Support Information

One-step synthesis two Wells–Dawson arsenotungstate hybrids via M-O-M bridges for efficient adsorption and selective separation of organic pollutants

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1. Structural figures

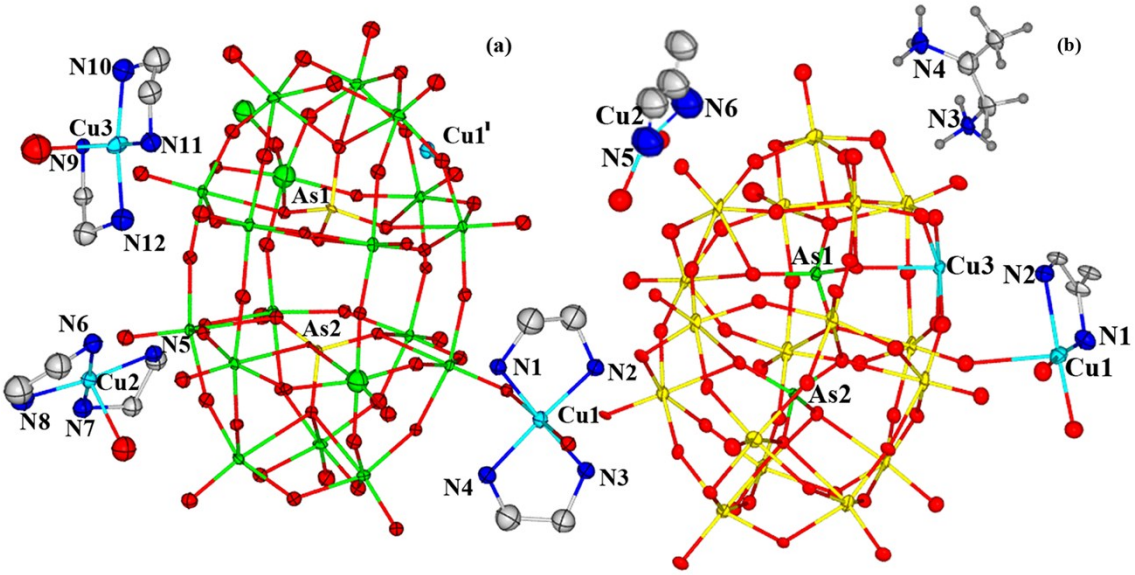


Fig.S1 ORTEP view of the basic units in (a) compound **1** (b) compound **2** with 50%thermal ellipsoid. Symmetry code: Cu1' (-1+x, y, z)

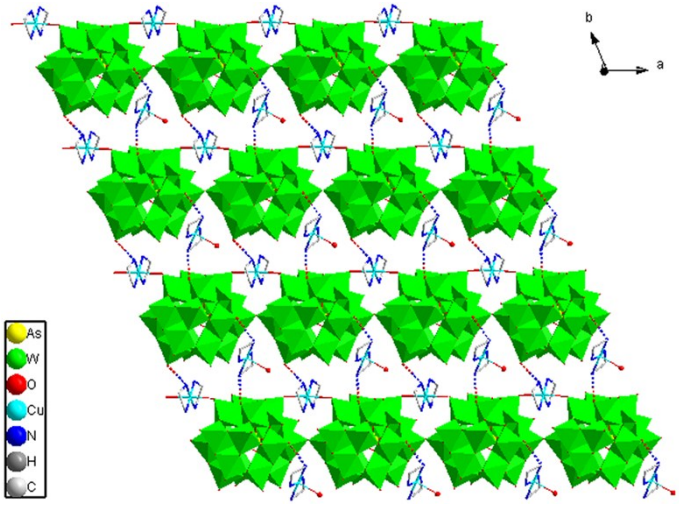


Fig.S2 Polyhedral/stick representation of a 2-D layer of compound **1**

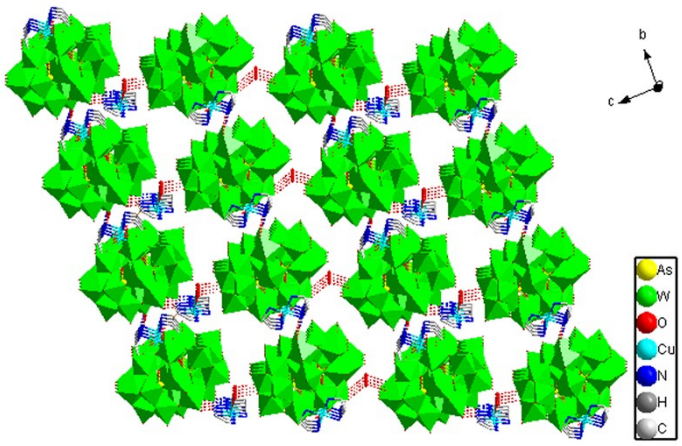


Fig.S3 Polyhedral/stick representation of the 3D network of **1**

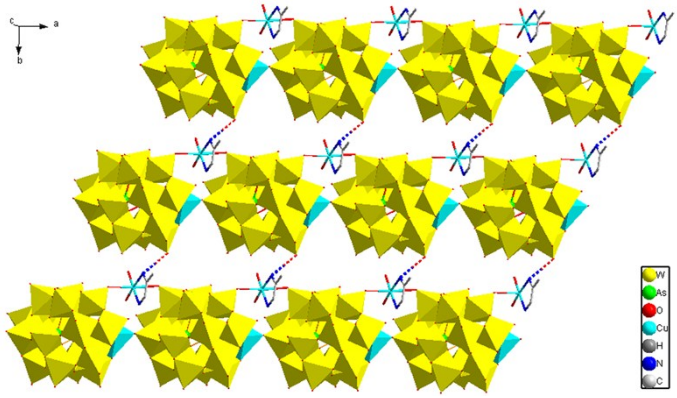


Fig.S4 Polyhedral/stick representation of a 2-D layer of compound **2**

2. Structural data

Table S1 Selected bond lengths (Å) and bond angles (°) of compound 1

W(1)-O(53)	1.69(2)	W(1)-O(62)	1.89(2)	W(1)-O(54)	1.90(2)
W(1)-O(8)	1.94(2)	W(1)-O(55)	1.94(2)	W(1)-O(7)	2.36(2)
W(2)-O(42)	1.74(2)	W(2)-O(14)	1.85(2)	W(2)-O(45)	1.92(2)
W(2)-O(11)	1.94(2)	W(2)-O(34)	1.95(2)	W(2)-O(35)	2.369(19)
W(3)-O(58)	1.72(2)	W(3)-O(16)	1.84(2)	W(3)-O(21)	1.89(2)
W(3)-O(33)	1.95(2)	W(3)-O(11)	1.97(2)	W(3)-O(35)	2.36(2)
W(4)-O(30)	1.70(2)	W(4)-O(1)	1.86(2)	W(4)-O(18)	1.88(2)
W(4)-O(2)	1.91(2)	W(4)-O(32)	1.93(2)	W(4)-O(5)	2.29(2)
W(5)-O(37) Mo(4)-O(23)	1.72(2)	W(5)-O(13)	1.85(2)	W(5)-O(38)	1.89(2)
W(5)-O(36)	1.96(2)	W(5)-O(8)	1.96(2)	W(5)-O(7)	2.34(2)
W(6)-O(28)	1.73(2)	W(6)-O(48)	1.87(2)	W(6)-O(46)	1.90(2)
W(6)-O(17)	1.89(2)	W(6)-O(45)	1.92(2)	W(6)-O(4)	2.31(2)
W(7)-O(22)	1.72(2)	W(7)-O(41)	1.88(2)	W(7)-O(25)	1.92(2)
W(7)-O(15)	1.92(2)	W(7)-O(10)	1.94(2)	W(7)-O(43)	2.33(2)
W(8)-O(52)	1.72(2)	W(8)-O(49)	1.85(2)	W(8)-O(51)	1.90(2)

W(8)-O(50)	1.91(2)	W(8)-O(54)	1.92(2)	W(8)-O(26)	2.32(2)
W(9)-O(57)	1.73(2)	W(9)-O(39)	1.83(2)	W(9)-O(17)	1.92(2)
W(9)-O(38)	1.97(2)	W(9)-O(49)	2.00(2)	W(9)-O(26)	2.34(2)
W(10)-O(31)	1.72(2)	W(10)-O(27)	1.86(2)	W(10)-O(51)	1.92(2)
W(10)-O(21)	1.96(2)	W(10)-O(48)	1.99(2)	W(10)-O(4)	2.30(2)
W(11)-O(12)	1.74(2)	W(11)-O(36)	1.91(2)	W(11)-O(24)	1.90(2)
W(11)-O(55)	1.92(2)	W(11)-O(18)	1.93(2)	W(11)-O(7)	2.36(2)
W(12)-O(29)	1.70(2)	W(12)-O(6)	1.89(2)	W(12)-O(2)	1.91(2)
W(12)-O(41)	1.96(2)	W(12)-O(23)	1.96(2)	W(12)-O(44)	2.322(17)
W(13)-O(47)	1.72(2)	W(13)-O(23)	1.88(2)	W(13)-O(33)	1.91(2)
W(13)-O(15)	1.92(2)	W(13)-O(34)	1.96(2)	W(13)-O(35)	2.33(2)
W(14)-O(20)	1.71(2)	W(14)-O(3)	1.86(2)	W(14)-O(25)	1.90(2)
W(14)-O(24)	1.95(2)	W(14)-O(1)	1.99(2)	W(14)-O(40)	2.27(2)
W(15)-O(59)	1.71(2)	W(15)-O(9)	1.85(2)	W(15)-O(50)	1.91(2)
W(15)-O(32)	1.949(19)	W(15)-O(62)	1.96(2)	W(15)-O(5)	2.33(2)
W(16)-O(60)	1.72(2)	W(16)-O(19)	1.81(2)	W(16)-O(46)	1.90(2)
W(16)-O(10)	1.95(2)	W(16)-O(14)	2.06(2)	W(16)-O(43)	2.32(2)
W(17)-O(56)#1	1.90(2)	W(17)-O(9)	1.95(2)	W(17)-O(16)	1.96(2)
W(17)-O(27)	1.95(2)	W(17)-O(6)	1.976(19)	W(17)-O(44)	2.283(18)
W(18)-O(56)	1.87(2)	W(18)-O(13)	1.95(2)	W(18)-O(19)	1.97(2)
W(18)-O(3)	1.97(2)	W(18)-O(39)	2.00(2)	W(18)-O(40)	2.29(2)
As(1)-O(26)	1.66(2)	As(1)-O(5)	1.68(2)	As(1)-O(40)	1.67(2)
As(1)-O(7)	1.69(2)	As(2)-O(43)	1.67(2)	As(2)-O(44)	1.648(18)
As(2)-O(4)	1.69(2)	As(2)-O(35)	1.70(2)		
Cu(1)-N(1)	2.01(3)	Cu(1)-N(2)	2.01(3)	Cu(1)-N(3)	2.04(3)
Cu(1)-N(4)	2.06(3)	Cu(2)-N(5)	2.00(3)	Cu(2)-N(6)	2.03(3)
Cu(2)-N(7)	2.03(3)	Cu(2)-N(8)	2.01(4)	Cu(2)-O(63)	2.30(3)
Cu(3)-N(9)	2.05(3)	Cu(3)-N(10)	2.04(3)	Cu(3)-N(11)	2.01(3)
Cu(3)-N(12)	2.06(3)	Cu(3)-O(61)	2.46(4)		
O(53)-W(1)-O(62)	104.1(10)	O(53)-W(1)-O(54)	104.3(10)	O(53)-W(1)-O(8)	101.1(10)
O(53)-W(1)-O(55)	99.8(10)	O(53)-W(1)-O(7)	170.2(10)	O(42)-W(2)-O(14)	104.7(10)
O(42)-W(2)-O(45)	101.7(10)	O(42)-W(2)-O(11)	98.8(10)	O(42)-W(2)-O(34)	100.9(10)
O(42)-W(2)-O(35)	169.7(9)	O(58)-W(3)-O(16)	104.1(10)	O(58)-W(3)-O(21)	102.1(9)
O(58)-W(3)-O(33)	102.2(9)	O(58)-W(3)-O(35)	169.6(8)	O(30)-W(4)-O(1)	101.8(10)
O(30)-W(4)-O(18)	95.1(10)	O(30)-W(4)-O(2)	98.6(10)	O(30)-W(4)-O(32)	100.6(10)
O(30)-W(4)-O(5)	173.9(10)	O(37)-W(5)-O(13)	105.1(11)	O(37)-W(5)-O(38)	103.7(10)
O(37)-W(5)-O(36)	98.9(10)	O(37)-W(5)-O(8)	97.6(10)	O(37)-W(5)-O(7)	166.8(9)
O(28)-W(6)-O(48)	100.8(10)	O(28)-W(6)-O(46)	102.1(10)	O(28)-W(6)-O(17)	97.7(9)
O(28)-W(6)-O(45)	96.8(10)	O(28)-W(6)-O(4)	173.1(9)	O(22)-W(7)-O(41)	102.3(10)
O(22)-W(7)-O(25)	97.3(10)	O(22)-W(7)-O(15)	96.5(10)	O(22)-W(7)-O(10)	101.0(10)
O(22)-W(7)-O(43)	173.2(9)	O(52)-W(8)-O(49)	99.2(10)	O(52)-W(8)-O(51)	98.0(10)
O(52)-W(8)-O(50)	103.6(10)	O(52)-W(8)-O(54)	95.8(10)	O(52)-W(8)-O(26)	171.8(9)
O(57)-W(9)-O(39)	101.5(10)	O(57)-W(9)-O(17)	98.4(9)	O(57)-W(9)-O(38)	96.6(9)
O(57)-W(9)-O(49)	99.9(10)	O(57)-W(9)-O(26)	169.9(9)	O(31)-W(10)-O(27)	101.0(9)

O(31)-W(10)-O(51)	99.2(9)	O(31)-W(10)-O(21)	97.0(9)	O(31)-W(10)-O(48)	100.3(9)
O(31)-W(10)-O(4)	171.0(8)	O(12)-W(11)-O(36)	101.0(10)	O(12)-W(11)-O(24)	101.4(10)
O(12)-W(11)-O(55)	101.3(10)	O(12)-W(11)-O(18)	103.0(10)	O(12)-W(11)-O(7)	171.9(10)
O(29)-W(12)-O(6)	100.9(9)	O(29)-W(12)-O(2)	97.6(10)	O(29)-W(12)-O(41)	101.3(10)
O(29)-W(12)-O(23)	96.6(9)	O(29)-W(12)-O(44)	175.6(9)	O(47)-W(13)-O(23)	102.1(10)
O(47)-W(13)-O(33)	101.5(10)	O(47)-W(13)-O(15)	102.6(10)	O(47)-W(13)-O(34)	99.5(10)
O(47)-W(13)-O(35)	171.4(9)	O(20)-W(14)-O(3)	102.0(10)	O(20)-W(14)-O(25)	97.7(10)
O(20)-W(14)-O(24)	96.5(10)	O(20)-W(14)-O(1)	99.2(9)	O(20)-W(14)-O(40)	177.2(9)
O(59)-W(15)-O(9)	99.0(9)	O(59)-W(15)-O(50)	101.7(9)	O(59)-W(15)-O(32)	101.4(9)
O(59)-W(15)-O(62)	95.3(9)	O(59)-W(15)-O(5)	172.6(8)	O(60)-W(16)-O(19)	101.3(10)
O(60)-W(16)-O(46)	103.6(10)	O(60)-W(16)-O(10)	98.3(10)	O(60)-W(16)-O(14)	92.1(10)
O(60)-W(16)-O(43)	169.2(9)	O(56)#1-W(17)-O(9)	96.5(9)	O(56)#1-W(17)-O(16)	95.0(9)
O(56)#1-W(17)-O(27)	100.8(9)	O(56)#1-W(17)-O(6)	97.4(9)	O(56)#1-W(17)-O(44)	171.5(8)
O(56)-W(18)-O(13)	95.3(10)	O(56)-W(18)-O(19)	97.0(9)	O(56)-W(18)-O(3)	99.6(9)
O(56)-W(18)-O(39)	98.5(9)	O(56)-W(18)-O(40)	172.6(8)		
O(26)-As(1)-O(5)	111.5(10)	O(26)-As(1)-O(40)	112.2(10)	O(26)-As(1)-O(7)	106.3(10)
O(43)-As(2)-O(44)	112.1(9)	O(43)-As(2)-O(4)	110.6(10)	O(43)-As(2)-O(35)	107.8(10)
N(2)-Cu(1)-N(1)	85.7(11)	N(2)-Cu(1)-N(3)	97.3(11)	N(2)-Cu(1)-N(4)	176.8(12)
N(5)-Cu(2)-N(8)	174.5(14)	N(5)-Cu(2)-N(6)	94.0(12)	N(5)-Cu(2)-N(7)	85.1(12)
N(5)-Cu(2)-O(63)	93.2(12)	N(11)-Cu(3)-N(9)	178.9(12)	N(11)-Cu(3)-N(10)	82.9(14)
N(11)-Cu(3)-N(12)	97.8(14)	N(11)-Cu(3)-O(61)	90.9(13)		

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

Table S2 Selected bond lengths (Å) and bond angles (º) of compound 2

W(1)-O(16)	1.72(3)	W(1)-O(21)	1.75(3)	W(1)-O(19)	1.88(4)
W(1)-O(36)	1.85(3)	W(1)-O(58)	1.98(3)	W(1)-O(8)	2.30(3)
W(2)-O(41)	1.72(3)	W(2)-O(47)	1.79(3)	W(2)-O(23)	1.96(4)
W(2)-O(43)	2.04(3)	W(2)-O(21)	2.05(3)	W(2)-O(8)	2.27(3)
W(3)-O(52)	1.73(3)	W(3)-O(37)	1.86(4)	W(3)-O(15)	1.85(3)
W(3)-O(6)	1.90(3)	W(3)-O(48)	2.02(3)	W(3)-O(56)	2.44(3)
W(4)-O(20)	1.66(3)	W(4)-O(13)	1.89(4)	W(4)-O(33)	1.93(3)
W(4)-O(36)	1.96(3)	W(4)-O(37)	1.96(4)	W(4)-O(12)	2.35(3)
W(5)-O(44)	1.65(4)	W(5)-O(14)	1.86(3)	W(5)-O(10)	1.90(3)
W(5)-O(13)	1.94(4)	W(5)-O(19)	1.99(3)	W(5)-O(34)	2.33(3)
W(6)-O(40)	1.75(3)	W(6)-O(43)	1.80(3)	W(6)-O(17)	1.85(3)
W(6)-O(35)	1.88(4)	W(6)-O(26	1.88(3)	W(6)-O(31)	2.38(3)
W(7)-O(18)	1.75(3)	W(7)-O(51)	1.82(3)	W(7)-O(55	1.83(4)
W(7)-O(1)	1.83(3)	W(7)-O(17)	2.02(3)	W(7)-O(45)	2.32(3)
W(8)-O(64)	1.74(3)	W(8)-O(29)	1.84(3)	W(8)-O(32)	1.94(3)
W(8)-O(15)	1.96(3)	W(8)-O(27)	2.01(3)	W(8)-O(4)	2.41(3)
W(9)-O(63)	1.71(4)	W(9)-O(23)	1.84(4)	W(9)-O(2)	1.84(3)

W(9)-O(11)	1.92(3)	W(9)-O(10)	1.96(3)	W(9)-O(34)	2.40(3)
W(10)-O(53)	1.71(3)	W(10)-O(9)	1.78(3)	W(10)-O(33)	1.93(3)
W(10)-O(42)	2.01(4)	W(10)-O(46)	2.04(3)	W(10)-O(12)	2.27(3)
W(11)-O(7)	1.67(2)	W(11)-O(27)	1.84(3)	W(11)-O(58)	1.87(3)
W(11)-O(6)	1.94(3)	W(11)-O(26)	2.06(3)	W(11)-O(31)	2.32(3)
W(12)-O(5)	1.76(3)	W(12)-O(50)	1.92(3)	W(12)-O(35)	1.96(3)
W(12)-O(32)	1.98(3)	W(12)-O(55)	2.00(3)	W(12)-O(4)	2.35(3)
W(13)-O(61)	1.75(3)	W(13)-O(42)	1.86(4)	W(13)-O(48)	1.84(3)
W(13)-O(49)	1.87(3)	W(13)-O(39)	1.95(4)	W(13)-O(56)	2.21(3)
W(14)-O(30)	1.75(3)	W(14)-O(22)	1.75(3)	W(14)-O(46)	1.83(3)
W(14)-O(11)	1.97(4)	W(14)-O(14)	2.06(3)	W(14)-O(34)	2.27(3)
W(15)-O(25)	1.74(3)	W(15)-O(54)	1.75(3)	W(15)-O(39)	1.87(3)
W(15)-O(50)	1.94(3)	W(15)-O(29)	2.01(3)	W(15)-O(4)	2.36(3)
W(16)-O(3)	1.70(4)	W(16)-O(28)	1.81(3)	W(16)-O(1)	1.97(3)
W(16)-O(2)	2.01(4)	W(16)-O(47)	2.07(3)	W(16)-O(38)	2.24(3)
W(17)-O(62)	1.66(3)	W(17)-O(24)	1.73(4)	W(17)-O(49)	1.94(3)
W(17)-O(51)	2.07(3)	W(17)-O(54)	2.11(3)	W(17)-O(45)	2.23(3)
As(1)-O(38)	1.68(3)	As(1)-O(8)	1.70(3)	As(1)-O(34)	1.74(4)
As(1)-O(12)	1.72(3)	As(2)-O(31)	1.61(3)	As(2)-O(56)	1.66(3)
As(2)-O(4)	1.64(3)	As(2)-O(45)	1.71(3)	Cu(1)-O(65)	1.93(3)
Cu(1)-O(57)	1.97(3)	Cu(1)-N(1)	2.00(4)	Cu(1)-N(2)	2.14(4)
Cu(2)-O(59)	2.06(4)	Cu(2)-O(60)	2.08(4)	Cu(2)-N(6)	1.95(9)
Cu(2)-N(5)	2.33(9)	Cu(3)-O(38)	2.19(3)	Cu(3)-O(7)#2	2.28(2)
O(16)-W(1)-O(21)	102.1(16)	O(16)-W(1)-O(19)	97.0(17)	O(16)-W(1)-O(36)	99.8(15)
O(16)-W(1)-O(58)	96.9(16)	O(16)-W(1)-O(8)	174.3(14)	O(41)-W(2)-O(47)	101.9(15)
O(41)-W(2)-O(23)	102.5(15)	O(41)-W(2)-O(43)	90.5(14)	O(41)-W(2)-O(21)	105.1(14)
O(41)-W(2)-O(8)	168.6(14)	O(52)-W(3)-O(37)	93.8(15)	O(52)-W(3)-O(15)	100.9(15)
O(52)-W(3)-O(6)	102.9(15)	O(52)-W(3)-O(48)	100.7(14)	O(52)-W(3)-O(56)	168.4(13)
O(20)-W(4)-O(13)	94.4(17)	O(20)-W(4)-O(33)	104.7(15)	O(20)-W(4)-O(36)	99.7(14)
O(20)-W(4)-O(37)	98.0(16)	O(20)-W(4)-O(12)	173.7(14)	O(44)-W(5)-O(14)	103.1(17)
O(44)-W(5)-O(10)	103.1(17)	O(44)-W(5)-O(13)	100.6(17)	O(44)-W(5)-O(19)	100.3(17)
O(44)-W(5)-O(34)	174.3(16)	O(40)-W(6)-O(43)	95.8(15)	O(40)-W(6)-O(17)	100.7(14)
O(40)-W(6)-O(35)	98.4(15)	O(40)-W(6)-O(26)	95.4(13)	O(40)-W(6)-O(31)	172.7(13)
O(18)-W(7)-O(51)	97.7(15)	O(18)-W(7)-O(55)	98.6(15)	O(18)-W(7)-O(1)	95.1(15)
O(18)-W(7)-O(17)	100.7(13)	O(18)-W(7)-O(45)	170.1(13)	O(64)-W(8)-O(29)	101.0(15)
O(64)-W(8)-O(32)	94.2(14)	O(64)-W(8)-O(15)	107.9(14)	O(64)-W(8)-O(27)	102.3(14)
O(64)-W(8)-O(4)	168.4(14)	O(63)-W(9)-O(23)	98.1(15)	O(63)-W(9)-O(2)	104.1(16)
O(63)-W(9)-O(11)	104.1(16)	O(63)-W(9)-O(10)	97.5(15)	O(63)-W(9)-O(34)	168.5(15)
O(53)-W(10)-O(9)	102.6(16)	O(53)-W(10)-O(33)	99.3(16)	O(53)-W(10)-O(42)	97.8(16)
O(53)-W(10)-O(46)	95.9(16)	O(53)-W(10)-O(12)	170.8(14)	O(7)-W(11)-O(27)	93.5(15)
O(7)-W(11)-O(58)	97.6(14)	O(7)-W(11)-O(6)	100.4(13)	O(7)-W(11)-O(26)	98.8(12)
O(7)-W(11)-O(31)	173.9(12)	O(5)-W(12)-O(50)	101.0(15)	O(5)-W(12)-O(35)	102.7(15)
O(5)-W(12)-O(32)	98.0(14)	O(5)-W(12)-O(55)	106.1(14)	O(5)-W(12)-O(4)	171.7(14)
O(61)-W(13)-O(42)	98.7(16)	O(61)-W(13)-O(48)	97.9(15)	O(61)-W(13)-O(49)	102.9(15)

O(61)-W(13)-O(39)	94.5(16)	O(61)-W(13)-O(56)	174.7(14)	O(30)-W(14)-O(22)	105.6(16)
O(30)-W(14)-O(46)	93.6(16)	O(30)-W(14)-O(11)	91.2(15)	O(30)-W(14)-O(14)	158.0(15)
O(30)-W(14)-O(34)	88.2(15)	O(25)-W(15)-O(54)	104.8(15)	O(25)-W(15)-O(39)	105.3(15)
O(25)-W(15)-O(50)	96.1(14)	O(25)-W(15)-O(29)	97.8(14)	O(25)-W(15)-O(4)	166.0(13)
O(3)-W(16)-O(28)	109.1(15)	O(3)-W(16)-O(1)	94.1(16)	O(3)-W(16)-O(2)	97.3(16)
O(3)-W(16)-O(47)	97.0(15)	O(3)-W(16)-O(38)	176.8(16)	O(62)-W(17)-O(24)	98.5(17)
O(62)-W(17)-O(49)	110.1(15)	O(62)-W(17)-O(51)	94.4(14)	O(62)-W(17)-O(54)	94.3(16)
O(62)-W(17)-O(45)	163.7(15)	O(38)-As(1)-O(8)	111.9(16)	O(38)-As(1)-O(34)	107.8(17)
O(38)-As(1)-O(12)	110.1(16)	O(31)-As(2)-O(56)	114.8(17)	O(31)-As(2)-O(45)	114.3(16)
O(28)-Cu(3)-O(24)	94.3(14)	O(28)-Cu(3)-O(9)	163.9(15)	O(28)-Cu(3)-O(30)	92.6(15)
O(28)-Cu(3)-O(38)	71.8(14)	O(28)-Cu(3)-O(7)#2	95.8(12)	O(65)-Cu(1)-O(57)	82.1(15)
O(65)-Cu(1)-N(1)	171.8(16)	O(65)-Cu(1)-N(2)	97.8(11)	N(1)-Cu(1)-N(2)	84.5(12)
N(6)-Cu(2)-O(59)	97(3)	N(6)-Cu(2)-O(60)	156(3)	N(6)-Cu(2)-N(5)	74(3)

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

Table S3 Selected Hydrogen Bond Lengths ( ) and Bond Angles (°) of complexes **1-2**

	D-H...A	d(D-H)	d(H...A)	<D-H...A	d(D...A)	Symmetry
1	N1-H1A...O30	0.90	2.28	157.1	3.13(4)	
	N1-H1B...O20	0.90	2.13	164.2	3.01(4)	
	N5-H5A...O29	0.90	2.16	151.5	2.98(4)	
	N5-H5B...O47	0.90	2.35	140.9	3.10(3)	
	N6-H6A...O1W	0.90	2.15	156.4	3.00(4)	
	N9-H9B...O30	0.90	2.17	141.5	2.93(4)	
	N11-H11B...O59	0.90	2.04	159.8	2.90(4)	
	N12-H12C...O6	0.90	2.38	139.6	3.12(4)	
	O63-H63A...O3W	0.85	2.19	124.4	2.76(4)	
	O1W-H1WA...O3W	0.85	2.13	128.5	2.74(4)	
	O2W-H2WB...O5W	0.85	3.08	101.0	3.35(5)	
	O3W-H3WB...O33	0.85	2.66	92.2	2.82(4)	
	N2-H2A...O27	0.90	2.08	159.0	2.94(4)	[x-1, y-1, z]
	N2-H2B...O39	0.90	2.63	142.4	3.39(3)	[x, y-1, z]
	N3-H3A...O39	0.90	2.22	149.4	3.03(4)	[x, y-1, z]
	N5-H5A...O28	0.90	2.53	113.2	3.00(3)	[x, y-1, z]
	N6-H6B...O48	0.90	2.44	135.5	3.15(4)	[x, y-1, z]
	N7-H7A...O11	0.90	2.38	158.2	3.23(4)	[-x+1, -y+1, -z]
	N7-H7B...O42	0.90	2.35	141.6	3.10(4)	[x, y-1, z]
	N8-H8A...O11	0.90	2.38	151.4	3.20(4)	[x, y-1, z]
	N8-H8A...O45	0.90	2.54	140.7	3.29(4)	[x, y-1, z]
	N8-H8B...O42	0.90	2.26	167.3	3.14(4)	[-x+1, -y+1, -z]
	N9-H9A...O49	0.90	2.18	129.5	2.84(3)	[x, y-1, z]
	N10-H10B...O53	0.90	2.14	146.7	2.93(4)	[-x+1,-y+1,-z+1]
	N11-H11A...O36	0.90	2.14	147.7	2.94(4)	[x+1, y, z]
	N12-H12D...O3	0.90	2.21	143.3	2.98(4)	[x+1, y, z]

	O63-H63B...O34	0.85	2.02	142.8	2.75(4)	[-x+1, -y+1, -z]
	O63-H63...O47	0.85	2.64	137.6	3.31(4)	[-x+1, -y+1, -z]
	O61-H61B...O52	0.85	2.84	92.5	3.00(4)	[x, y-1, z]
	O1W-H1WB...O19	0.85	2.60	120.4	3.12(4)	[x+1, y, z]
	O1W-H1WB...O10	0.85	2.61	142.6	3.33(3)	[x+1, y, z]
	O2W-H2WA...O37	0.85	1.96	171.0	2.81(4)	[x+1, y, z]
	O3W-H3WB...O47	0.85	2.80	134.5	3.45(4)	[-x+1, -y+1, -z]
	O4W-H4WA...O5W	0.85	2.63	122.5	3.17(5)	[-x+1, -y+2, -z+1]
	O4W-H4WB...O52	0.85	2.22	132.3	2.86(4)	[-x+1, -y+2, -z+1]
	O5W-H5WB...O49	0.85	2.31	173.8	3.16(4)	[-x+1, -y+2, -z+1]
	O5W-H5WB...O38	0.85	2.63	115.9	3.10(4)	[-x+1, -y+2, -z+1]
	O6W-H6WB...O10	0.85	2.77	88.8	2.88(4)	[x+1, y, z]
	O6W-H6WB...O14	0.85	2.71	130.9	3.33(4)	[x+1, y, z]
2	O59-H59A...O60	0.93	2.49	88.3	2.63(6)	
	O59-H59B...O2W	0.93	2.40	134.6	3.12(6)	
	N5-H5B...O21	0.90	2.13	133.1	2.82(9)	
	N5-H5B...O19	0.90	2.42	130.8	3.09(8)	
	N5-H5B...O23	0.90	2.59	145.2	3.37(9)	
	N6-H6D...O10	0.90	1.80	163.6	2.68(10)	
	N6-H6E...O2W	0.90	2.66	130.6	3.32(8)	
	O60-H60B...O16	0.93	2.14	133.1	2.86(6)	
	N2-H2A...O30	0.90	2.64	154.6	3.48(5)	
	N3-H3A...O1W	0.89	1.93	174.2	2.82(6)	
	N3-H3B...O28	0.89	2.29	135.8	3.00(5)	
	N3-H3B...O2	0.89	2.48	153.0	3.30(5)	
	N4-H4A...O1W	0.89	2.65	143.7	3.41(6)	
	O65-H65A...O57	0.93	2.42	87.9	2.56(5)	
	O57-H57...O17	0.82	2.43	147.3	3.15(4)	[x+1/2, y-1/2, z]
	N1-H1A...O3	0.90	2.10	153.3	2.93(5)	[x+1/2, y-1/2, z]
	N1-H1B...O41	0.90	2.35	154.0	3.19(5)	[x+1/2, y-1/2, z]
	N1-H1B...O47	0.90	2.65	127.4	3.27(5)	[x+1/2, y-1/2, z]
	O59-H59B...O51	0.93	2.62	116.9	3.15(6)	[x-1/2,-y+1/2,z-1/2]
	N5-H5A...O1W	0.90	2.65	154.6	3.48(9)	[x-1, y, z]
	N2-H2B...O6	0.90	2.27	148.6	3.07(5)	[x+1, y, z]
	N3-H3C...O58	0.89	2.46	140.7	3.20(4)	[x+1, y, z]
	O65-H65B...O7	0.93	2.45	154.1	3.31(4)	[x+1, y, z]
	O1W-H1WB...O25	0.85	2.48	163.8	3.30(6)	[x+1/2,-y+1/2,z-1/2]
	O2W-H2WA...O32	0.85	2.32	154.4	3.11(5)	[x+1/2,-y+1/2,z-1/2]
	O2W-H2WB...O62	0.85	2.83	99.0	3.08(5)	[x-1/2,-y+1/2,z-1/2]
	O3W-H3WB...O46	0.85	2.34	154.1	3.12(6)	[x+1/2, y+1/2, z]
	O4W-H4WA...O33	0.85	2.53	145.9	3.27(5)	[x+1/2, y+1/2, z]
	O4W-H4WB...O48	0.85	2.57	126.7	3.16(5)	[x+1/2, y+1/2, z]

3. Physical characterization

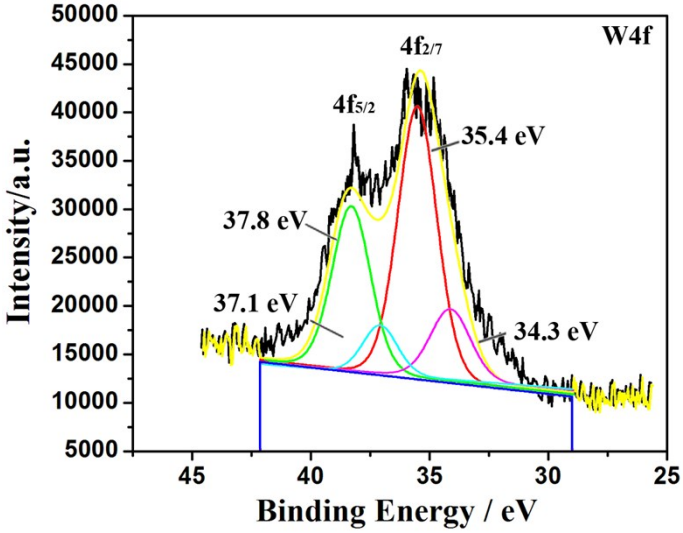


Fig. S5 The XPS spectra of W in compound **1.**

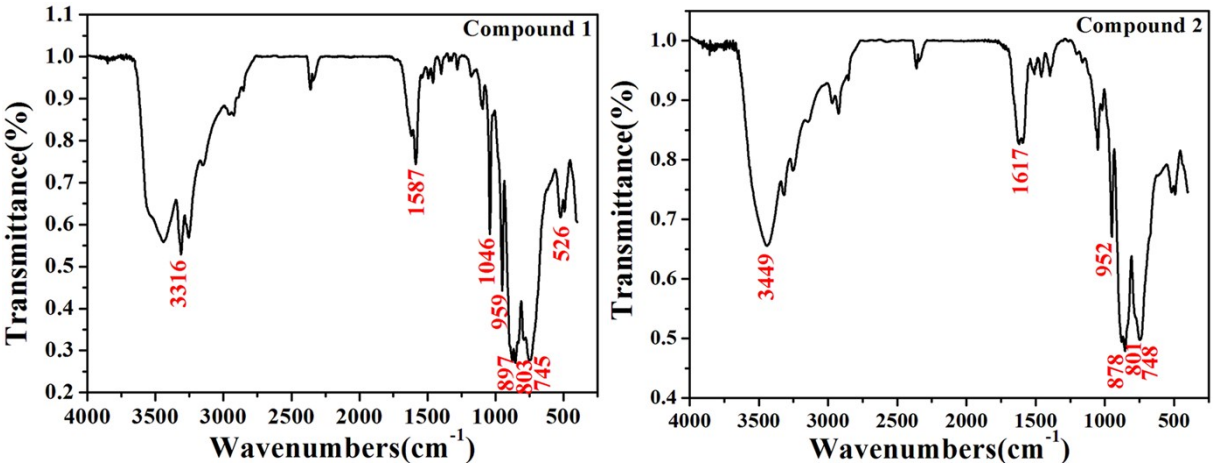


Fig. S6 IR spectras of compounds **1-2**

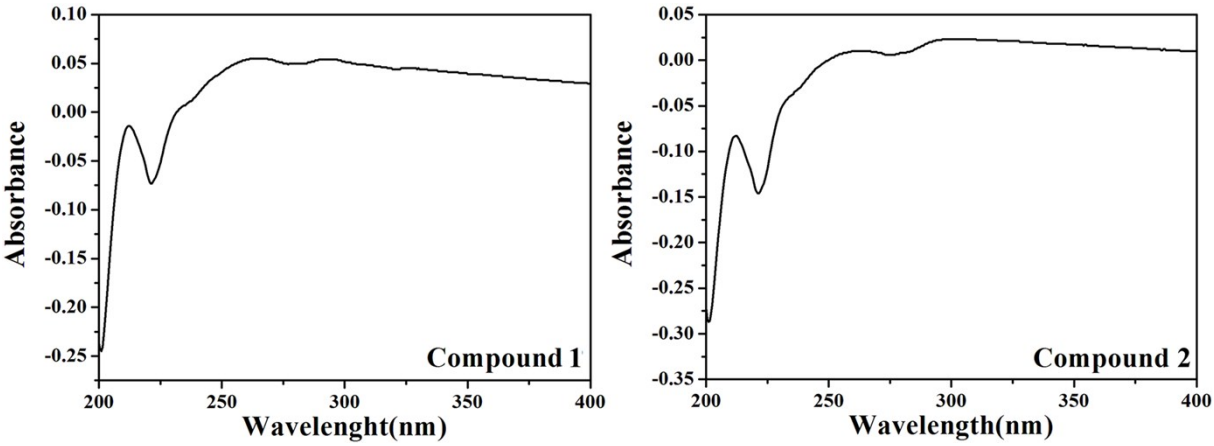


Fig.S7 UV-vis spectras of compounds **1-2**

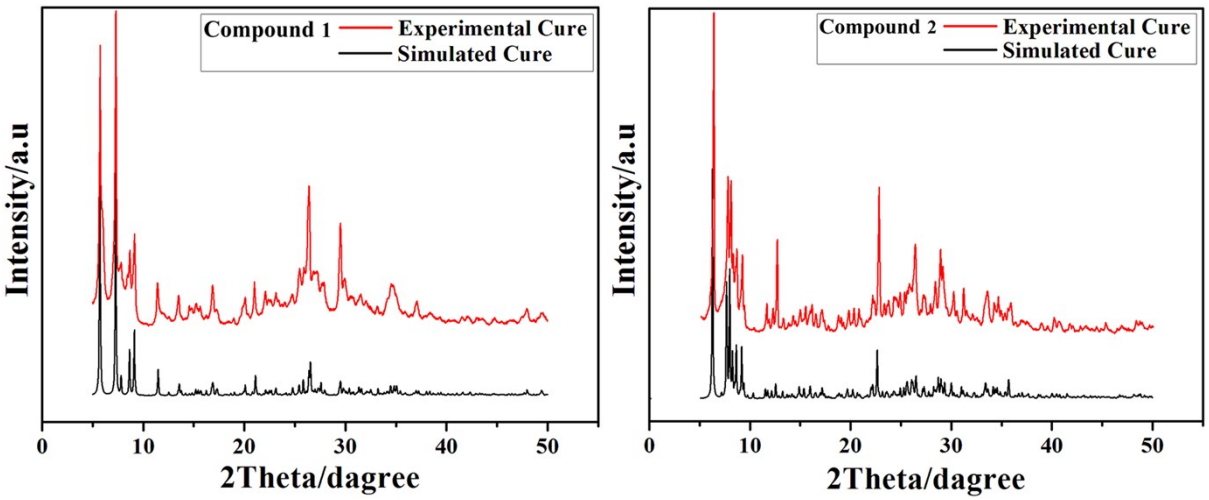


Fig.S8 Simulated and experimental XRD spectras of **1-2**

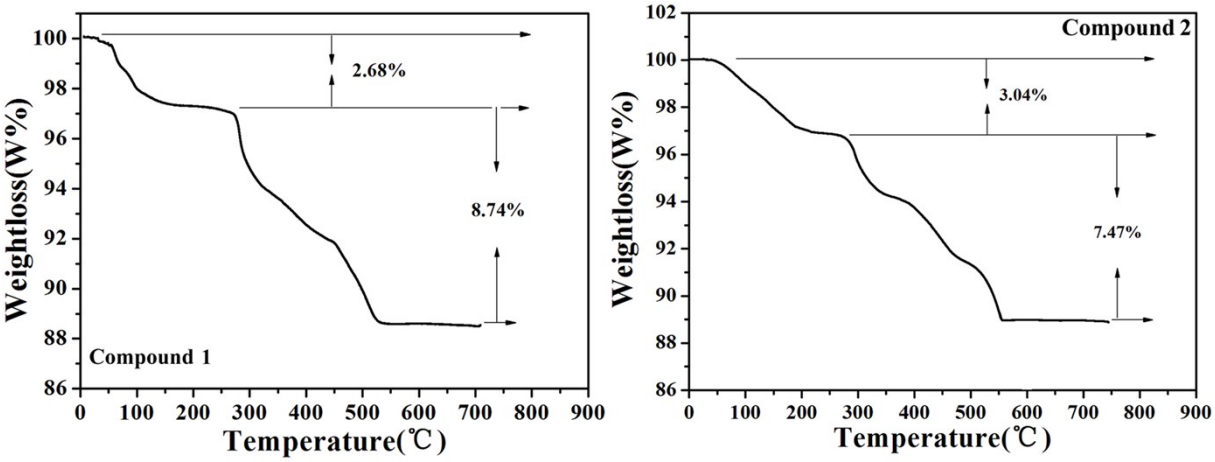


Fig.S9 TG curves of compounds **1-2**

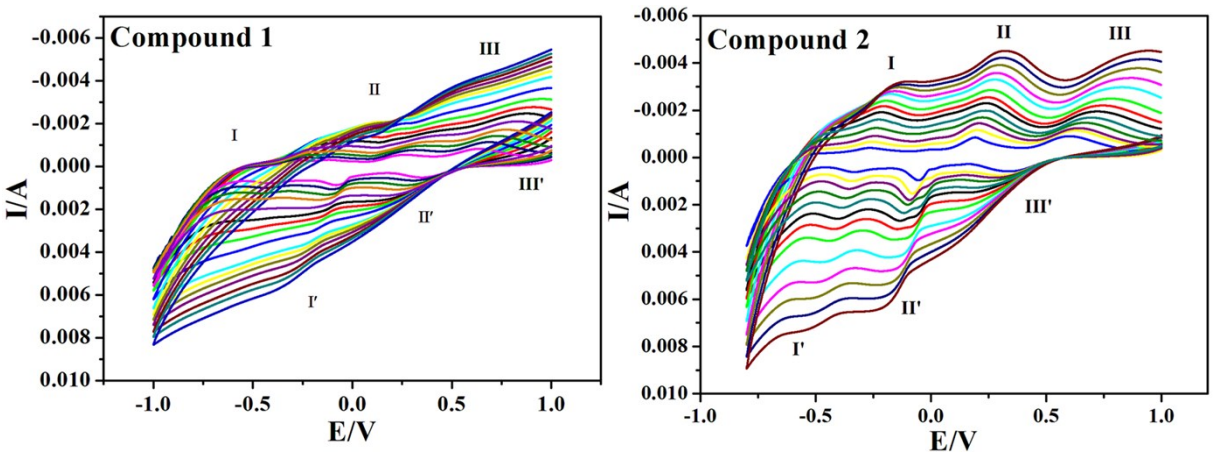


Fig. S10 Cyclic voltammograms of **1-CPE** and **2-CPE** in the 1.0 M H_2SO_4 solution at different scan rates

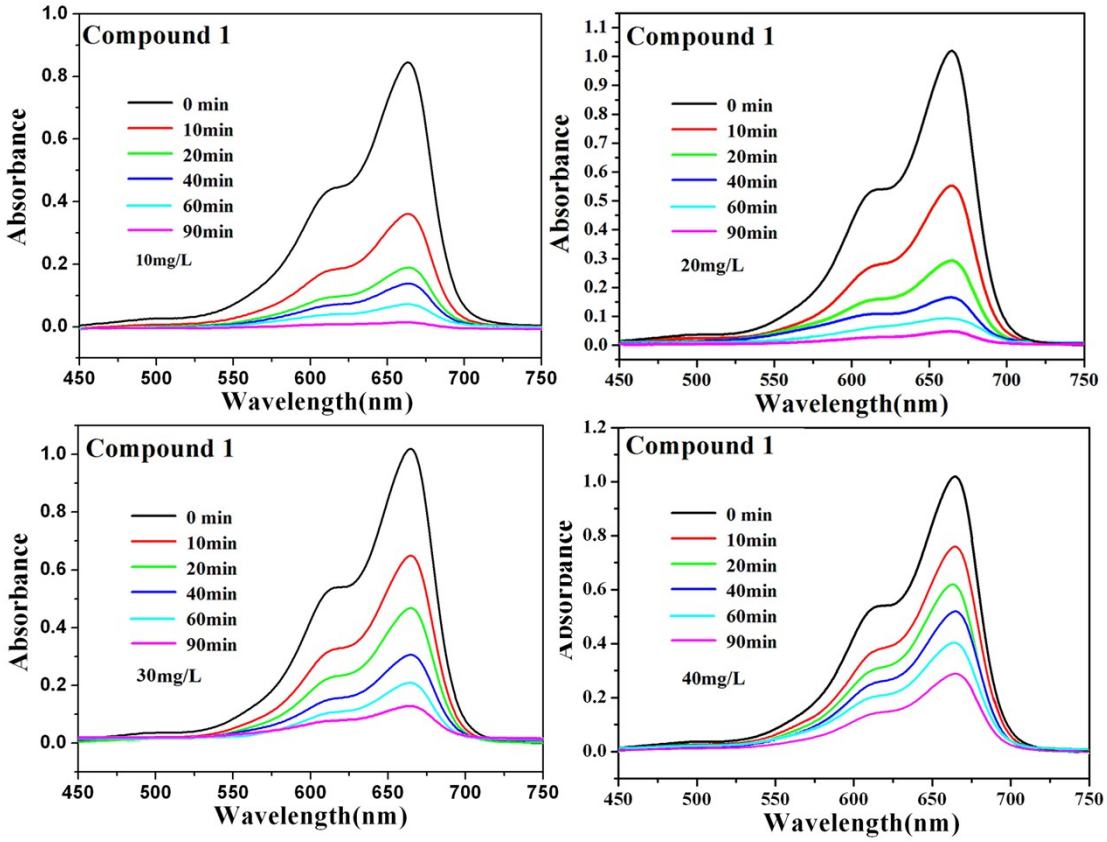


Fig. S11 Compound **1** (10 mg) was used to adsorb MB in 100 mL aqueous solution with different concentrations of dyes: 10 mg $\cdot L^{-1}$; 20 mg $\cdot L^{-1}$; 30 mg $\cdot L^{-1}$; 40mg $\cdot L^{-1}$.

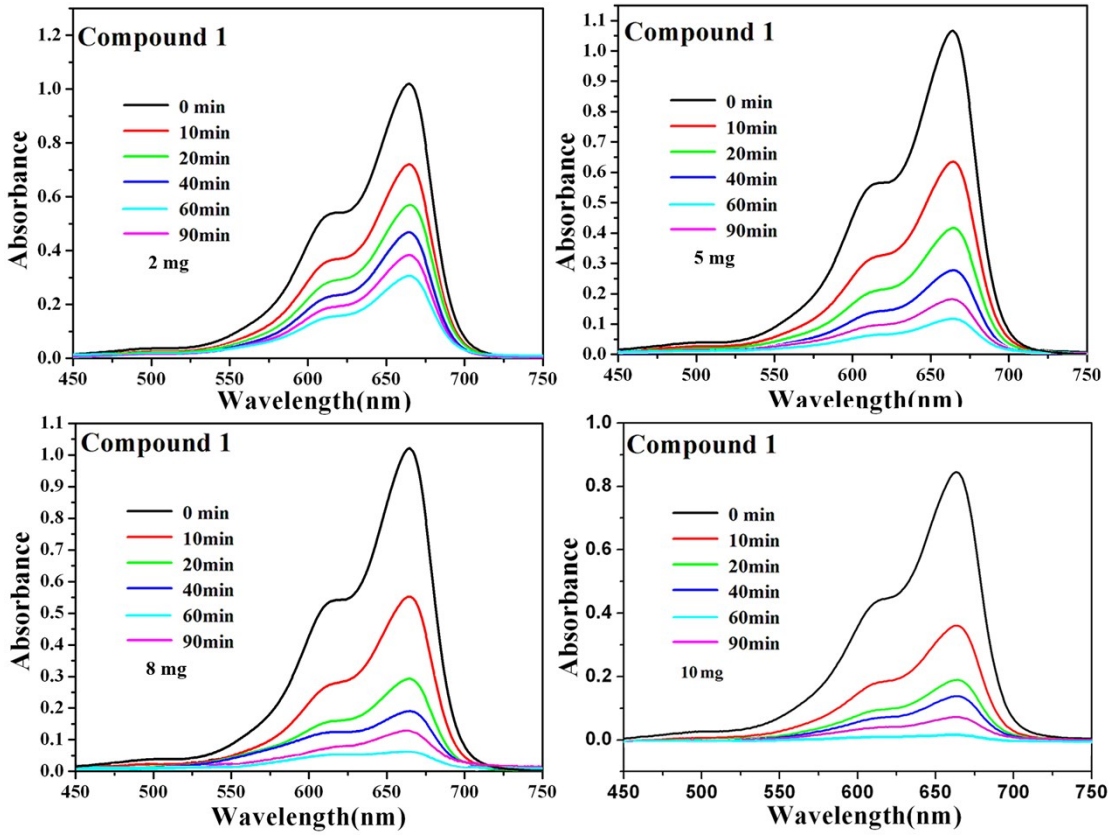


Fig. S12 Compound **1** was used to adsorb MB (10 mg/L, 100 mL) aqueous solution

with different quality (mg) of absorbent: 2 mg, 5mg, 8 mg, and 10mg.

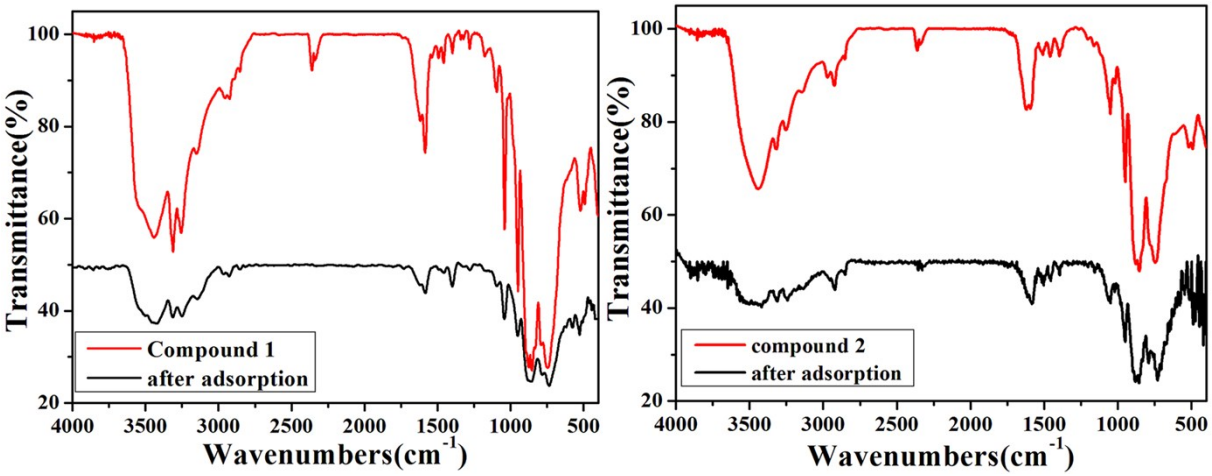


Fig. S13 The IR spectra of catalyst **1** and **2** before and after adsorption experiment.

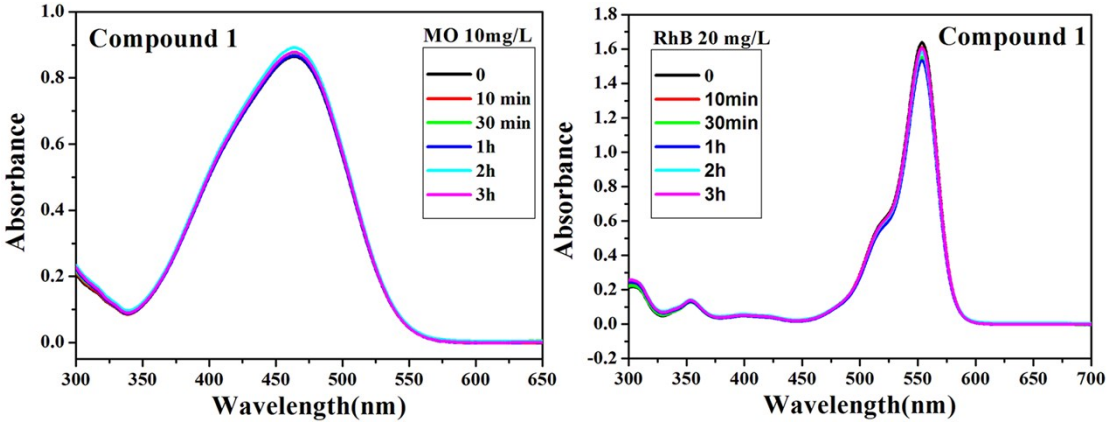


Fig. S14 The adsorption activity of compound **1** (10.0 mg) toward different dye aqueous solutions: MO and RhB.

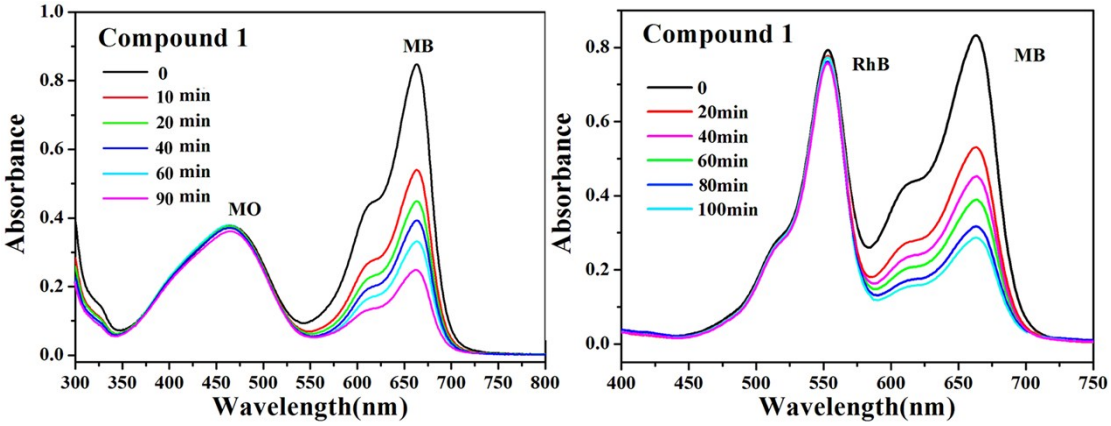
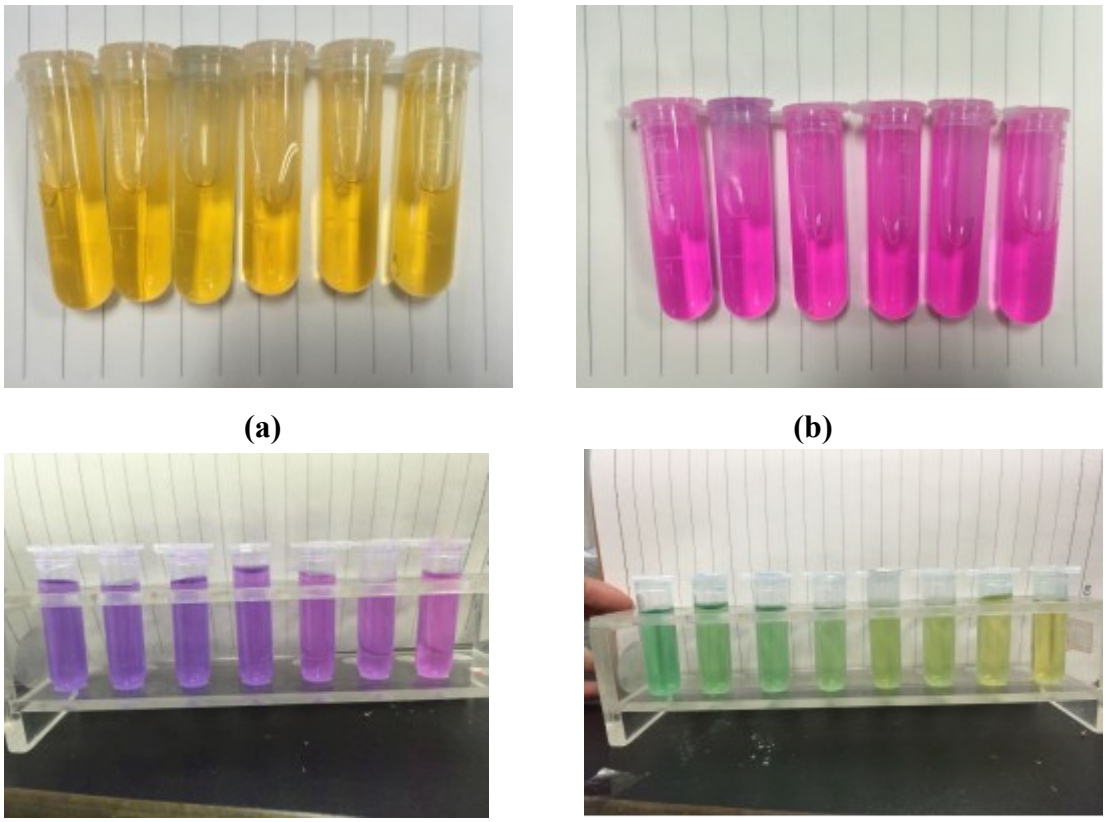


Fig. S15 The selective adsorption capability of compound **1** toward the mixed dyes: MO and MB; RhB and MB.



(a) **(b)**

(c) **(d)**

Fig S16 (a) The photographs of initial MO solution; (b) The photographs of initial RhB solution; (c) The photographs of dye selective adsorption of compound **2** toward the mixed dyes: RhB and MB**;** (d)The photographs of dye selective adsorption of compound **2** toward the mixed dyes: MO and MB