15)	O(5)-Mo(2)-O(4)	105.95(16)	O(5)-Mo(2)-O(6)	89.30(13)
O(5)-Mo(2)-O(7)	100.13(15)	O(5)-Mo(2)- O(13) [1]	165.22(13)	O(7)-Mo(2)-O(3)	141.43(12)
O(7)-Mo(2)-O(6)	78.09(11)	O(7)-Mo(2)- O(13) [1]	71.99(12)	O(13)[1]-Mo(2)-O(6)	76.95(10)
O(7)-Mo(3)-O(11)	78.13(11)	O(7)-Mo(3)- O(13)[1]	72.30(12)	O(8)-Mo(3)-O(7)	103.36(14)
O(8)-Mo(3)-O(9)	100.57(14)	O(8)-Mo(3)-O(11)	165.46(14)	O(8)-Mo(3)- O(13)[1]	89.66(14)
O(9)-Mo(3)-O(7)	142.30(12)	O(9)-Mo(3)-O(11)	71.69(11)	O(9)-Mo(3)- O(13)[1]	79.20(12)
O(10)-Mo(3)-O(7)	100.52(15)	O(10)-Mo(3)-O(8)	105.38(16)	O(10)-Mo(3)-O(9)	100.68(15)
O(10)-Mo(3)-O(11)	88.38(13)	O(10)-Mo(3)- O(13)[1]	164.63(13)	O(13)[1]-Mo(3)-O(11)	76.94(10)
O(6)-Mo(4)-O(11)	109.66(14)	O(12)-Mo(4)-O(6)	109.28(15)	O(12)-Mo(4)-O(11)	109.72(15)
O(12)-Mo(4)-O(13)	109.24(15)	O(13)-Mo(4)-O(6)	109.27(14)	O(13)-Mo(4)-O(11)	109.65(14)
O(14)-Mo(5)-O(16)	100.52(13)	O(14)-Mo(5)-O(17)	161.10(12)	O(14)-Mo(5)-O(19)[2]	91.64(12)
O(14)-Mo(5)-O(26)	93.99(13)	O(15)-Mo(5)-O(14)	104.92(15)	O(15)-Mo(5)-O(16)	103.20(14)
O(15)-Mo(5)-O(17)	93.50(13)	O(15)-Mo(5)-O(19)[2]	163.44(13)	O(15)-Mo(5)-O(26)	103.52(14)
O(16)-Mo(5)-O(17)	78.87(11)	O(16)-Mo(5)-O(19)[2]	73.56(11)	O(16)-Mo(5)-O(26)	145.01(12)
O(17)-Mo(5)-O(19)[2]	69.95(10)	O(26)-Mo(5)-O(17)	77.34(11)	O(17)-Mo(5)- O(19)[2]	74.37(11)
O(17)-Mo(6)- Mo(7)	133.81(9)	O(17)-Mo(6)-O(19)[2]	80.78(12)	O(17)-Mo(6)-O(19)	156.17(12)
O(17)-Mo(6)-O(20)	97.46(12)	O(17)-Mo(6)-O(23)[2]	96.10(12)	O(18)-Mo(6)-Mo(7)	89.90(10)
O(18)-Mo(6)-O(17)	104.76(14)	O(18)-Mo(6)- O(19)[2]	174.46(13)	O(18)-Mo(6)- O(19)	99.06(13)
O(18)-Mo(6)-O(20)	100.67(13	O(18)-Mo(6)- O(23)[2]	101.32(13)	O(19)[2]-Mo(6)-Mo(7)	86.19(7)
O(19)-Mo(6)-Mo(7)	45.60(7)	O(19)-Mo(6)- O(19)[2]	75.39(11)	O(20)-Mo(6)-Mo(7)	36.36(8)
O(20)-Mo(6)- O(19)	78.41(11)	O(20)-Mo(6)- O(19)[2]	78.42(10)	O(23)[2]-Mo(6)-Mo(7)	124.09(8)
O(23)[2]-Mo(6)- O(19)[2]	77.76(10)	O(23)[2]-Mo(6)- O(19)	78.49(11)	O(23)[2]-Mo(6)- O(20)	150.21(12)
O(16)[2]-Mo(7)-Mo(6)	119.41(8)	O(16)[2]-Mo(7)- O(19)	77.95(11)	O(16)[2]-Mo(7)- O(20)	147.90(11)
O(16)[2]-Mo(7)- O(23)	86.06(11)	O(19) -Mo(7)-Mo(6)	41.52(7)	O(19) -Mo(7)-O(23)	71.71(9)
O(20) -Mo(7)-Mo(6)	35.45(8)	O(20) -Mo(7)-O(19)	73.68(10)	O(20) -Mo(7)-O(23)	71.12(11)
O(21) -Mo(7)- Mo(6)	84.98(10)	O(21) -Mo(7)- O(16)[2]	101.13(14)	O(21) -Mo(7)-O(19)	95.01(12)
O(21) -Mo(7)-O(20)	96.04(13)	O(21) -Mo(7)-O(23)	163.44(12)	O(22) -Mo(7)- Mo(6)	135.58(11)
O(22) -Mo(7)- O(16)[2]	101.35(14)	O(22) -Mo(7)-O(19)	159.79(13)	O(22) -Mo(7)-O(20	100.15(13)
O(22) -Mo(7)-O(21)	104.86(15)	O(22) -Mo(7)-O(23)	88.08(12)	O(23) -Mo(7)- Mo(6)	78.51(7)
O(20)-Mo(8)- O(19)[2]	72.08(9)	O(23)-Mo(8)- O(19)[2]	72.79(10)	O(23)-Mo(8)- O(20)	72.45(11)
O(24)-Mo(8)- O(19)[2]	164.31(13)	O(24)-Mo(8)- O(20)	92.27(12)	O(24)-Mo(8)- O(23)	102.05(13)
O(24)-Mo(8)- O(25)	105.27(14)	O(24)-Mo(8)- O(26)	101.06(14)	O(25)-Mo(8)- O(19)[2]	90.30(12)
O(25)-Mo(8)- O(20)	162.12(12)	O(25)-Mo(8)- O(23)	99.93(13)	O(25)-Mo(8)- O(26)	98.49(13)
O(26)-Mo(8)- O(19)[2]	78.00(11)	O(26)-Mo(8)- O(20)	81.17(11)	O(26)-Mo(8)- O(23)	145.33(12)
O(14)-Co(1)-O(14)[3]	180.0	O(25)-Co(1)-O(14)[3]	96.74(11)	O(25)[3]-Co(1)-O(14)[3]	83.26(11)
O(25)-Co(1)-O(14)	83.26(11)	O(25)[3]-Co(1)-O(14)	96.74(11)	O(25)-Co(1)-O(25)[3]	180.0
O(27)-Co(1)-O(14)[3]	87.67(13)	O(27)-Co(1)-O(14)	92.33(13)	O(27)[3]-Co(1)-O(14)[3]	92.33(13)
O(27)[3]-Co(1)-O(14)	87.67(13)	O(27)-Co(1)-O(25)	89.23(12)	O(27)[3]-Co(1)-O(25)	90.77(12)
O(27)-Co(1)-O(25)[3]	90.77(12)	O(27)[3]-Co(1)-O(25)[3]	89.23(12)	O(27)-Co(1)- O(27)[3]	180.0

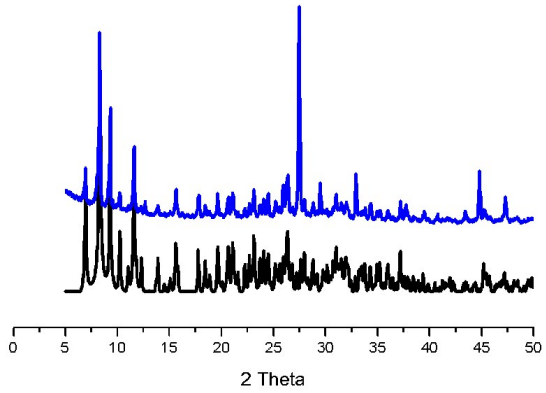


Fig. S1. Powder X-ray diffraction (PXRD) patterns for **1**. Blue: experimental data ; black: simulated pattern from single-crystal X-ray structure data.

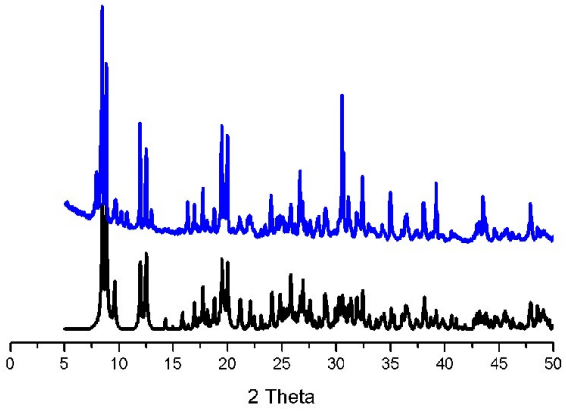


Fig. S2. Powder X-ray diffraction (PXRD) patterns for **2**. Blue: experimental data ; black: simulated pattern from single-crystal X-ray structure data.

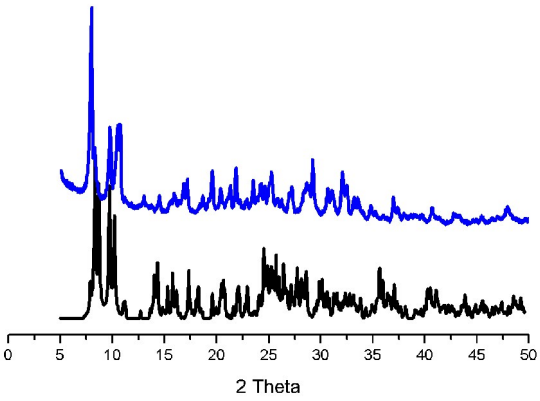


Fig. S3. Powder X-ray diffraction (PXRD) patterns for **3**. Blue: experimental data ; black: simulated pattern from single-crystal X-ray structure data.

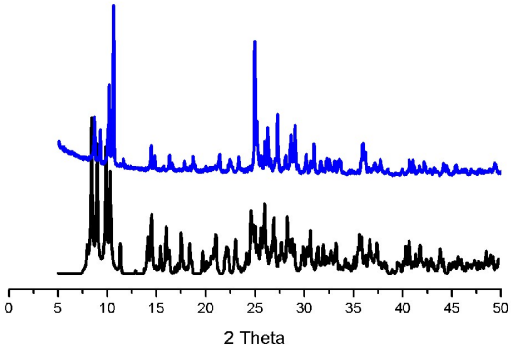


Fig. S4. Powder X-ray diffraction (PXRD) patterns for **4**. Blue: experimental data ; black: simulated pattern from single-crystal X-ray structure data.

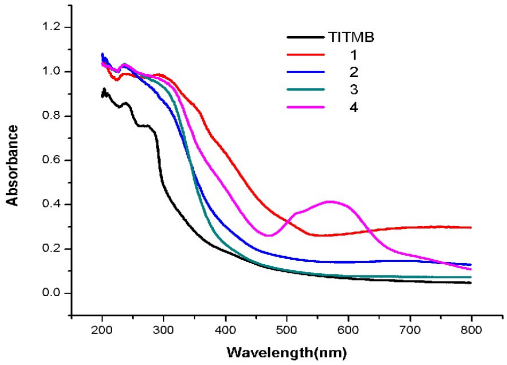


Fig. S5 UV/Vis absorption spectra of ligand TITMB and compounds **1**, **2**, **3** and **4**.

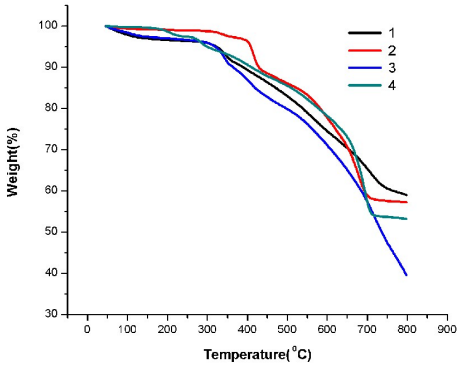


Fig. S6 TG plot of compounds **1** to **4.**

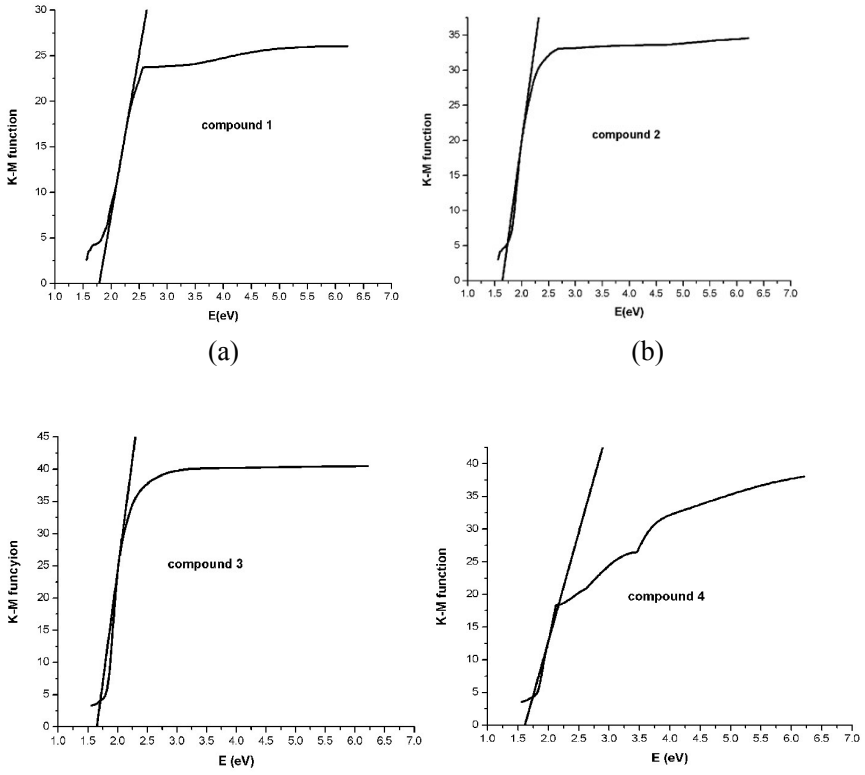
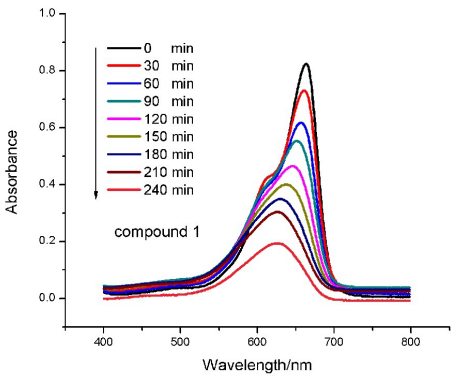
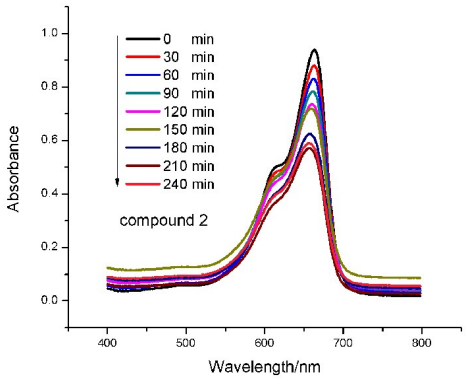


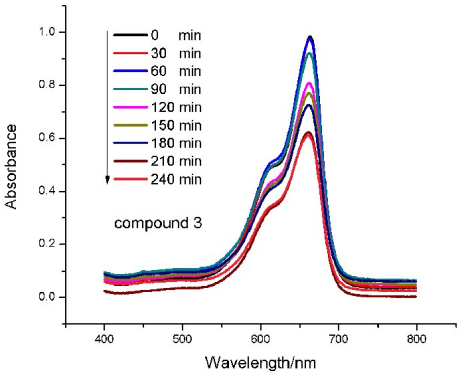
Fig. S7 K-M function versus energy (eV) curve compounds **1**, **2**, **3** and **4**.


0 min
30 min
60 min
90 min
120 min
150 min
180 min
210 min
240 min
compound 1
Absorbance
Wavelength/nm

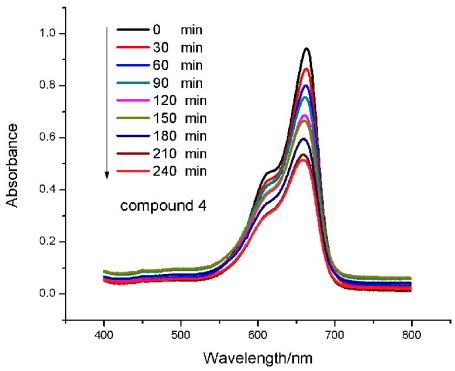
(a)


0 min
30 min
60 min
90 min
120 min
150 min
180 min
210 min
240 min
compound 2
Absorbance
Wavelength/nm

(b)


0 min
30 min
60 min
90 min
120 min
150 min
180 min
210 min
240 min
compound 3
Absorbance
Wavelength/nm

(c)


0 min
30 min
60 min
90 min
120 min
150 min
180 min
210 min
240 min
compound 4
Absorbance
Wavelength/nm

(d)

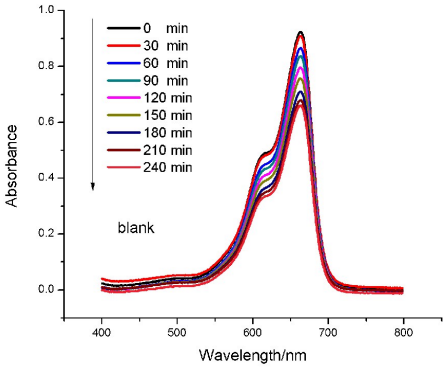
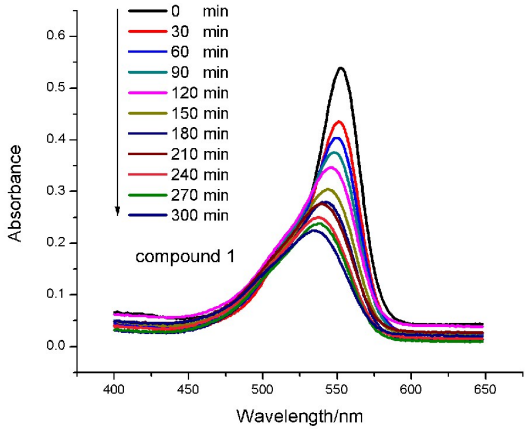
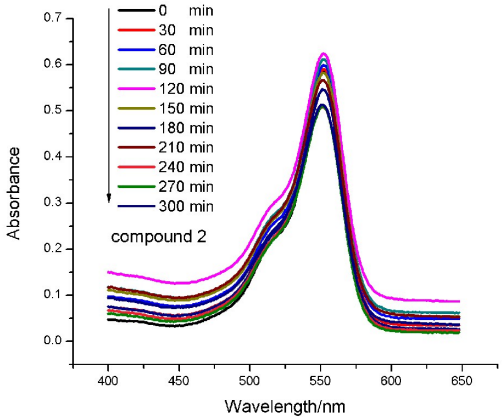

0 min
30 min
60 min
90 min
120 min
150 min
180 min
210 min
240 min
blank
Absorbance
Wavelength/nm

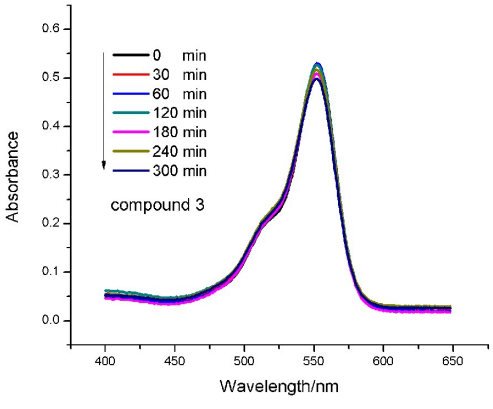
Fig.S8 Absorption spectra of the MB aqueous solution during the decomposition reaction with the use of compounds **1** (a), **2** (b), **3** (c), **4** (d) and **blank** (e).



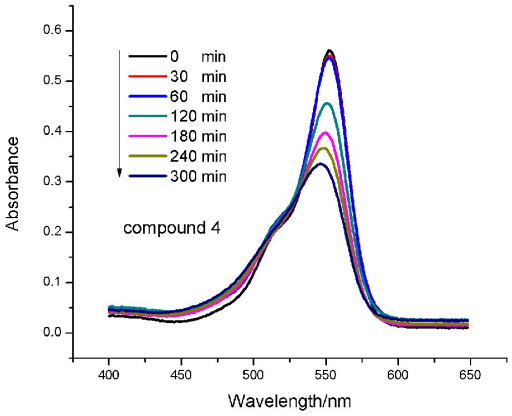
(a)



(b)



(c)



(d)

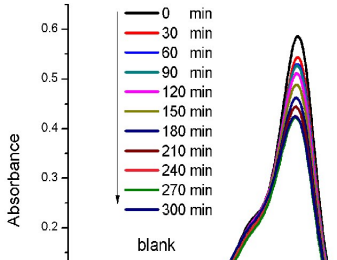
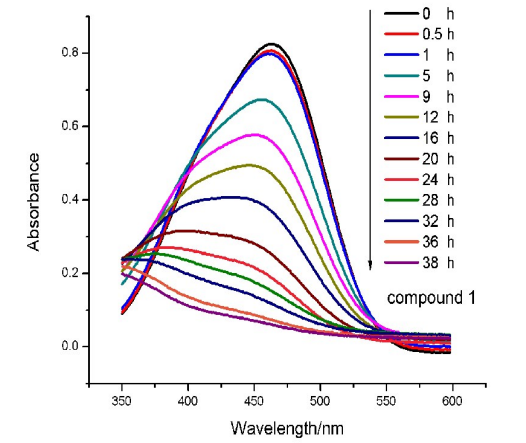
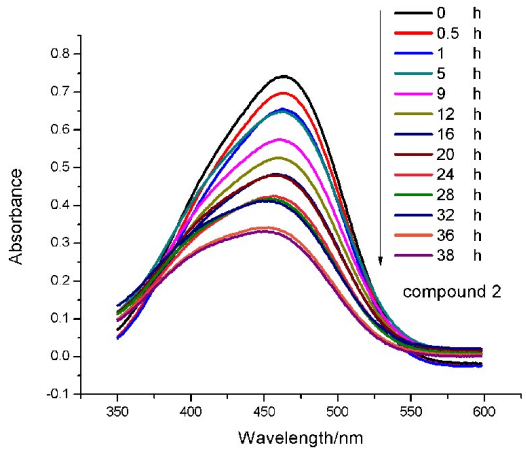
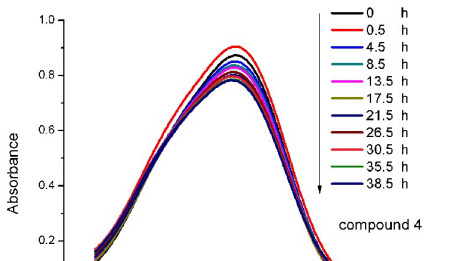


Fig.S9 Absorption spectra of the RhB aqueous solution during the decomposition reaction with the use of compounds **1** (a), **2** (b), **3** (c), **4** (d) and **blank** (e).





(a) (b)



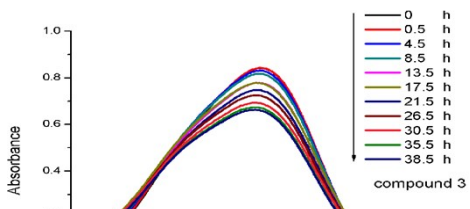


Fig.S10 Absorption spectra of the MO aqueous solution during the decomposition reaction with the use of compounds **1** (a), **2** (b), **3** (c), **4** (d) and **blank** (e).