

Support Information

Long Rigid ligand induced basket-type phosphomolybdate photo-/ electro-catalytic materials

Fan-xue Meng^{a,b}, Jing-hua Lv,^a Kai Yu,^{a,b*} Mao-lin Zhang,^{a,b} Kun-peng Wang,^{a,b} Bai-bin Zhou^{a,b*}

1. Structural figures

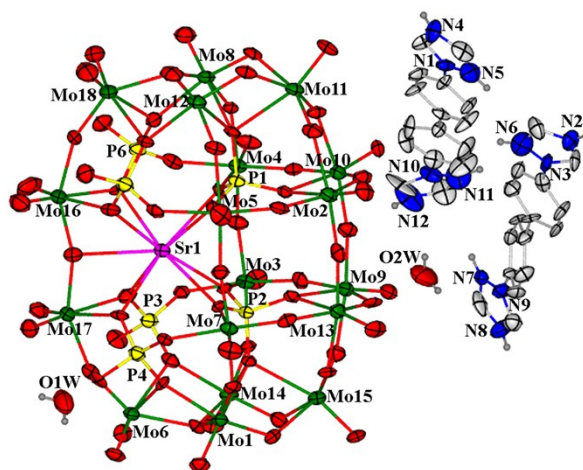


Figure S1 ORTEP view of the basic units in compound 1 with 50% thermal ellipsoid.

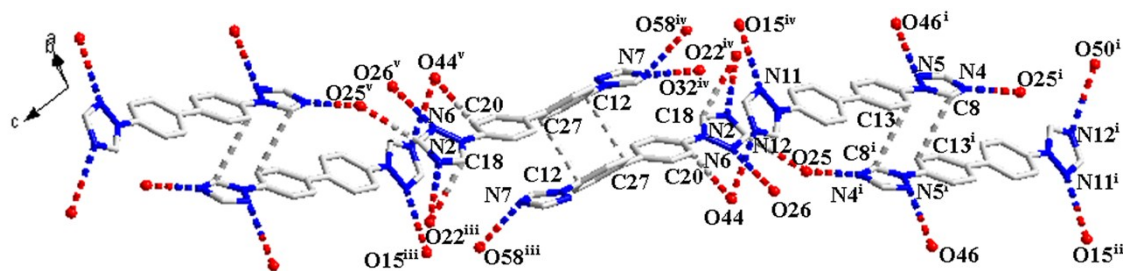


Figure S2 The supramolecular organic ligand dimeric chain linked by hydrogen bond and π - π interactions. [Symmetry code: (i) $-x, 1-y, -z$; (ii) $-1-x, -y, -z$; (iii) $1-x, -y, 1-z$; (iv) $1+x, 1+y, z$; (v) $2-x, 1-y, 1-z$]

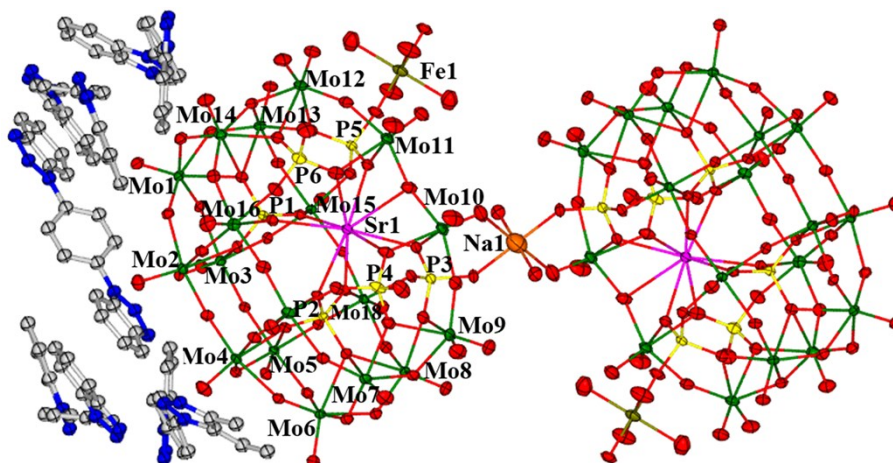


Figure S3 ORTEP view of the basic units in compound **2** with 50% thermal ellipsoid.

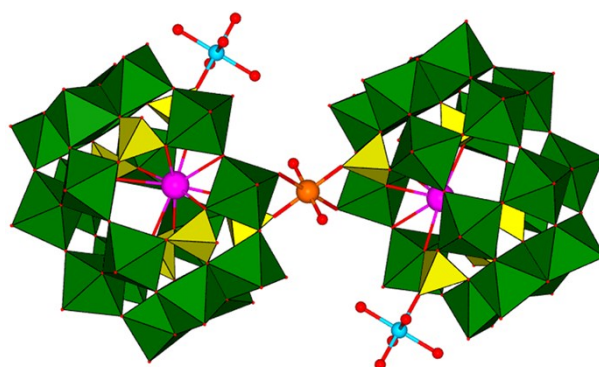


Figure S4 The basket dimeric cluster linked by $\{\text{Na}(\text{H}_2\text{O})_2\}$.

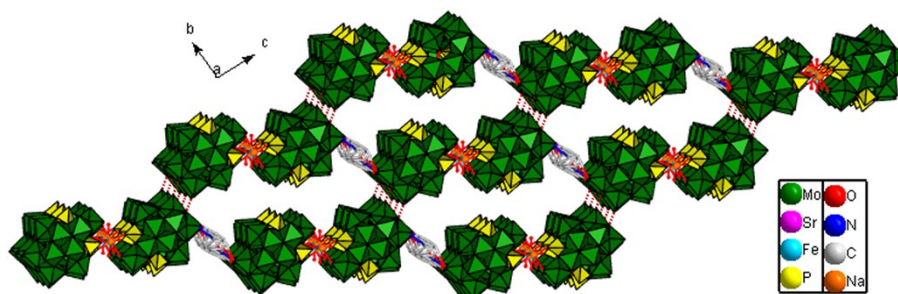


Figure S5 The 3D supramolecular network of compound **2**.

2. Structural data

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

Mo(1)-O(60)	1.667(8)	Mo(2)-O(44)	1.668(9)	Mo(3)-O(41)	1.664(9)
Mo(1)-O(3)	1.772(9)	Mo(2)-O(61)	1.856(9)	Mo(3)-O(17)	1.854(9)
Mo(1)-O(45)	1.788(8)	Mo(2)-O(2)	1.890(9)	Mo(3)-O(6)	1.895(9)
Mo(1)-O(49)	2.054(9)	Mo(2)-O(26)	1.956(9)	Mo(3)-O(9)	2.026(8)
Mo(1)-O(23)	2.143(8)	Mo(2)-O(24)	2.067(9)	Mo(3)-O(28)	2.037(8)
Mo(1)-O(16)	2.447(8)	Mo(2)-O(62)	2.319(9)	Mo(3)-O(20)	2.246(8)
Mo(4)-O(30)	1.666(9)	Mo(5)-O(63)	1.672(10)	Mo(6)-O(38)	1.683(9)

Mo(4)-O(6)	1.846(9)	Mo(5)-O(13)	1.886(8)	Mo(6)-O(34)	1.708(9)
Mo(4)-O(8)	1.894(9)	Mo(5)-O(61)	1.903(9)	Mo(6)-O(15)	1.851(9)
Mo(4)-O(19)	2.050(9)	Mo(5)-O(36)	2.036(8)	Mo(6)-O(49)	2.072(8)
Mo(4)-O(4)	2.063(8)	Mo(5)-O(43)	2.044(9)	Mo(6)-O(27)	2.321(8)
Mo(4)-O(21)	2.223(8)	Mo(5)-O(37)	2.235(8)	Mo(6)-O(23)	2.332(9)
Mo(7)-O(51)	1.660(8)	Mo(8)-O(53)	1.677(9)	Mo(9)-O(70)	1.687(9)
Mo(7)-O(13)	1.843(8)	Mo(8)-O(4)	1.788(8)	Mo(9)-O(17)	1.899(9)
Mo(7)-O(11)	1.877(9)	Mo(8)-O(57)	1.806(8)	Mo(9)-O(1)	1.906(9)
Mo(7)-O(40)	2.055(8)	Mo(8)-O(33)	2.038(9)	Mo(9)-O(35)	1.940(9)
Mo(7)-O(3)	2.067(8)	Mo(8)-O(39)	2.124(9)	Mo(9)-O(64)	2.046(9)
Mo(7)-O(52)	2.231(8)	Mo(8)-O(5)	2.392(8)	Mo(9)-O(14)	2.305(8)
Mo(10)-O(25)	1.686(8)	Mo(11)-O(55)	1.691(8)	Mo(12)-O(59)	1.662(9)
Mo(10)-O(1)	1.865(9)	Mo(11)-O(73)	1.796(9)	Mo(12)-O(36)	1.792(9)
Mo(10)-O(26)	1.887(9)	Mo(11)-O(24)	1.797(9)	Mo(12)-O(47)	1.812(9)
Mo(10)-O(8)	1.888(9)	Mo(11)-O(47)	2.083(9)	Mo(12)-O(33)	2.047(9)
Mo(10)-O(73)	2.121(8)	Mo(11)-O(57)	2.080(9)	Mo(12)-O(56)	2.130(9)
Mo(10)-O(62)	2.271(8)	Mo(11)-O(5)	2.411(8)	Mo(12)-O(5)	2.420(8)
Mo(13)-O(54)	1.685(9)	Mo(14)-O(68)	1.662(9)	Mo(15)-O(69)	1.676(9)
Mo(13)-O(2)	1.870(9)	Mo(14)-O(9)	1.796(8)	Mo(15)-O(64)	1.805(9)
Mo(13)-O(11)	1.904(9)	Mo(14)-O(46)	1.806(9)	Mo(15)-O(7)	1.822(9)
Mo(13)-O(35)	1.912(9)	Mo(14)-O(49)	2.069(8)	Mo(15)-O(46)	2.070(10)
Mo(13)-O(7)	2.089(8)	Mo(14)-O(27)	2.161(9)	Mo(15)-O(45)	2.071(9)
Mo(13)-O(14)	2.286(8)	Mo(14)-O(16)	2.399(8)	Mo(15)-O(16)	2.422(8)
Mo(16)-O(71)	1.674(10)	Mo(17)-O(22)	1.684(9)	Mo(18)-O(48)	1.683(10)
Mo(16)-O(67)	1.703(11)	Mo(17)-O(32)	1.724(9)	Mo(18)-O(72)	1.723(11)
Mo(16)-O(18)	1.894(8)	Mo(17)-O(18)	1.918(9)	Mo(18)-O(10)	1.837(8)
Mo(16)-O(10)	1.973(8)	Mo(17)-O(15)	1.971(9)	Mo(18)-O(33)	2.085(9)
Mo(16)-O(65)	2.266(10)	Mo(17)-O(31)	2.280(9)	Mo(18)-O(39)	2.337(9)
Mo(16)-O(29)	2.270(9)	Mo(17)-O(12)	2.286(9)	Mo(18)-O(56)	2.349(9)
Sr(1)-O(12)	2.576(8)	Sr(1)-O(65)	2.598(9)	Sr(1)-O(31)	2.599(9)
Sr(1)-O(29)	2.616(8)	Sr(1)-O(52)	2.670(8)	Sr(1)-O(21)	2.672(7)
Sr(1)-O(37)	2.672(8)	Sr(1)-O(20)	2.676(8)	Sr(1)-O(18)	2.807(9)
P(1)-O(37)	1.512(8)	P(2)-O(52)	1.516(9)	P(3)-O(31)	1.501(9)
P(1)-O(5)	1.578(8)	P(2)-O(20)	1.517(8)	P(3)-O(28)	1.536(9)
P(1)-O(21)	1.517(9)	P(2)-O(14)	1.532(9)	P(3)-O(27)	1.555(9)
P(1)-O(62)	1.535(9)	P(2)-O(16)	1.571(8)	P(3)-O(42)	1.586(9)
P(4)-O(12)	1.511(9)	P(5)-O(29)	1.501(9)	P(6)-O(65)	1.517(10)
P(4)-O(40)	1.544(9)	P(5)-O(19)	1.535(10)	P(6)-O(43)	1.553(9)
P(4)-O(23)	1.565(9)	P(5)-O(39)	1.544(9)	P(6)-O(56)	1.570(9)
P(4)-O(58)	1.567(8)	P(5)-O(50)	1.559(9)	P(6)-O(66)	1.569(10)
O(60)-Mo(1)-O(3)	104.7(4)	O(44)-Mo(2)-O(61)	101.4(4)	O(41)-Mo(3)-O(17)	101.4(4)
O(60)-Mo(1)-O(45)	102.3(4)	O(44)-Mo(2)-O(2)	98.4(4)	O(41)-Mo(3)-O(6)	98.1(4)
O(60)-Mo(1)-O(49)	98.4(4)	O(44)-Mo(2)-O(26)	102.5(4)	O(41)-Mo(3)-O(9)	94.8(4)
O(60)-Mo(1)-O(23)	98.2(4)	O(44)-Mo(2)-O(24)	95.2(4)	O(41)-Mo(3)-O(28)	96.6(4)
O(60)-Mo(1)-O(16)	169.9(4)	O(44)-Mo(2)-O(62)	171.8(4)	O(41)-Mo(3)-O(20)	173.7(4)

O(30)-Mo(4)-O(6)	100.0(4)	O(63)-Mo(5)-O(13)	98.6(4)	O(38)-Mo(6)-O(34)	102.8(5)
O(30)-Mo(4)-O(8)	100.1(4)	O(63)-Mo(5)-O(61)	101.1(4)	O(38)-Mo(6)-O(15)	104.6(4)
O(30)-Mo(4)-O(19)	96.9(4)	O(63)-Mo(5)-O(36)	94.0(4)	O(38)-Mo(6)-O(49)	97.5(4)
O(30)-Mo(4)-O(4)	92.2(4)	O(63)-Mo(5)-O(43)	96.2(4)	O(38)-Mo(6)-O(27)	85.7(4)
O(30)-Mo(4)-O(21)	172.7(4)	O(63)-Mo(5)-O(37)	173.9(4)	O(38)-Mo(6)-O(23)	164.1(4)
O(51)-Mo(7)-O(13)	99.4(4)	O(53)-Mo(8)-O(4)	104.3(4)	O(70)-Mo(9)-O(17)	101.8(4)
O(51)-Mo(7)-O(11)	102.8(4)	O(53)-Mo(8)-O(57)	101.5(4)	O(70)-Mo(9)-O(1)	99.7(4)
O(51)-Mo(7)-O(40)	94.1(4)	O(53)-Mo(8)-O(33)	98.3(4)	O(70)-Mo(9)-O(35)	101.5(4)
O(51)-Mo(7)-O(3)	92.5(4)	O(53)-Mo(8)-O(39)	98.0(4)	O(70)-Mo(9)-O(64)	92.4(4)
O(51)-Mo(7)-O(52)	170.8(4)	O(53)-Mo(8)-O(5)	170.7(4)	O(70)-Mo(9)-O(14)	170.4(4)
O(25)-Mo(10)-O(1)	100.3(4)	O(55)-Mo(11)-O(73)	103.0(4)	O(59)-Mo(12)-O(36)	103.2(4)
O(25)-Mo(10)-O(26)	102.3(4)	O(55)-Mo(11)-O(24)	105.0(4)	O(59)-Mo(12)-O(47)	100.6(4)
O(25)-Mo(10)-O(8)	99.1(4)	O(55)-Mo(11)-O(47)	97.7(4)	O(59)-Mo(12)-O(33)	99.8(4)
O(25)-Mo(10)-O(73)	90.7(4)	O(55)-Mo(11)-O(57)	94.0(4)	O(59)-Mo(12)-O(56)	99.6(4)
O(25)-Mo(10)-O(62)	168.1(4)	O(55)-Mo(11)-O(5)	162.9(4)	O(59)-Mo(12)-O(5)	170.7(4)
O(54)-Mo(13)-O(2)	99.8(4)	O(68)-Mo(14)-O(9)	104.8(4)	O(69)-Mo(15)-O(64)	105.1(4)
O(54)-Mo(13)-O(11)	100.8(4)	O(68)-Mo(14)-O(46)	102.5(4)	O(69)-Mo(15)-O(7)	103.9(5)
O(54)-Mo(13)-O(35)	100.5(5)	O(68)-Mo(14)-O(49)	97.4(4)	O(69)-Mo(15)-O(46)	97.4(4)
O(54)-Mo(13)-O(7)	92.1(4)	O(68)-Mo(14)-O(27)	98.0(4)	O(69)-Mo(15)-O(45)	96.0(4)
O(54)-Mo(13)-O(14)	169.5(4)	O(68)-Mo(14)-O(16)	170.4(4)	O(69)-Mo(15)-O(16)	163.9(4)
O(71)-Mo(16)-O(67)	101.0(6)	O(22)-Mo(17)-O(32)	103.4(5)	O(48)-Mo(18)-O(72)	102.5(5)
O(71)-Mo(16)-O(18)	100.5(4)	O(22)-Mo(17)-O(18)	100.4(4)	O(48)-Mo(18)-O(10)	103.5(5)
O(71)-Mo(16)-O(10)	97.5(4)	O(22)-Mo(17)-O(15)	97.2(4)	O(48)-Mo(18)-O(33)	98.3(4)
O(71)-Mo(16)-O(65)	92.5(5)	O(22)-Mo(17)-O(31)	88.8(4)	O(48)-Mo(18)-O(39)	87.2(4)
O(71)-Mo(16)-O(29)	170.0(5)	O(22)-Mo(17)-O(12)	165.7(4)	O(48)-Mo(18)-O(56)	164.9(4)
O(37)-P(1)-O(21)	107.5(5)	O(52)-P(2)-O(20)	106.9(5)	O(31)-P(3)-O(28)	110.5(5)
O(37)-P(1)-O(62)	110.9(5)	O(52)-P(2)-O(14)	112.6(5)	O(31)-P(3)-O(27)	107.7(5)
O(37)-P(1)-O(5)	110.2(5)	O(52)-P(2)-O(16)	109.7(5)	O(31)-P(3)-O(42)	112.5(5)
O(12)-P(4)-O(40)	110.8(5)	O(29)-P(5)-O(19)	109.8(5)	O(65)-P(6)-O(43)	111.6(5)
O(12)-P(4)-O(23)	110.2(5)	O(29)-P(5)-O(39)	109.5(5)	O(65)-P(6)-O(56)	108.3(5)
O(12)-P(4)-O(58)	108.2(5)	O(29)-P(5)-O(50)	111.3(5)	O(65)-P(6)-O(66)	109.7(6)
O(12)-Sr(1)-O(65)	81.8(3)	O(12)-Sr(1)-O(29)	117.6(3)	O(12)-Sr(1)-O(20)	101.8(2)
O(12)-Sr(1)-O(31)	66.6(3)	O(12)-Sr(1)-O(52)	72.6(3)	O(12)-Sr(1)-O(18)	58.9(3)
O(12)-Sr(1)-O(37)	119.0(3)	O(12)-Sr(1)-O(21)	169.2(3)		

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

Mo(1)-O(22)	1.673(5)	Mo(2)-O(25)	1.687(5)	Mo(3)-O(71)	1.682(5)
Mo(1)-O(4)	1.790(4)	Mo(2)-O(43)	1.883(5)	Mo(3)-O(1)	1.868(5)
Mo(1)-O(5)	1.834(5)	Mo(2)-O(6)	1.886(5)	Mo(3)-O(35)	1.912(5)
Mo(1)-O(14)	2.021(5)	Mo(2)-O(10)	1.956(5)	Mo(3)-O(10)	1.938(5)
Mo(1)-O(66)	2.078(5)	Mo(2)-O(4)	2.080(5)	Mo(3)-O(5)	2.074(5)
Mo(1)-O(19)	2.425(5)	Mo(2)-O(26)	2.289(4)	Mo(3)-O(26)	2.281(4)
Mo(4)-O(9)	1.682(5)	Mo(5)-O(23)	1.681(5)	Mo(6)-O(15)	1.665(5)
Mo(4)-O(6)	1.868(5)	Mo(5)-O(1)	1.879(5)	Mo(6)-O(28)	1.788(5)
Mo(4)-O(60)	1.891(5)	Mo(5)-O(36)	1.887(4)	Mo(6)-O(2)	1.817(5)

Mo(4)-O(3)	1.947(5)	Mo(5)-O(3)	1.966(5)	Mo(6)-O(52)	2.040(5)
Mo(4)-O(2)	2.068(5)	Mo(5)-O(28)	2.072(5)	Mo(6)-O(46)	2.102(5)
Mo(4)-O(31)	2.300(4)	Mo(5)-O(31)	2.270(4)	Mo(6)-O(24)	2.413(5)
Mo(7)-O(65)	1.679(5)	Mo(8)-O(72)	1.674(5)	Mo(9)-O(32)	1.668(6)
Mo(7)-O(41)	1.788(5)	Mo(8)-O(33)	1.777(5)	Mo(9)-O(30)	1.702(6)
Mo(7)-O(46)	1.793(5)	Mo(8)-O(52)	1.814(5)	Mo(9)-O(57)	1.851(5)
Mo(7)-O(53)	2.061(5)	Mo(8)-O(53)	2.051(5)	Mo(9)-O(53)	2.054(5)
Mo(7)-O(54)	2.163(5)	Mo(8)-O(55)	2.123(5)	Mo(9)-O(54)	2.333(5)
Mo(7)-O(24)	2.414(5)	Mo(8)-O(24)	2.415(5)	Mo(9)-O(55)	2.346(5)
Mo(10)-O(69)	1.688(6)	Mo(11)-O(64)	1.679(6)	Mo(12)-O(20)	1.676(6)
Mo(10)-O(70)	1.709(6)	Mo(11)-O(68)	1.702(6)	Mo(12)-O(16)	1.707(5)
Mo(10)-O(40)	1.911(5)	Mo(11)-O(40)	1.899(5)	Mo(12)-O(61)	1.833(5)
Mo(10)-O(57)	1.983(5)	Mo(11)-O(61)	2.008(5)	Mo(12)-O(12)	2.048(5)
Mo(10)-O(48)	2.237(5)	Mo(11)-O(73)	2.248(5)	Mo(12)-O(29)	2.318(5)
Mo(10)-O(8)	2.261(5)	Mo(11)-O(11)	2.276(5)	Mo(12)-O(18)	2.355(5)
Mo(13)-O(7)	1.680(5)	Mo(14)-O(21)	1.674(5)	Mo(15)-O(47)	1.677(4)
Mo(13)-O(44)	1.787(5)	Mo(14)-O(51)	1.786(5)	Mo(15)-O(34)	1.865(5)
Mo(13)-O(66)	1.800(5)	Mo(14)-O(14)	1.814(5)	Mo(15)-O(35)	1.873(5)
Mo(13)-O(12)	2.064(5)	Mo(14)-O(12)	2.037(5)	Mo(15)-O(39)	2.039(5)
Mo(13)-O(18)	2.119(5)	Mo(14)-O(29)	2.141(5)	Mo(15)-O(44)	2.043(5)
Mo(13)-O(19)	2.425(4)	Mo(14)-O(19)	2.402(5)	Mo(15)-O(13)	2.219(4)
Mo(16)-O(62)	1.672(5)	Mo(17)-O(50)	1.666(5)	Mo(18)-O(56)	1.679(5)
Mo(16)-O(42)	1.875(5)	Mo(17)-O(42)	1.856(5)	Mo(18)-O(36)	1.870(5)
Mo(16)-O(43)	1.880(5)	Mo(17)-O(60)	1.881(5)	Mo(18)-O(34)	1.883(5)
Mo(16)-O(51)	2.014(5)	Mo(17)-O(41)	2.032(5)	Mo(18)-O(45)	2.033(5)
Mo(16)-O(59)	2.054(5)	Mo(17)-O(49)	2.062(5)	Mo(18)-O(33)	2.037(5)
Mo(16)-O(38)	2.237(4)	Mo(17)-O(37)	2.208(4)	Mo(18)-O(17)	2.215(5)
P(1)-O(38)	1.515(5)	P(2)-O(37)	1.520(5)	P(3)-O(48)	1.528(5)
P(1)-O(13)	1.524(5)	P(2)-O(17)	1.521(5)	P(3)-O(45)	1.532(5)
P(1)-O(26)	1.535(5)	P(2)-O(31)	1.538(5)	P(3)-O(58)	1.536(5)
P(1)-O(19)	1.567(5)	P(2)-O(24)	1.570(5)	P(3)-O(55)	1.561(5)
P(4)-O(49)	1.514(6)	P(5)-O(63)	1.514(5)	P(6)-O(11)	1.513(6)
P(4)-O(8)	1.517(5)	P(5)-O(73)	1.517(5)	P(6)-O(59)	1.520(5)
P(4)-O(27)	1.553(6)	P(5)-O(39)	1.530(5)	P(6)-O(67)	1.551(5)
P(4)-O(54)	1.556(6)	P(5)-O(18)	1.564(5)	P(6)-O(29)	1.559(5)
Fe(1)-O(63)	1.882(5)	Sr(1)-O(11)	2.573(5)	Sr(1)-O(37)	2.667(4)
Fe(1)-O(63)#1	1.882(5)	Sr(1)-O(73)	2.580(5)	Sr(1)-O(38)	2.706(5)
Fe(1)-O(2W)	2.036(6)	Sr(1)-O(48)	2.586(5)	Sr(1)-O(40)	2.829(5)
Fe(1)-O(2W)#1	2.036(6)	Sr(1)-O(8)	2.586(5)	Sr(1)-O(17)	2.663(5)
Fe(1)-O(3W)	2.040(6)	Fe(1)-O(3W)#1	2.040(6)	Sr(1)-O(13)	2.644(5)
O(58)-Na(1)	1.952(5)	O(69)-Na(1)	2.575(7)	O(1W)-Na(1)	1.954(9)
Na(1)-O(58)#3	1.952(5)	Na(1)-O(1W)#3	1.954(9)	Na(1)-O(69)#3	2.575(7)
O(22)-Mo(1)-O(4)	104.6(2)	O(25)-Mo(2)-O(43)	103.0(2)	O(71)-Mo(3)-O(1)	101.5(2)
O(22)-Mo(1)-O(5)	103.1(2)	O(25)-Mo(2)-O(6)	99.5(2)	O(71)-Mo(3)-O(35)	99.7(2)
O(22)-Mo(1)-O(14)	99.2(2)	O(25)-Mo(2)-O(10)	98.2(2)	O(71)-Mo(3)-O(10)	100.9(2)

O(22)-Mo(1)-O(66)	96.7(2)	O(25)-Mo(2)-O(4)	94.8(2)	O(71)-Mo(3)-O(5)	92.9(2)
O(22)-Mo(1)-O(19)	166.0(2)	O(25)-Mo(2)-O(26)	168.5(2)	O(71)-Mo(3)-O(26)	169.5(2)
O(9)-Mo(4)-O(6)	100.6(2)	O(23)-Mo(5)-O(1)	100.2(2)	O(15)-Mo(6)-O(28)	106.3(2)
O(9)-Mo(4)-O(60)	101.6(2)	O(23)-Mo(5)-O(36)	98.9(2)	O(15)-Mo(6)-O(2)	103.7(2)
O(9)-Mo(4)-O(3)	100.1(2)	O(23)-Mo(5)-O(3)	102.3(2)	O(15)-Mo(6)-O(52)	97.0(2)
O(9)-Mo(4)-O(2)	93.8(2)	O(23)-Mo(5)-O(28)	93.8(2)	O(15)-Mo(6)-O(46)	94.5(2)
O(9)-Mo(4)-O(31)	169.6(2)	O(23)-Mo(5)-O(31)	171.7(2)	O(15)-Mo(6)-O(24)	163.0(2)
O(65)-Mo(7)-O(41)	103.6(3)	O(72)-Mo(8)-O(33)	103.6(2)	O(32)-Mo(9)-O(30)	104.4(3)
O(65)-Mo(7)-O(46)	103.5(2)	O(72)-Mo(8)-O(52)	100.8(2)	O(32)-Mo(9)-O(57)	103.9(3)
O(65)-Mo(7)-O(53)	99.3(2)	O(72)-Mo(8)-O(53)	100.2(2)	O(32)-Mo(9)-O(53)	99.4(2)
O(65)-Mo(7)-O(54)	96.9(2)	O(72)-Mo(8)-O(55)	98.9(2)	O(32)-Mo(9)-O(54)	85.8(2)
O(65)-Mo(7)-O(24)	171.9(2)	O(72)-Mo(8)-O(24)	171.5(2)	O(32)-Mo(9)-O(55)	165.3(2)
O(69)-Mo(10)-O(70)	102.6(3)	O(64)-Mo(11)-O(68)	102.9(3)	O(20)-Mo(12)-O(16)	102.5(3)
O(69)-Mo(10)-O(40)	99.0(3)	O(64)-Mo(11)-O(40)	101.4(3)	O(20)-Mo(12)-O(61)	104.0(3)
O(69)-Mo(10)-O(57)	98.2(3)	O(64)-Mo(11)-O(61)	94.5(2)	O(20)-Mo(12)-O(12)	99.1(2)
O(69)-Mo(10)-O(48)	90.2(2)	O(64)-Mo(11)-O(73)	91.5(2)	O(20)-Mo(12)-O(29)	85.7(2)
O(69)-Mo(10)-O(8)	167.2(3)	O(64)-Mo(11)-O(11)	167.0(2)	O(20)-Mo(12)-O(18)	164.9(2)
O(7)-Mo(13)-O(44)	103.6(2)	O(21)-Mo(14)-O(51)	103.1(3)	O(47)-Mo(15)-O(34)	98.9(2)
O(7)-Mo(13)-O(66)	103.3(2)	O(21)-Mo(14)-O(14)	101.8(3)	O(47)-Mo(15)-O(35)	101.2(2)
O(7)-Mo(13)-O(12)	99.9(2)	O(21)-Mo(14)-O(12)	99.8(2)	O(47)-Mo(15)-O(39)	95.1(2)
O(7)-Mo(13)-O(18)	97.0(2)	O(21)-Mo(14)-O(29)	97.3(2)	O(47)-Mo(15)-O(44)	93.0(2)
O(7)-Mo(13)-O(19)	171.9(2)	O(21)-Mo(14)-O(19)	172.2(2)	O(47)-Mo(15)-O(13)	172.0(2)
O(62)-Mo(16)-O(42)	99.5(2)	O(50)-Mo(17)-O(42)	98.7(2)	O(56)-Mo(18)-O(36)	99.9(2)
O(62)-Mo(16)-O(43)	101.0(2)	O(50)-Mo(17)-O(60)	100.6(2)	O(56)-Mo(18)-O(34)	100.0(2)
O(62)-Mo(16)-O(51)	95.8(2)	O(50)-Mo(17)-O(41)	93.1(2)	O(56)-Mo(18)-O(45)	96.0(2)
O(62)-Mo(16)-O(59)	96.1(2)	O(50)-Mo(17)-O(49)	96.0(2)	O(56)-Mo(18)-O(33)	93.3(2)
O(62)-Mo(16)-O(38)	173.5(2)	O(50)-Mo(17)-O(37)	172.6(2)	O(56)-Mo(18)-O(17)	173.9(2)
O(38)-P(1)-O(13)	108.3(3)	O(37)-P(2)-O(17)	107.4(3)	O(48)-P(3)-O(45)	109.8(3)
O(38)-P(1)-O(26)	110.9(3)	O(37)-P(2)-O(31)	110.4(3)	O(48)-P(3)-O(58)	113.0(3)
O(38)-P(1)-O(19)	109.9(3)	O(37)-P(2)-O(24)	110.2(3)	O(48)-P(3)-O(55)	108.7(3)
O(49)-P(4)-O(8)	110.7(3)	O(63)-P(5)-O(73)	110.5(3)	O(11)-P(6)-O(59)	111.9(3)
O(49)-P(4)-O(27)	106.8(3)	O(63)-P(5)-O(39)	108.7(3)	O(11)-P(6)-O(67)	111.0(3)
O(49)-P(4)-O(54)	112.2(3)	O(63)-P(5)-O(18)	108.2(3)	O(11)-P(6)-O(29)	109.2(3)
O(63)-Fe(1)-O(2W)	92.6(2)	O(1W)#3-Na(1)-O(1W)	179.999(1)	O(11)-Sr(1)-O(13)	101.74(16)
O(63)#1-Fe(1)-O(2W)	87.4(2)	O(1W)#3-Na(1)-O(58)#3	87.4(3)	O(11)-Sr(1)-O(17)	168.92(16)
O(63)-Fe(1)-O(3W)#1	88.2(2)	O(1W)-Na(1)-O(58)#3	92.6(3)	O(11)-Sr(1)-O(40)	59.84(16)
O(63)-Fe(1)-O(2W)#1	87.4(2)	O(1W)#3-Na(1)-O(58)	92.6(3)	O(11)-Sr(1)-O(73)	65.60(15)
O(63)#1-Fe(1)-O(2W)#1	92.6(2)	O(1W)-Na(1)-O(58)	87.4(3)	O(11)-Sr(1)-O(48)	118.06(16)
O(63)#1-Fe(1)-O(3W)#1	91.8(2)	O(1W)#3-Na(1)-O(69)	79.6(3)	O(11)-Sr(1)-O(8)	81.23(16)
O(63)-Fe(1)-O(63)#1	180.0(3)	O(1W)-Na(1)-O(69)	100.4(3)	O(11)-Sr(1)-O(38)	71.99(16)
O(63)-Fe(1)-O(3W)	91.8(2)	O(1W)#3-Na(1)-O(69)#3	100.4(3)	O(11)-Sr(1)-O(37)	117.36(15)
O(63)#1-Fe(1)-O(3W)	88.2(2)	O(1W)-Na(1)-O(69)#3	79.6(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+2,-z #2 -x,-y+1,-z+1 #3 -x,-y+2,-z

Table S3 Bond valence sum calculations for Mo atoms in **1**

	Mo ^V	Mo ^{VI}	Average
Mo1	5.89	6.17	6.03
Mo2	5.69	5.96	5.83
Mo3	5.94	5.68	5.81
Mo4	5.63	5.89	5.76
Mo5	5.51	5.76	5.64
Mo6	5.72	6.00	5.86
Mo7	5.69	5.96	5.83
Mo8	5.81	6.08	5.95
Mo9	5.52	5.79	5.66
Mo10	5.71	5.98	5.85
Mo11	5.72	6.00	5.86
Mo12	5.81	6.08	5.95
Mo13	5.63	5.89	5.76
Mo14	5.75	6.02	5.89
Mo15	5.71	5.93	5.85
Mo16	5.96	6.24	6.10
Mo17	5.82	6.10	5.96
Mo18	5.87	6.15	5.79
Sum	5.74	6.00	5.87

Table S4 Bond valence sum calculations for Mo atoms in **2**

	Mo ^V	Mo ^{VI}	Average
Mo1	5.81	6.08	5.95
Mo2	5.54	5.80	5.67
Mo3	5.59	5.86	5.73
Mo4	5.62	5.88	5.75
Mo5	5.58	5.84	5.71
Mo6	5.85	6.12	5.99
Mo7	5.74	6.01	5.88
Mo8	5.80	6.07	5.94
Mo9	5.83	6.11	5.97
Mo10	5.84	6.11	5.98
Mo11	5.87	6.14	6.01
Mo12	5.84	6.12	5.98
Mo13	5.76	6.03	5.90
Mo14	5.78	6.05	5.92
Mo15	5.64	5.90	5.77
Mo16	5.62	5.88	5.75
Mo17	5.69	5.95	5.82
Mo18	5.61	5.87	5.74
Sum	5.72	6.00	5.86

Table S5 Selected Hydrogen Bond Lengths () and Bond Angles (°) of complexes **1** and **2**

D-H...A	d(D-H)	d(H...A)	<D-H...A	d(D...A)	Symmetry	
1	N4-H4...O25	0.860	2.095	153.04	2.888	[-x, -y+1, -z]
	N5-H5...O46	0.860	2.628	152.04	3.412	[x, y+1, z]
	O1W-H1WA...O66	0.850	2.112	152.59	2.893	
	O1W-H1WB...O66	0.850	2.150	132.19	2.793	[-x, -y, -z+1]
	N6-H6...O26	0.860	2.524	158.49	3.339	
	O2W-H2WA	0.850				
	O2W-H2WB...O42	0.850	1.939	127.33	2.546	[x+1, y+1, z]
	O2W-H2WB...O22	0.850	2.579	142.43	3.293	[x+1, y+1, z]
	N7-H7...O32	0.860	2.059	154.96	2.862	[-x+1, -y, -z+1]
	N7-H7...O58	0.860	2.587	110.38	2.997	[-x+1, -y, -z+1]
	N8-H8A...O72	0.860	2.636	161.41	3.462	[x+1, y, z]
	N11-H11...O15	0.860	2.644	158.00	3.456	[x+1, y+1, z]
	N12-H12...O50	0.860	2.216	157.83	3.030	[x+1, y, z]
2	O2W-H2WA...O16	0.850	1.842	166.01	2.675	
	O2W-H2WB...N4	0.850	2.441	168.99	3.279	[x, y+1, z]
	O3W-H3WA...O64	0.850	2.076	149.25	2.840	[-x+1, -y+2, -z]
	O3W-H3WB...O7W	0.850	2.50	89.4	2.633	
	N1-H1...O27	0.860	2.469	127.59	3.070	[x+1, y, z]
	N1-H1...O32	0.860	2.533	150.92	3.311	[x+1, y, z]
	N4-H4A...O7	0.860	2.371	133.23	3.026	[x, y-1, z]
	N4-H4A...O30	0.860	2.591	128.62	3.199	[x+1, y-1, z]
	N4-H4A...O2W	0.860	2.653	130.65	3.279	[x, y-1, z]
	N6-H6...O5	0.860	1.907	170.91	2.759	[x, y-1, z]
	N14-H14...O23	0.860	2.399	156.54	3.206	[x+1, y-1, z]
	N10-H10A...O22	0.860	2.095	133.70	2.760	[-x+1, -y+1, -z+1]
	N10-H10A...O15	0.860	2.413	127.46	3.014	[-x, -y+1, -z+1]
	N16-H16A...O2	0.860	2.219	169.15	3.068	[-x, -y+1, -z+1]
	O9W-H9WA...O49	0.850	2.317	155.25	3.110	
	O9W-H9WB...O59	0.850	2.331	156.54	3.130	
	O1W-H1WA...O58	0.850	2.104	142.05	2.823	[-x, -y+2, -z]
	O1W-H1WA...O30	0.850	2.542	123.80	3.096	[-x, -y+2, -z]
	O1W-H1WA...O57	0.850	2.656	120.86	3.177	[-x, -y+2, -z]
	O1W-H1WB...O58	0.850	2.268	111.66	2.700	
	O1W-H1WB...O69	0.850	2.286	133.58	2.937	[-x, -y+2, -z]
	O4W-H4WA...N5	0.850	2.061	124.06	2.633	[x-1, y, z]
	O4W-H4WA...N14	0.850	2.192	142.14	2.910	[x-1, y, z]
	O4W-H4WB...O9	0.850	2.256	147.95	3.010	[-x, -y+1, -z+1]
	O4W-H4WB...O3	0.850	2.329	135.82	2.998	[-x, -y+1, -z+1]
	O5W-H5WA...O73	0.850	2.229	162.96	3.052	
	O5W-H5WA...O64	0.850	2.573	122.87	3.117	
	O5W-H5WB	0.850				
	O6W-H6WA...O70	0.850	2.151	147.25	2.902	
	O6W-H6WB...O67	0.850	2.060	116.05	2.550	[-x+1, -y+1, -z]
	O6W-H6WB...O68	0.850	2.305	150.50	3.073	[-x+1, -y+1, -z]

O7W-H7WA	0.850				
O7W-H7WB	0.850				
O8W-H8WA...O70	0.850	2.114	169.06	2.953	[x, y, z+1]
O8W-H8WB...N12	0.850	2.435	163.36	3.259	[-x+1, -y+1, -z+1]

3. Physical characterization

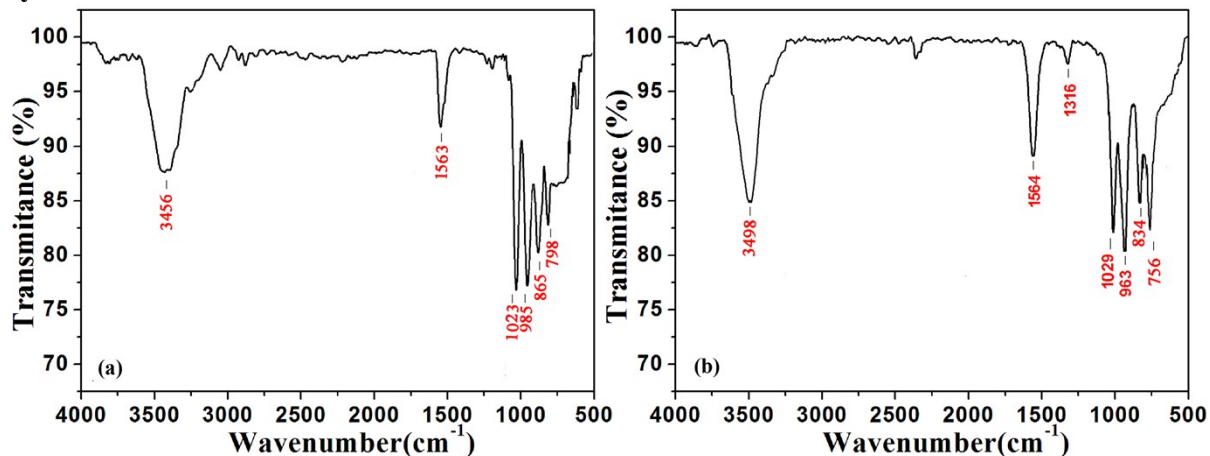


Fig. S6 IR spectra of (a) compound 1 and (b) compound 2.

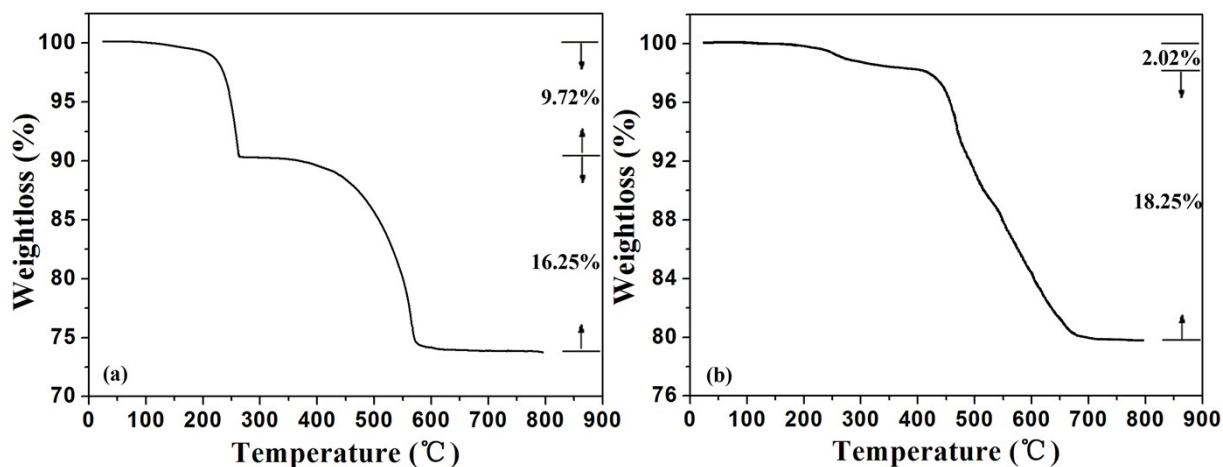


Fig. S7 TG curves of (a) compound 1 and (b) compound 2.

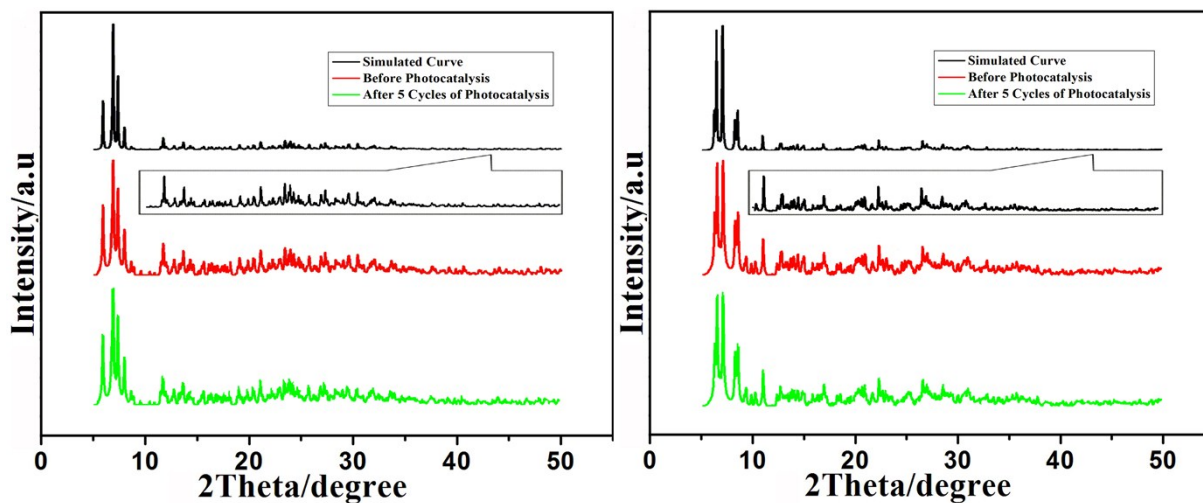


Fig. S8 The PXRD contrast curves of (a) compound 1 and (b) compound 2.

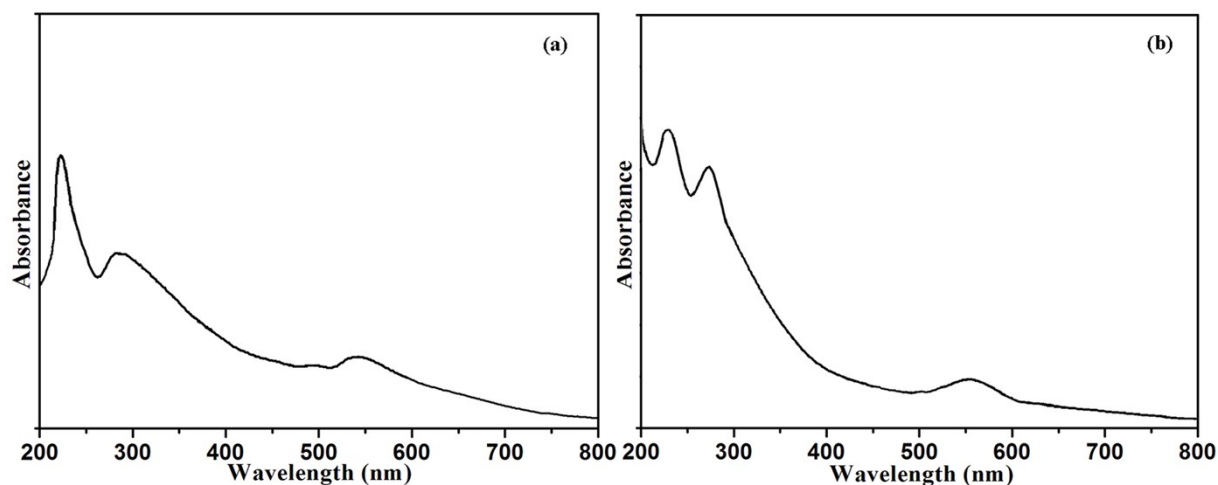


Fig. S9 UV-vis spectra of compounds **1** and **2** in solid state at room temperature.

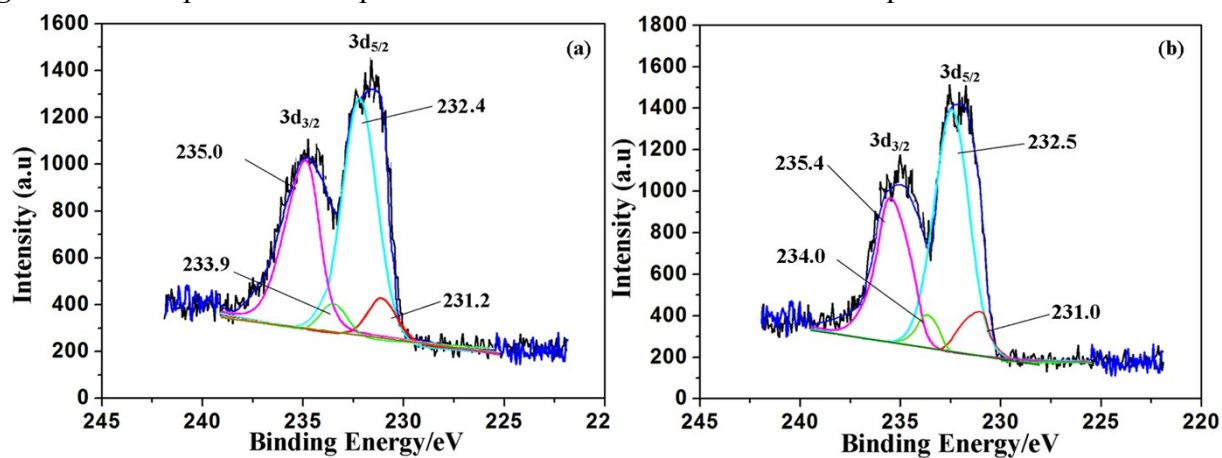


Fig. S10 XPS spectra of (a) compound **1** and (b) compound **2**.

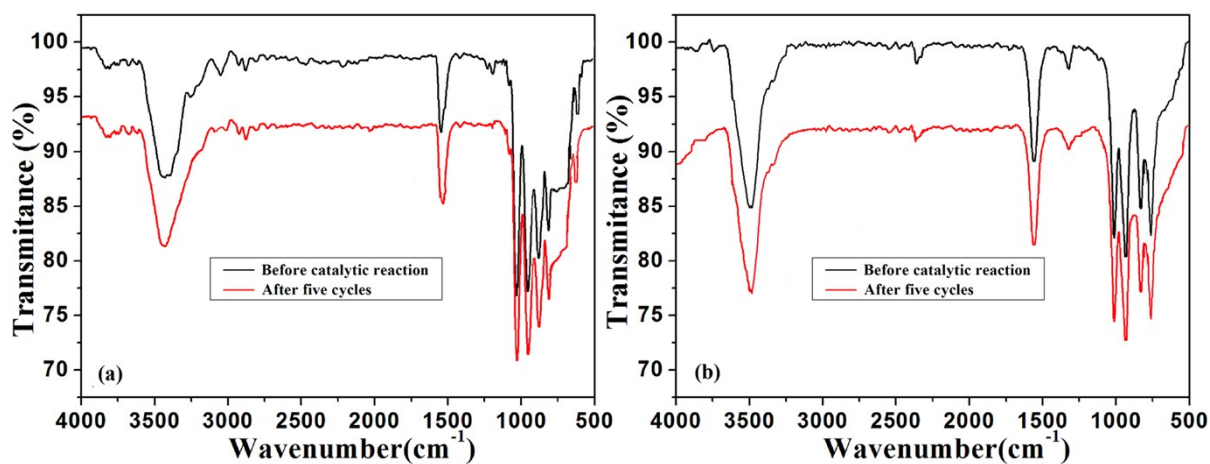


Fig. S11 The IR spectra of compounds **1** and **2** before photocatalytic reaction and after five cycles.

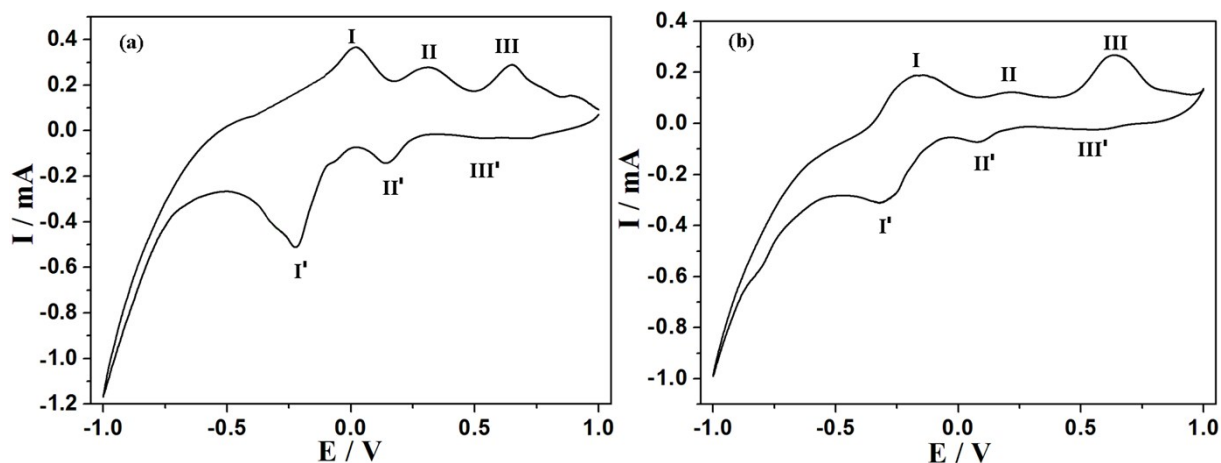


Fig. S12 Cyclic voltammograms of (a) 1-CPE and (b) 2-CPE in the 0.1 M H₂SO₄ solution at 20 mV s⁻¹ (Potentials vs. SCE).

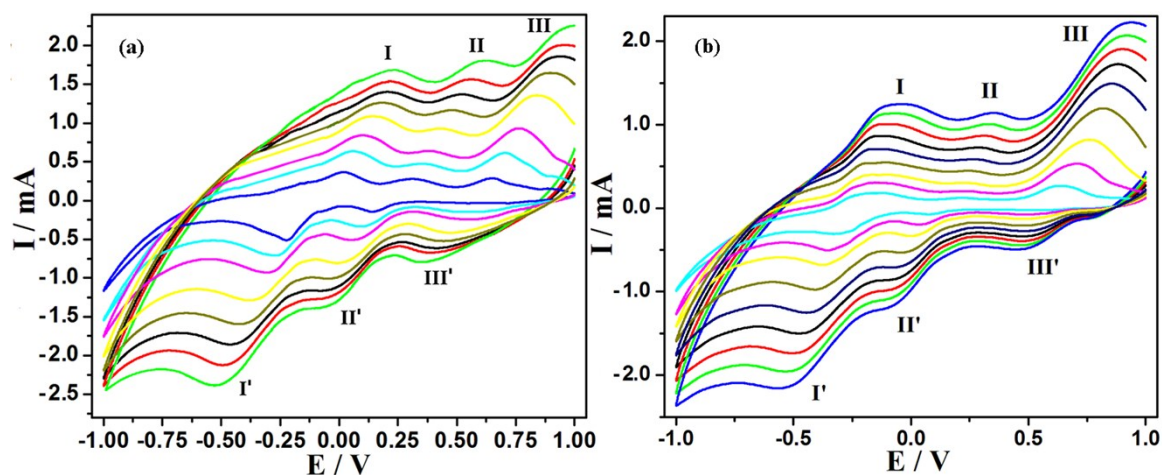


Fig. S13 Cyclic voltammograms of (a) 1-CPE and (b) 2-CPE in the 0.1 M H₂SO₄ solution at different scan rate. rates (from inner to outer: 20, 40, 60, 80, 100, 120, 140, and 160, mV s⁻¹ (Potentials vs. SCE).

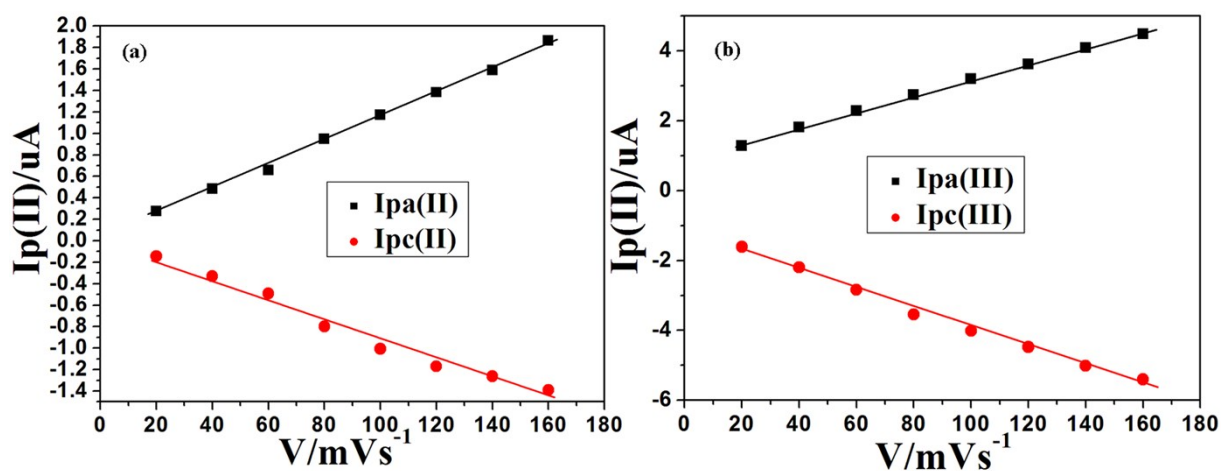


Fig. S14 The dependence of anodic and cathodic peak II current for 1 and peak III current for 2 on scan rates. (Potentials vs. SCE).