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Support Information

The basket-type dimer layers based on tetra-electron reduced heteropoly blue directed by copper/nickel and Strontium Linkers

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1. Structural figures

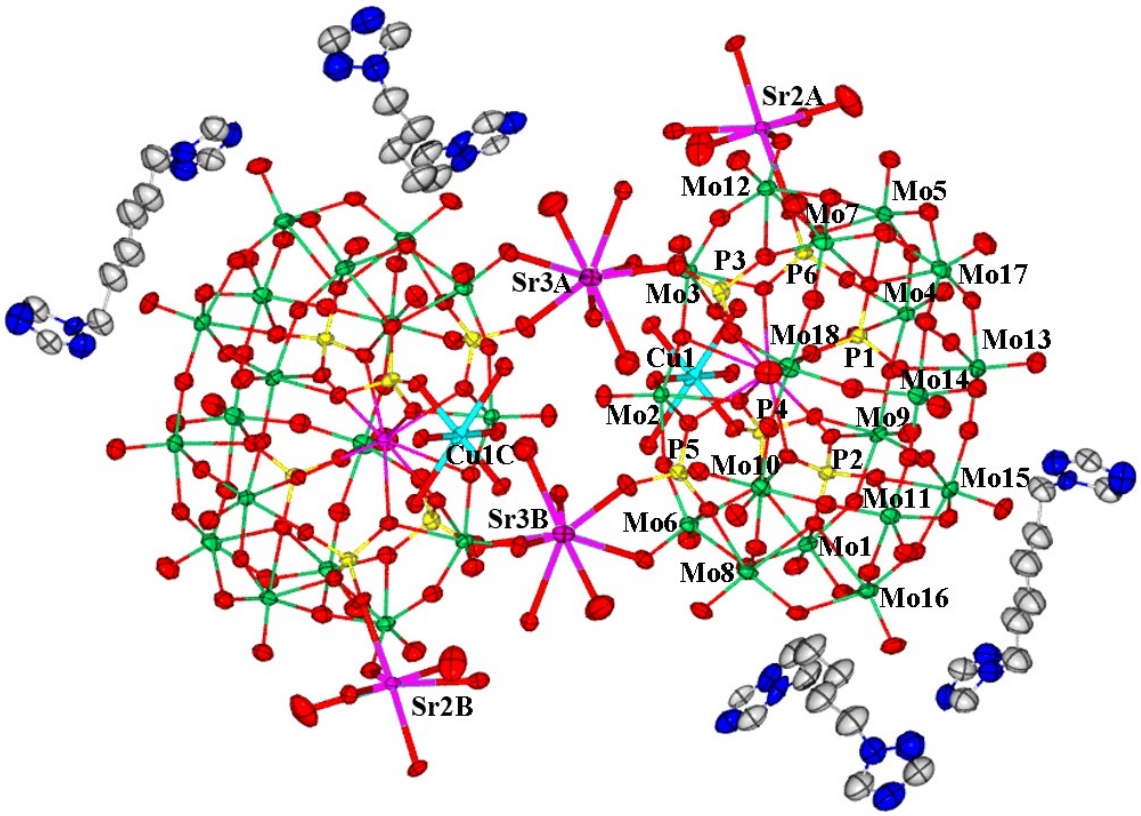

Fig. S1 ORTEP view of the basic units in compound **1** with 50% thermal ellipsoid. Symmetry code: A, -1+x, -1+y, z; B, 1-x, -y, 2-z; C, x, -1+y, z.

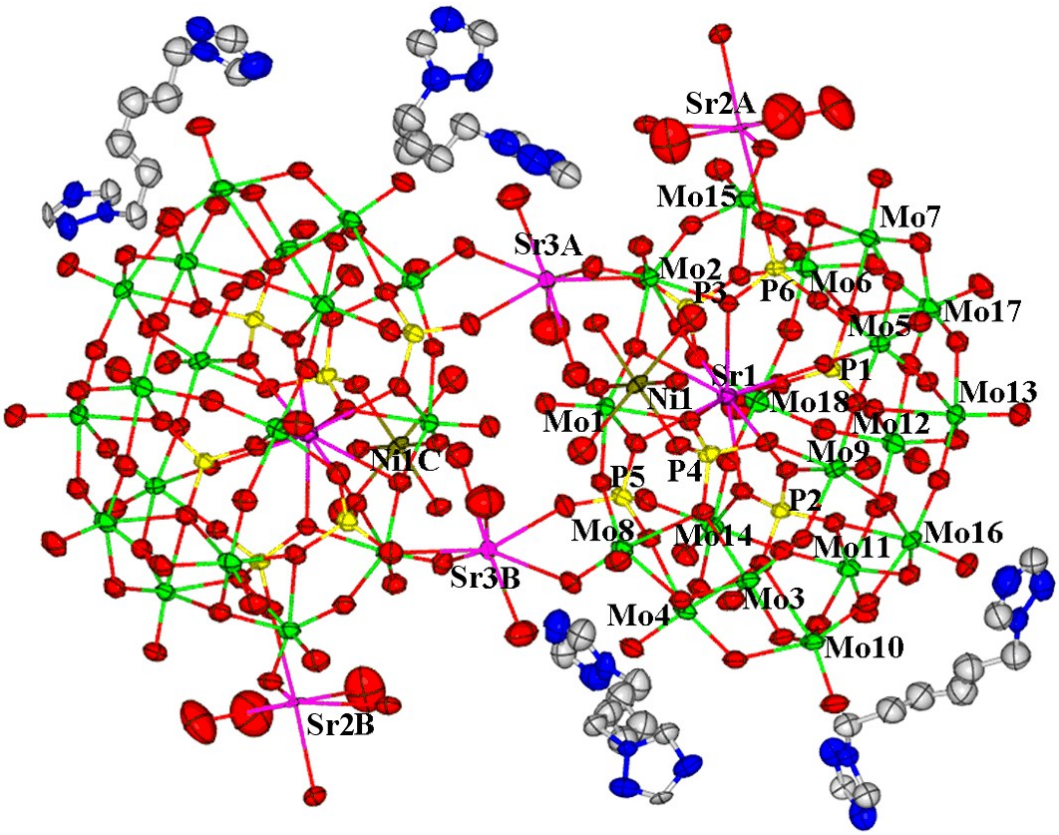

Fig. S2 ORTEP view of the basic units in compound **2** with 50% thermal ellipsoid. Symmetry code: A, -1+x, -1+y, z; B, 1-x, -y, 2-z; C, x, -1+y, z.

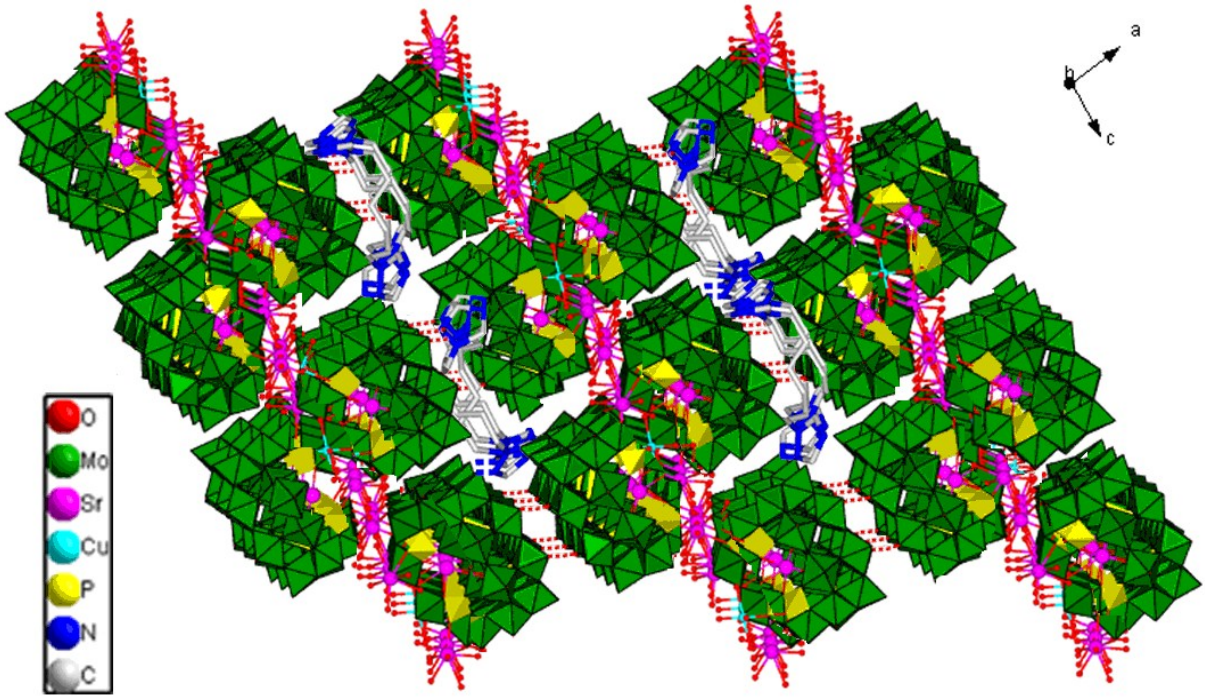

Fig. S3 The 3-D supramolecular network on the ac plane of compound **1**.

2. Structural data

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

Mo(1)-O(63)	1.685(10)	Mo(2)-O(48)	1.696(9)	Mo(3)-O(70)	1.691(10)
Mo(1)-O(25)	1.782(10)	Mo(2)-O(61)	1.735(9)	Mo(3)-O(49)	1.720(10)
Mo(1)-O(65)	1.817(9)	Mo(2)-O(1)	1.855(9)	Mo(3)-O(1)	1.947(9)
Mo(1)-O(33)	2.064(10)	Mo(2)-O(2)	2.026(9)	Mo(3)-O(18)	1.967(9)
Mo(1)-O(35)	2.115(9)	Mo(2)-O(10)	2.165(9)	Mo(3)-O(8)	2.258(9)
Mo(1)-O(22)	2.406(10)	Mo(2)-O(11)	2.244(9)	Mo(3)-O(9)	2.266(9)
Mo(4)-O(55)	1.683(10)	Mo(5)-O(47)	1.691(10)	Mo(6)-O(60)	1.714(10)
Mo(4)-O(16)	1.837(9)	Mo(5)-O(17)	1.775(10)	Mo(6)-O(44)	1.721(10)
Mo(4)-O(6)	1.889(9)	Mo(5)-O(38)	1.797(10)	Mo(6)-O(2)	1.811(9)
Mo(4)-O(14)	2.027(9)	Mo(5)-O(34)	2.063(10)	Mo(6)-O(33)	2.055(9)
Mo(4)-O(17)	2.057(10)	Mo(5)-O(13)	2.131(9)	Mo(6)-O(36)	2.304(9)
Mo(4)-O(28)	2.206(9)	Mo(5)-O(21)	2.394(9)	Mo(6)-O(35)	2.334(9)
Mo(7)-O(46)	1.690(11)	Mo(8)-O(64)	1.685(10)	Mo(9)-O(56)	1.681(10)
Mo(7)-O(19)	1.777(9)	Mo(8)-O(72)	1.767(10)	Mo(9)-O(16)	1.899(9)
Mo(7)-O(67)	1.812(10)	Mo(8)-O(32)	1.800(10)	Mo(9)-O(50)	1.899(9)
Mo(7)-O(34)	2.047(10)	Mo(8)-O(33)	2.045(10)	Mo(9)-O(25)	2.019(9)
Mo(7)-O(37)	2.110(9)	Mo(8)-O(36)	2.114(9)	Mo(9)-O(15)	2.044(9)
Mo(7)-O(21)	2.429(10)	Mo(8)-O(22)	2.406(9)	Mo(9)-O(26)	2.195(9)
Mo(10)-O(52)	1.696(10)	Mo(11)-O(57)	1.690(10)	Mo(12)-O(69)	1.703(10)
Mo(10)-O(20)	1.865(9)	Mo(11)-O(3)	1.870(10)	Mo(12)-O(45)	1.719(10)
Mo(10)-O(7)	1.890(10)	Mo(11)-O(7)	1.880(10)	Mo(12)-O(18)	1.831(9)
Mo(10)-O(40)	2.021(9)	Mo(Mo(11)-O(42) 11)-	1.955(11)	Mo(12)-O(34)	2.060(10)
Mo(10)-O(72)	2.047(9)	Mo(11)-O(31)	2.063(10)	Mo(12)-O(37)	2.317(9)
Mo(10)-O(27)	2.225(9)	Mo(11)-O(5)	2.256(9)	Mo(12)-O(13)	2.317(9)
Mo(13)-O(71)	1.685(11)	Mo(14)-O(58)	1.687(11)	Mo(15)-O(43)	1.676(10)
Mo(13)-O(12)	1.871(10)	Mo(14)-O(3)	1.877(10)	Mo(15)-O(50)	1.893(9)
Mo(13)-O(6)	1.901(10)	Mo(14)-O(51)	1.897(10)	Mo(15)-O(12)	1.891(10)
Mo(13)-O(41)	1.913(10)	Mo(14)-O(41)	1.928(11)	Mo(15)-O(42)	1.943(10)
Mo(13)-O(23)	2.077(10)	Mo(14)-O(39)	2.098(10)	Mo(15)-O(24)	2.066(10)
Mo(13)-O(4)	2.291(10)	Mo(14)-O(4)	2.273(9)	Mo(15)-O(5)	2.299(10)
Mo(16)-O(66)	1.704(10)	Mo(17)-O(68)	1.688(10)	Mo(18)-O(59)	1.672(10)
Mo(16)-O(24)	1.802(10)	Mo(17)-O(23)	1.792(11)	Mo(18)-O(20)	1.870(9)
Mo(16)-O(31)	1.815(10)	Mo(17)-O(39)	1.789(10)	Mo(18)-O(51)	1.873(10)
Mo(16)-O(65)	2.049(10)	Mo(17)-O(67)	2.076(11)	Mo(18)-O(30)	2.032(10)
Mo(16)-O(32)	2.091(10)	Mo(17)-O(38)	2.087(10)	Mo(18)-O(19)	2.050(9)
Mo(16)-O(22)	2.427(9)	Mo(17)-O(21)	2.406(9)	Mo(18)-O(29)	2.201(9)
Sr(1)-O(11)	2.520(9)	Sr(1)-O(9)	2.558(9)	Sr(1)-O(8)	2.616(9)
Sr(1)-O(29)	2.622(9)	Sr(1)-O(28)	2.646(9)	Sr(1)-O(10)	2.652(9)
Sr(1)-O(27)	2.661(9)	Sr(1)-O(26)	2.709(9)	Sr(1)-O(1)	2.846(9)
Sr(2)-O(73)#3	2.479(6)	Sr(2)-O(78)#3	2.573(13)	Sr(2)-O(78)	2.572(13)
Sr(2)-O(45)	2.627(10)	Sr(2)-O(73)	2.478(9)	Sr(2)-O(45)#3	2.627(10)
Sr(2)-O(80)	2.501(16)	Sr(3)-O(81)	2.915(16)	Sr(3)-O(53)	2.555(7)
Sr(3)-O(49)	2.600(7)	Sr(3)-O(54)#2	2.485(10)	Sr(3)-O(74)	2.562(13)
Sr(3)-O(79)	2.549(15)	Sr(3)-O(77)	2.617(12)	Sr(3)-O(44)#2	2.750(8)
Cu(1)-O(61)	1.984(7)	Cu(1)-O(62)#1	1.943(6)	Cu(1)-O(62)	1.943(6)
Cu(1)-O(61)#1	1.984(7)	Cu(1)-O(75)	2.495(6)	Cu(1)-O(75)#1	2.495(6)
P(1)-O(28)	1.508(9)	P(1)-O(29)	1.527(10)	P(1)-O(4)	1.529(10)
P(1)-O(21)	1.575(9)	P(2)-O(27)	1.518(10)	P(2)-O(26)	1.518(9)
P(2)-O(5)	1.548(10)	P(2)-O(22)	1.579(9)	P(3)-O(53)	1.496(10)
P(3)-O(9)	1.516(9)	P(3)-O(30)	1.539(10)	P(3)-O(37)	1.589(10)
P(4)-O(11)	1.506(9)	P(4)-O(62)	1.528(9)	P(4)-O(15)	1.532(10)
P(4)-O(35)	1.566(9)	P(5)-O(54)	1.492(10)	P(5)-O(10)	1.535(9)

P(5)-O(40)	1.548(10)	P(5)-O(36)	1.585(10)	P(6)-O(73)	1.504(9)
P(6)-O(8)	1.524(9)	P(6)-O(14)	1.568(9)	P(6)-O(13)	1.563(10)
O(63)-Mo(1)-O(25)	104.9(5)	O(48)-Mo(2)-O(61)	102.4(4)	O(70)-Mo(3)-O(49)	103.5(5)
O(63)-Mo(1)-O(65)	101.7(5)	O(48)-Mo(2)-O(1)	101.0(4)	O(70)-Mo(3)-O(1)	98.3(4)
O(63)-Mo(1)-O(33)	98.1(5)	O(48)-Mo(2)-O(2)	95.8(4)	O(70)-Mo(3)-O(18)	98.8(4)
O(63)-Mo(1)-O(35)	97.9(4)	O(48)-Mo(2)-O(10)	92.8(4)	O(70)-Mo(3)-O(8)	89.2(4)
O(63)-Mo(1)-O(22)	169.6(4)	O(48)-Mo(2)-O(11)	169.7(4)	O(70)-Mo(3)-O(9)	166.1(4)
O(55)-Mo(4)-O(16)	99.4(5)	O(47)-Mo(5)-O(17)	104.4(5)	O(60)-Mo(6)-O(44)	102.6(5)
O(55)-Mo(4)-O(6)	100.2(5)	O(47)-Mo(5)-O(38)	101.9(5)	O(60)-Mo(6)-O(2)	104.5(5)
O(55)-Mo(4)-O(14)	95.9(4)	O(47)-Mo(5)-O(34)	97.8(5)	O(60)-Mo(6)-O(33)	98.6(4)
O(55)-Mo(4)-O(17)	92.3(5)	O(47)-Mo(5)-O(13)	97.8(4)	O(60)-Mo(6)-O(36)	166.0(4)
O(55)-Mo(4)-O(28)	173.4(4)	O(47)-Mo(5)-O(21)	170.3(4)	O(60)-Mo(6)-O(35)	86.7(4)
O(46)-Mo(7)-O(19)	104.8(5)	O(64)-Mo(8)-O(72)	104.3(5)	O(56)-Mo(9)-O(16)	98.0(5)
O(46)-Mo(7)-O(67)	101.4(5)	O(64)-Mo(8)-O(32)	101.7(5)	O(56)-Mo(9)-O(50)	99.9(5)
O(46)-Mo(7)-O(34)	98.8(5)	O(64)-Mo(8)-O(33)	98.3(5)	O(56)-Mo(9)-O(25)	94.6(5)
O(46)-Mo(7)-O(37)	98.4(5)	O(64)-Mo(8)-O(36)	98.4(4)	O(56)-Mo(9)-O(15)	96.6(4)
O(46)-Mo(7)-O(21)	170.3(5)	O(64)-Mo(8)-O(22)	170.1(4)	O(56)-Mo(9)-O(26)	174.6(4)
O(52)-Mo(10)-O(20)	99.3(5)	O(57)-Mo(11)-O(3)	99.8(5)	O(69)-Mo(12)-O(45)	103.1(5)
O(52)-Mo(10)-O(7)	100.2(5)	O(57)-Mo(11)-O(7)	101.3(5)	O(69)-Mo(12)-O(18)	105.3(5)
O(52)-Mo(10)-O(40)	96.5(4)	O(57)-Mo(11)-O(42)	99.8(5)	O(69)-Mo(12)-O(34)	96.2(5)
O(52)-Mo(10)-O(72)	93.5(4)	O(57)-Mo(11)-O(31)	92.8(4)	O(69)-Mo(12)-O(13)	164.6(4)
O(52)-Mo(10)-O(27)	174.4(4)	O(57)-Mo(11)-O(5)	169.1(5)	O(69)-Mo(12)-O(37)	87.0(4)
O(71)-Mo(13)-O(12)	99.1(5)	O(58)-Mo(14)-O(3)	101.0(5)	O(43)-Mo(15)-O(50)	101.8(5)
O(71)-Mo(13)-O(6)	101.6(5)	O(58)-Mo(14)-O(51)	100.7(5)	O(43)-Mo(15)-O(12)	99.4(5)
O(71)-Mo(13)-O(41)	101.8(5)	O(58)-Mo(14)-O(41)	100.9(5)	O(43)-Mo(15)-O(42)	100.5(5)
O(71)-Mo(13)-O(23)	93.6(5)	O(58)-Mo(14)-O(39)	91.9(5)	O(43)-Mo(15)-O(24)	93.3(5)
O(71)-Mo(13)-O(4)	170.2(5)	O(58)-Mo(14)-O(4)	169.1(4)	O(43)-Mo(15)-O(5)	169.4(4)
O(66)-Mo(16)-O(24)	104.5(5)	O(68)-Mo(17)-O(23)	104.4(4)	O(59)-Mo(18)-O(20)	98.3(5)
O(66)-Mo(16)-O(31)	104.6(5)	O(68)-Mo(17)-O(39)	103.7(4)	O(59)-Mo(18)-O(51)	100.6(5)
O(66)-Mo(16)-O(65)	97.6(5)	O(68)-Mo(17)-O(67)	96.9(4)	O(59)-Mo(18)-O(30)	96.0(5)
O(66)-Mo(16)-O(32)	97.2(5)	O(68)-Mo(17)-O(38)	97.1(3)	O(59)-Mo(18)-O(19)	93.9(5)
O(66)-Mo(16)-O(22)	164.3(4)	O(68)-Mo(17)-O(21)	164.3(3)	O(59)-Mo(18)-O(29)	173.8(5)
O(28)-P(1)-O(29)	107.4(5)	O(27)-P(2)-O(26)	108.3(5)	O(53)-P(3)-O(9)	112.1(6)
O(28)-P(1)-O(4)	110.8(5)	O(27)-P(2)-O(5)	111.3(5)	O(53)-P(3)-O(30)	109.5(6)
O(28)-P(1)-O(21)	109.9(5)	O(27)-P(2)-O(22)	109.8(5)	O(53)-P(3)-O(37)	111.0(6)
O(11)-P(4)-O(62)	111.3(5)	O(54)-P(5)-O(10)	112.9(6)	O(73)-P(6)-O(8)	114.1(5)
O(11)-P(4)-O(15)	110.6(5)	O(54)-P(5)-O(40)	111.0(6)	O(73)-P(6)-O(14)	108.6(5)
O(11)-P(4)-O(35)	107.5(5)	O(54)-P(5)-O(36)	110.8(6)	O(73)-P(6)-O(13)	109.4(4)
O(11)-Sr(1)-O(9)	117.5(3)	O(11)-Sr(1)-O(8)	83.2(3)	O(11)-Sr(1)-O(29)	168.9(3)
O(11)-Sr(1)-O(28)	119.4(3)	O(11)-Sr(1)-O(10)	64.2(3)	O(11)-Sr(1)-O(27)	98.5(3)
O(11)-Sr(1)-O(26)	70.9(3)	O(11)-Sr(1)-O(1)	59.1(3)	O(62)#1-Cu(1)-O(62)	180.0(4)
O(62)#1-Cu(1)-O(61)#1	93.4(3)	O(62)#1-Cu(1)-O(61)	86.6(3)	O(61)#1-Cu(1)-O(61)	86.6(3)
O(73)#3-Sr(2)-O(73)	173.9(5)	O(73)#3-Sr(2)-O(80)	87.0(2)	O(73)#3-Sr(2)-O(78)#3	90.4(4)
O(73)#3-Sr(2)-O(78)	87.7(4)	O(73)#3-Sr(2)-O(45)	106.6(3)	O(73)#3-Sr(2)-O(45)#3	78.1(2)
O(54)#2-Sr(3)-O(74)	90.6(4)	O(54)#2-Sr(3)-O(53)	150.3(2)	O(54)#2-Sr(3)-O(79)	99.5(3)
O(54)#2-Sr(3)-O(49)	92.9(3)	O(54)#2-Sr(3)-O(77)	74.0(4)	O(54)#2-Sr(3)-O(44)#2	76.1(3)
O(54)#2-Sr(3)-O(81)	151.3(8)				

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

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

Mo(1)-O(50)	1.686(7)	Mo(2)-O(70)	1.693(7)	Mo(3)-O(49)	1.683(7)
Mo(1)-O(15)	1.729(6)	Mo(2)-O(40)	1.710(7)	Mo(3)-O(38)	1.791(7)
Mo(1)-O(1)	1.868(6)	Mo(2)-O(1)	1.937(6)	Mo(3)-O(46)	1.815(7)
Mo(1)-O(2)	2.034(6)	Mo(2)-O(17)	1.974(7)	Mo(3)-O(32)	2.054(7)
Mo(1)-O(3)	2.160(6)	Mo(2)-O(5)	2.244(6)	Mo(3)-O(23)	2.111(6)
Mo(1)-O(4)	2.254(7)	Mo(2)-O(6)	2.263(7)	Mo(3)-O(20)	2.399(7)

Mo(4)-O(71)	1.693(7)	Mo(5)-O(53)	1.675(7)	Mo(6)-O(66)	1.681(8)
Mo(4)-O(58)	1.767(7)	Mo(5)-O(7)	1.848(7)	Mo(6)-O(9)	1.775(7)
Mo(4)-O(45)	1.806(7)	Mo(5)-O(16)	1.894(7)	Mo(6)-O(69)	1.811(7)
Mo(4)-O(32)	2.057(7)	Mo(5)-O(12)	2.024(7)	Mo(6)-O(18)	2.044(7)
Mo(4)-O(30)	2.109(7)	Mo(5)-O(37)	2.058(7)	Mo(6)-O(31)	2.114(7)
Mo(4)-O(20)	2.412(7)	Mo(5)-O(24)	2.203(7)	Mo(6)-O(19)	2.423(7)
Mo(7)-O(47)	1.693(7)	Mo(8)-O(64)	1.700(7)	Mo(9)-O(52)	1.688(8)
Mo(7)-O(37)	1.768(7)	Mo(8)-O(48)	1.721(7)	Mo(9)-O(7)	1.889(7)
Mo(7)-O(34)	1.800(7)	Mo(8)-O(2)	1.800(7)	Mo(9)-O(39)	1.901(7)
Mo(7)-O(18)	2.065(7)	Mo(8)-O(32)	2.055(7)	Mo(9)-O(38)	2.019(7)
Mo(7)-O(22)	2.124(7)	Mo(8)-O(30)	2.303(7)	Mo(9)-O(11)	2.038(6)
Mo(7)-O(19)	2.393(7)	Mo(8)-O(23)	2.339(7)	Mo(9)-O(27)	2.206(7)
Mo(10)-O(63)	1.694(7)	Mo(11)-O(72)	1.693(7)	Mo(12)-O(56)	1.692(7)
Mo(10)-O(44)	1.795(8)	Mo(11)-O(8)	1.881(7)	Mo(12)-O(8)	1.868(7)
Mo(10)-O(43)	1.808(8)	Mo(11)-O(28)	1.887(7)	Mo(12)-O(55)	1.887(8)
Mo(10)-O(46)	2.041(7)	Mo(11)-O(54)	1.947(8)	Mo(12)-O(67)	1.937(8)
Mo(10)-O(45)	2.088(8)	Mo(11)-O(43)	2.070(7)	Mo(12)-O(42)	2.102(7)
Mo(10)-O(20)	2.426(6)	Mo(11)-O(33)	2.251(7)	Mo(12)-O(13)	2.266(7)
Mo(13)-O(62)	1.685(8)	Mo(14)-O(14)	1.685(7)	Mo(15)-O(65)	1.697(7)
Mo(13)-O(61)	1.873(7)	Mo(14)-O(21)	1.873(7)	Mo(15)-O(57)	1.711(7)
Mo(13)-O(16)	1.896(7)	Mo(14)-O(28)	1.884(7)	Mo(15)-O(17)	1.822(7)
Mo(13)-O(67)	1.918(7)	Mo(14)-O(35)	2.022(7)	Mo(15)-O(18)	2.045(7)
Mo(13)-O(68)	2.086(7)	Mo(14)-O(58)	2.051(7)	Mo(15)-O(22)	2.308(7)
Mo(13)-O(13)	2.289(7)	Mo(14)-O(26)	2.221(6)	Mo(15)-O(31)	2.325(7)
Mo(16)-O(41)	1.679(8)	Mo(17)-O(60)	1.699(7)	Mo(18)-O(78)	1.670(8)
Mo(16)-O(39)	1.884(7)	Mo(17)-O(68)	1.786(8)	Mo(18)-O(21)	1.860(7)
Mo(16)-O(61)	1.890(7)	Mo(17)-O(42)	1.784(7)	Mo(18)-O(55)	1.877(7)
Mo(16)-O(54)	1.949(7)	Mo(17)-O(69)	2.068(8)	Mo(18)-O(36)	2.029(7)
Mo(16)-O(44)	2.075(7)	Mo(17)-O(34)	2.090(7)	Mo(18)-O(9)	2.050(7)
Mo(16)-O(33)	2.289(7)	Mo(17)-O(19)	2.412(7)	Mo(18)-O(25)	2.209(7)
Sr(1)-O(4)	2.512(6)	Sr(1)-O(6)	2.554(7)	Sr(1)-O(5)	2.616(6)
Sr(1)-O(25)	2.627(6)	Sr(1)-O(3)	2.648(6)	Sr(1)-O(24)	2.657(6)
Sr(1)-O(26)	2.666(6)	Sr(1)-O(27)	2.697(6)	Sr(1)-O(1)	2.838(7)
Sr(2)-O(51)#1	2.477(7)	Sr(2)-O(51)	2.477(7)	Sr(2)-O(79)	2.570(10)
Sr(2)-O(79)#1	2.570(10)	Sr(2)-O(80)	2.550(15)	Sr(2)-O(57)#1	2.639(8)
Sr(2)-O(57)	2.639(8)	Sr(3)-O(59)#3	2.475(7)	Sr(3)-O(81)	2.506(10)
Sr(3)-O(75B)	2.71(3)	Sr(3)-O(10)	2.572(7)	Sr(3)-O(40)	2.610(7)
Sr(3)-O(76)	2.625(8)	Sr(3)-O(48)#3	2.759(8)	P(1)-O(24)	1.504(7)
P(1)-O(25)	1.509(7)	P(1)-O(13)	1.541(7)	P(1)-O(19)	1.581(7)
P(2)-O(27)	1.517(7)	P(2)-O(26)	1.514(7)	P(2)-O(33)	1.557(7)
P(2)-O(20)	1.585(7)	P(3)-O(10)	1.494(8)	P(3)-O(6)	1.519(7)
P(3)-O(36)	1.543(8)	P(3)-O(31)	1.580(7)	P(4)-O(4)	1.511(7)
P(4)-O(29)	1.518(7)	P(4)-O(11)	1.540(7)	P(4)-O(23)	1.568(7)
P(5)-O(59)	1.493(7)	P(5)-O(3)	1.540(7)	P(5)-O(35)	1.540(7)
P(5)-O(30)	1.591(7)	P(6)-O(51)	1.504(7)	P(6)-O(5)	1.536(7)
P(6)-O(12)	1.547(7)	P(6)-O(22)	1.583(7)	Ni(1)-O(29)#2	1.953(6)
Ni(1)-O(29)	1.953(6)	Ni(1)-O(15)#2	1.995(7)	Ni(1)-O(15)	1.995(7)
Ni(1)- O(74A)	2.348(15)	Ni(1)- O(74A) #2	2.348(15)		
O(50)-Mo(1)-O(15)	102.7(3)	O(70)-Mo(2)-O(40)	102.9(3)	O(49)-Mo(3)-O(38)	104.5(4)
O(50)-Mo(1)-O(1)	101.1(3)	O(70)-Mo(2)-O(1)	98.7(3)	O(49)-Mo(3)-O(46)	102.1(3)
O(50)-Mo(1)-O(2)	96.0(3)	O(70)-Mo(2)-O(17)	98.7(3)	O(49)-Mo(3)-O(32)	97.8(3)
O(50)-Mo(1)-O(3)	92.9(3)	O(70)-Mo(2)-O(5)	89.5(3)	O(49)-Mo(3)-O(23)	97.9(3)
O(50)-Mo(1)-O(4)	169.6(3)	O(70)-Mo(2)-O(6)	166.5(3)	O(49)-Mo(3)-O(20)	169.8(3)
O(71)-Mo(4)-O(58)	103.9(4)	O(53)-Mo(5)-O(7)	99.7(3)	O(66)-Mo(6)-O(9)	104.6(4)
O(71)-Mo(4)-O(45)	101.5(3)	O(53)-Mo(5)-O(16)	100.2(3)	O(66)-Mo(6)-O(69)	101.6(4)
O(71)-Mo(4)-O(32)	98.7(3)	O(53)-Mo(5)-O(12)	96.3(3)	O(66)-Mo(6)-O(18)	99.3(3)
O(71)-Mo(4)-O(30)	98.9(3)	O(53)-Mo(5)-O(37)	92.5(3)	O(66)-Mo(6)-O(31)	98.4(3)

O(71)-Mo(4)-O(20)	170.2(3)	O(53)-Mo(5)-O(24)	172.9(3)	O(66)-Mo(6)-O(19)	170.5(3)
O(47)-Mo(7)-O(37)	104.6(4)	O(64)-Mo(8)-O(48)	102.7(4)	O(52)-Mo(9)-O(7)	97.9(3)
O(47)-Mo(7)-O(34)	101.6(3)	O(64)-Mo(8)-O(2)	104.6(3)	O(52)-Mo(9)-O(39)	100.2(3)
O(47)-Mo(7)-O(18)	98.2(3)	O(64)-Mo(8)-O(32)	98.0(3)	O(52)-Mo(9)-O(38)	94.3(3)
O(47)-Mo(7)-O(22)	98.1(3)	O(64)-Mo(8)-O(30)	165.6(3)	O(52)-Mo(9)-O(11)	96.6(3)
O(47)-Mo(7)-O(19)	170.3(3)	O(64)-Mo(8)-O(23)	86.7(3)	O(52)-Mo(9)-O(27)	174.6(3)
O(63)-Mo(10)-O(44)	104.7(4)	O(72)-Mo(11)-O(8)	99.6(3)	O(56)-Mo(12)-O(8)	100.4(3)
O(63)-Mo(10)-O(43)	104.3(4)	O(72)-Mo(11)-O(28)	100.7(4)	O(56)-Mo(12)-O(55)	100.6(4)
O(63)-Mo(10)-O(46)	97.9(3)	O(72)-Mo(11)-O(54)	100.0(4)	O(56)-Mo(12)-O(67)	101.0(4)
O(63)-Mo(10)-O(45)	96.6(4)	O(72)-Mo(11)-O(43)	92.7(3)	O(56)-Mo(12)-O(42)	92.4(3)
O(63)-Mo(10)-O(20)	164.1(3)	O(72)-Mo(11)-O(33)	168.8(4)	O(56)-Mo(12)-O(13)	169.6(3)
O(62)-Mo(13)-O(61)	99.3(4)	O(14)-Mo(14)-O(21)	99.2(3)	O(65)-Mo(15)-O(57)	103.1(4)
O(62)-Mo(13)-O(16)	101.7(4)	O(14)-Mo(14)-O(28)	100.2(3)	O(65)-Mo(15)-O(17)	105.0(3)
O(62)-Mo(13)-O(67)	101.1(4)	O(14)-Mo(14)-O(35)	96.4(3)	O(65)-Mo(15)-O(18)	96.7(3)
O(62)-Mo(13)-O(68)	93.5(3)	O(14)-Mo(14)-O(58)	93.5(3)	O(65)-Mo(15)-O(22)	164.3(3)
O(62)-Mo(13)-O(13)	169.8(3)	O(14)-Mo(14)-O(26)	174.3(3)	O(65)-Mo(15)-O(31)	86.5(3)
O(41)-Mo(16)-O(39)	101.9(3)	O(60)-Mo(17)-O(68)	103.8(4)	O(78)-Mo(18)-O(21)	99.0(4)
O(41)-Mo(16)-O(61)	99.2(4)	O(60)-Mo(17)-O(42)	104.7(4)	O(78)-Mo(18)-O(55)	100.6(4)
O(41)-Mo(16)-O(54)	100.8(3)	O(60)-Mo(17)-O(69)	96.8(4)	O(78)-Mo(18)-O(36)	96.2(4)
O(41)-Mo(16)-O(44)	93.5(3)	O(60)-Mo(17)-O(34)	96.9(3)	O(78)-Mo(18)-O(9)	93.2(3)
O(41)-Mo(16)-O(33)	169.4(3)	O(60)-Mo(17)-O(19)	164.0(3)	O(78)-Mo(18)-O(25)	173.3(3)
O(24)-P(1)-O(25)	108.1(6)	O(27)-P(2)-O(26)	108.4(6)	O(10)-P(3)-O(6)	112.7(6)
O(24)-P(1)-O(13)	111.2(6)	O(27)-P(2)-O(33)	110.5(6)	O(10)-P(3)-O(36)	109.1(7)
O(24)-P(1)-O(19)	109.5(6)	O(27)-P(2)-O(20)	109.5(6)	O(10)-P(3)-O(31)	110.6(6)
O(4)-P(4)-O(29)	111.9(6)	O(59)-P(5)-O(3)	112.6(6)	O(51)-P(6)-O(5)	113.9(6)
O(4)-P(4)-O(11)	109.8(6)	O(59)-P(5)-O(35)	110.9(6)	O(51)-P(6)-O(12)	109.4(6)
O(4)-P(4)-O(23)	107.6(6)	O(59)-P(5)-O(30)	110.6(6)	O(51)-P(6)-O(22)	109.1(6)
O(4)-Sr(1)-O(6)	117.5(2)	O(4)-Sr(1)-O(5)	82.8(2)	O(4)-Sr(1)-O(25)	168.8(2)
O(4)-Sr(1)-O(3)	64.2(2)	O(4)-Sr(1)-O(24)	119.2(2)	O(4)-Sr(1)-O(26)	98.7(2)
O(4)-Sr(1)-O(27)	70.9(2)	O(4)-Sr(1)-O(1)	59.33(19)	O(51)#1-Sr(2)-O(51)	174.0(3)
O(51)#1-Sr(2)-O(79)	90.8(3)	O(51)#1-Sr(2)-O(79)#1	87.4(3)	O(51)#1-Sr(2)-O(80)	87.01(17
O(51)#1-Sr(2)-O(57)#1	78.2(2)	O(51)#1-Sr(2)-O(57)	106.5(2)	O(59)#3-Sr(3)-O(81)	88.4(3)
O(59)#3-Sr(3)-O(77)	99.2(3)	O(59)#3-Sr(3)-O(10)	151.1(2)	O(59)#3-Sr(3)-O(40)	93.9(2)
O(59)#3-Sr(3)-O(76)	72.7(3)	O(59)#3-Sr(3)-O(48)#3	75.6(2)	O(29)#2-Ni(1)-O(29)	179.997(1)
O(29)#2-Ni(1)-O(15)#2	93.0(3)	O(29)#2-Ni(1)-O(15)	93.0(3)	O(29)#2-Ni(1)-	94.7(4)
O(29)#2-Ni(1)-O(74A)	85.3(4)	O(59)#3-Sr(3)-O(75B)	140.5(7)	O(59)#3-Sr(3)-O(75A)	152.5(4)

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

Table S3 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	O4W-H4WA ...O77	0.922	2.473	130.86	3.096(18)	[-x+1, -y+1, -z+1]
	O4W-H4WB...O79	0.844	2.110	168.27	2.95(4)	[-x+1, -y+1, -z+1]
	O81-H81A...O81	0.851	2.290	112.95	2.74(3)	[-x, y, -z+3/2]
	O81-H81A...O69	0.851	2.521	112.44	2.95(3)	[-x, y, -z+3/2]
	O3W-H3WA...O2W	0.850	2.720	91.97	2.88(5)	[-x+1, -y+1, -z+1]
	O3W-H3WA...O75	0.850	2.278	137.82	2.96(4)	[-x+1, -y+2, -z+1]
	O3W-H3WB...O73	0.850	1.921	150.07	2.69(2)	[x, y+1, z]
	O2W-H2WA...O15	0.850	2.606	111.96	3.03(2)	[-x+1, -y, -z+1]
	O2W-H2WB...O75	0.850	2.161	136.49	2.84(3)	[x, y-1, z]
	O2W-H2WB...O14	0.850	2.611	108.02	2.988(13)	[-x+1, -y, -z+1]
	O2W-H2WA...O4W	0.851	2.954	110.70	3.345(18)	
	N8-H8A...O68	0.860	2.378	138.19	3.07(2)	
	N9-H9...O57	0.860	2.152	143.59	2.89(2)	[x, -y+1, z-1/2]

	N9-H9...O58	0.860	2.139	129.32	2.766(19)	[-x+1, y, -z+3/2]
	N12-H12...O42	0.860	1.882	174.47	2.74(2)	
	N13-H13...O52	0.860	2.395	157.52	3.21(2)	[-x+1,-y+1, -z+2]
	N11-H11A...O50	0.860	2.470	163.39	3.30(2)	[x, y+1, z]
	N15-H15A...O40	0.860	2.605	156.99	3.41(3)	[-x+1, -y+1, -z+2]
	O77-H77A...O9	0.850	2.367	126.90	2.956(15)	
	O77-H77B...O48	0.849	2.453	122.87	3.000(15)	[-x, -y+1, -z+2]
	O74-H74A...O49	0.850	2.602	112.20	3.027(17)	
	O74-H74B...O64	0.850	2.131	165.94	2.963(17)	[-x, -y+1, -z+2]
	O75-H75A...O61	0.850	2.520	134.45	3.173(18)	[-x+1, -y+1, -z+1]
	O78-H78B...O60	0.850	2.002	164.88	2.832(16)	[-x, -y, -z+2]
	O78-H78A...O47	0.850	2.035	174.29	2.882(17)	[-x, y, -z+3/2]
	O79-H79A...O2	0.850	2.327	152.10	3.104(19)	[-x, -y+1, -z+2]
2	O75A H75D...O65	0.831	1.953	178.42	2.78(2)	[-x+1, y, -z+1/2]
	O75A H75C.. O65	0.928	2.459	140.30	3.23(2)	[-x+1, y, -z+1/2]
	N8 H8...O62	0.860	2.521	137.35	3.206(19)	[x, y+1, z]
	O74A H74A...O1W	0.894	2.167	147.20	2.96(3)	[x, y-1, z]
	O74A H74B... O4	0.894	2.387	129.41	3.034(15)	
	O74A-H74B...O5	0.894	2.421	138.09	3.143(16)	
	O81-H81A...O65	0.850	2.143	154.47	2.933(13)	[-x+1, y, -z+1/2]
	O81-H81B...O71	0.850	2.066	167.27	2.901(13)	[-x+1, -y+1, -z]
	N3-H3A...O54	0.860	1.911	173.16	2.767 (3)	[x+1, y, z]
	N2-H2...O14	0.860	2.445	158.97	3.262 (3)	[-x+1, -y+1, -z]
	N6-H6...O29	0.860	2.074	174.93	2.93(3)	[-x+1, -y, -z]
	O76 H76B... O2W	0.850	2.149	174.13	2.997(15)	
	O76 H76A... O6	0.850	2.200	163.08	3.023(11)	
	O79 H79A...O47	0.850	2.315	122.87	2.866(13)	
	O2W H2WA...O77	0.851	2.207	142.75	2.930(17)	
	O2W H2WA...O1W	0.851	2.524	127.41	3.12(3)	[-x+1, -y+1, -z]
	O2W H2WB...O36	0.849	2.140	179.51	2.989(14)	
	O77 H77A... O2	0.907	2.280	146.23	3.076(15)	
	O77 H77B...O75B	0.910	2.738	107.70	3.13(4)	
	O75B H75B...O81	0.850	2.923	101.73	3.21(4)	[x, y-1, z]
	O74B H74D...O70	0.850	2.394	139.74	3.09(2)	
	O74B H74C...O1W	0.850	2.720	110.30	3.12(3)	[x, y-1, z]
	O1W H1WA...O74A	0.850	2.920	163.06	3.74(2)	[x, y+1, z]
	O1W H1WA...O74B	0.850	2.366	147.85	3.12(3)	
	N11 H11...O43	0.860	2.288	140.29	3.001(15)	[x, -y+1, z+1/2]

3. Physical characterization

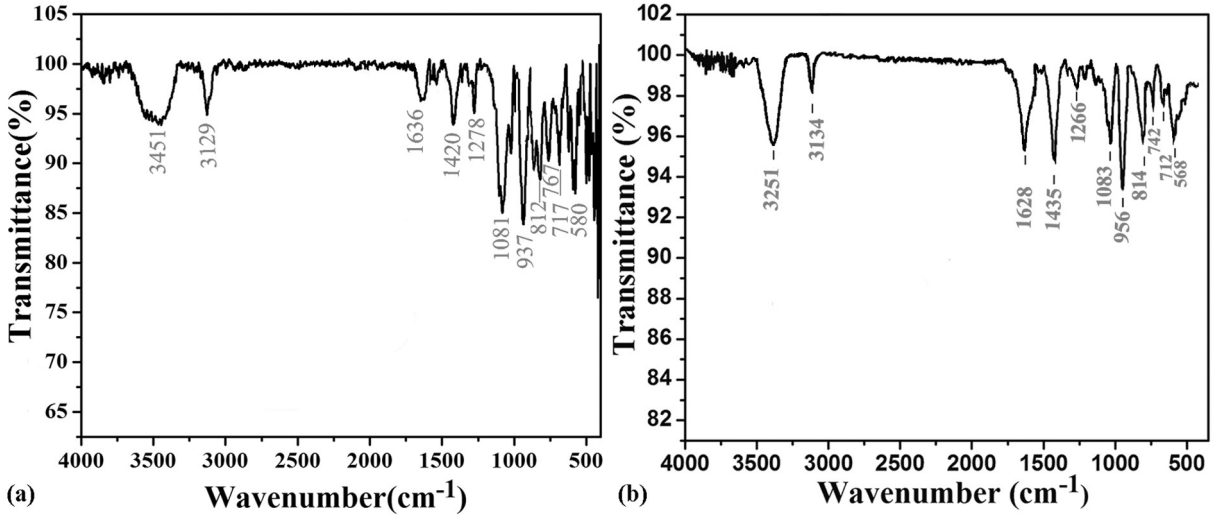

Fig. S4 IR spectra of compounds **1** and **2.**

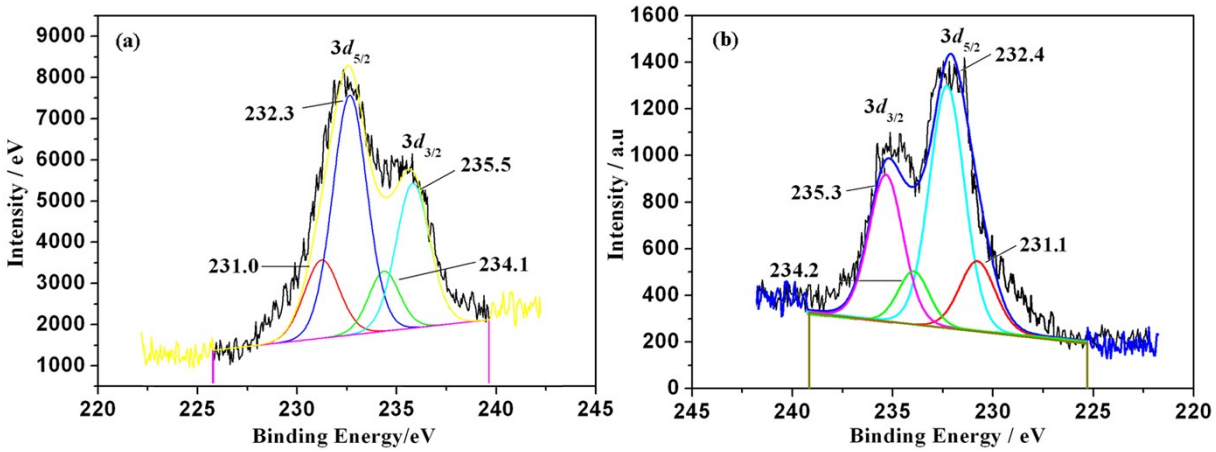

Fig. S5 The XPS spectrum of compounds **1** and **2**

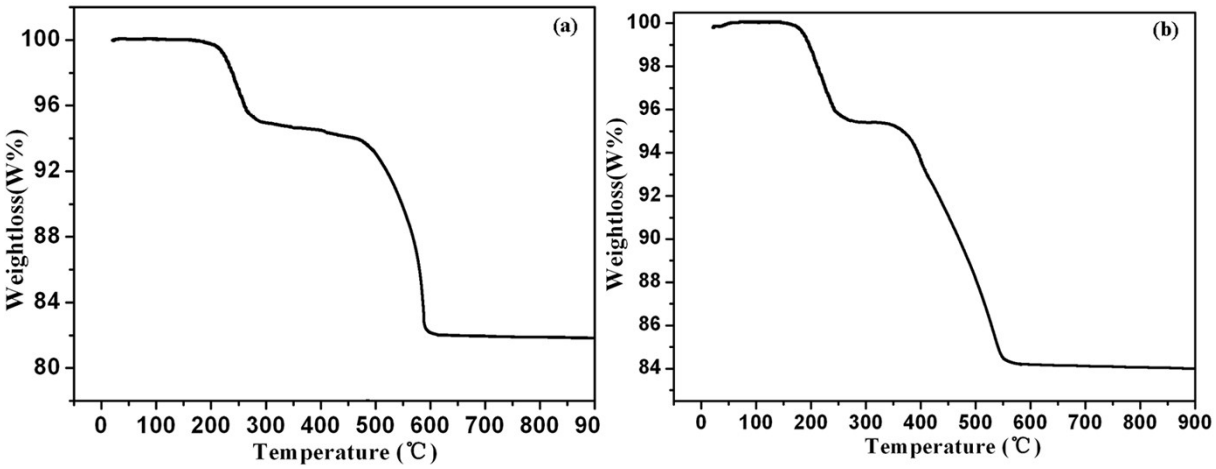

Fig. S6 TG curve of compounds **1** and **2**

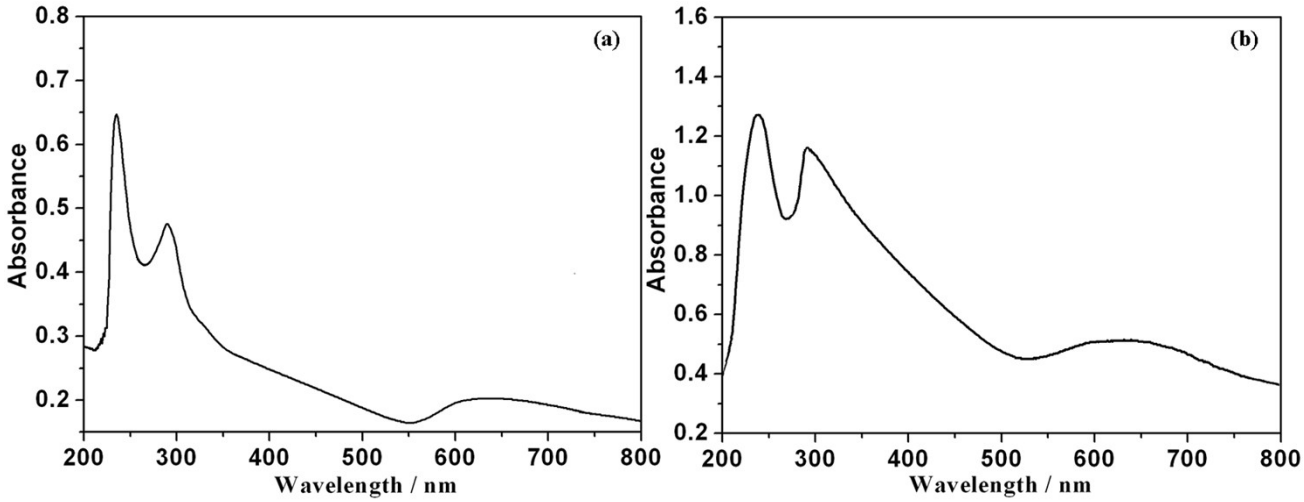

Fig. S7 Solid state UV-vis spectra of compounds **1** and **2**.

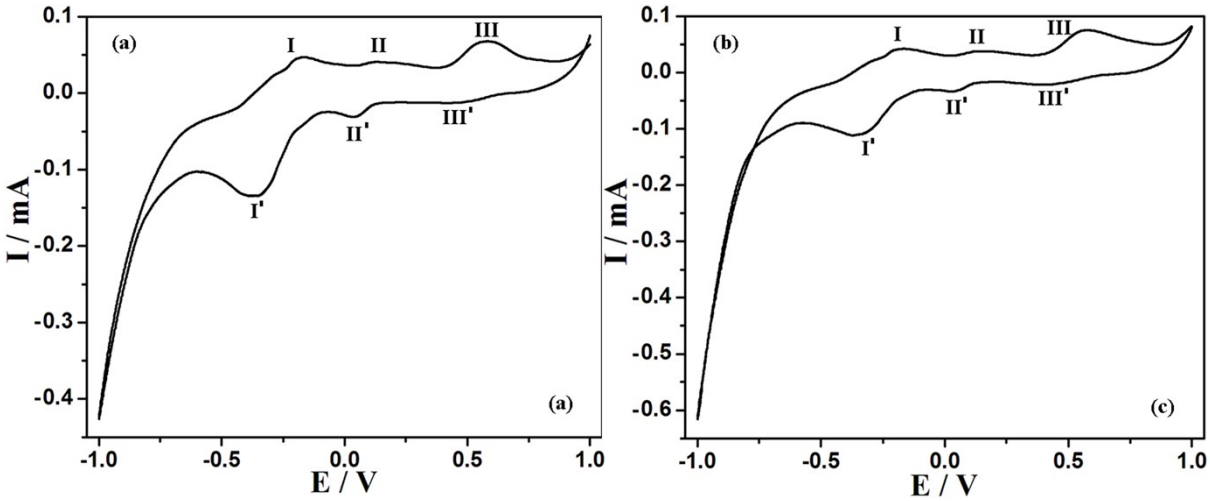

Fig. S8 Cyclic voltammograms of (a) **1-CPE** and (b) **2-CPE** in the 1 M H_2SO_4 solution at scan rate of 20 mV s^{-1} (Potentials vs. SCE).

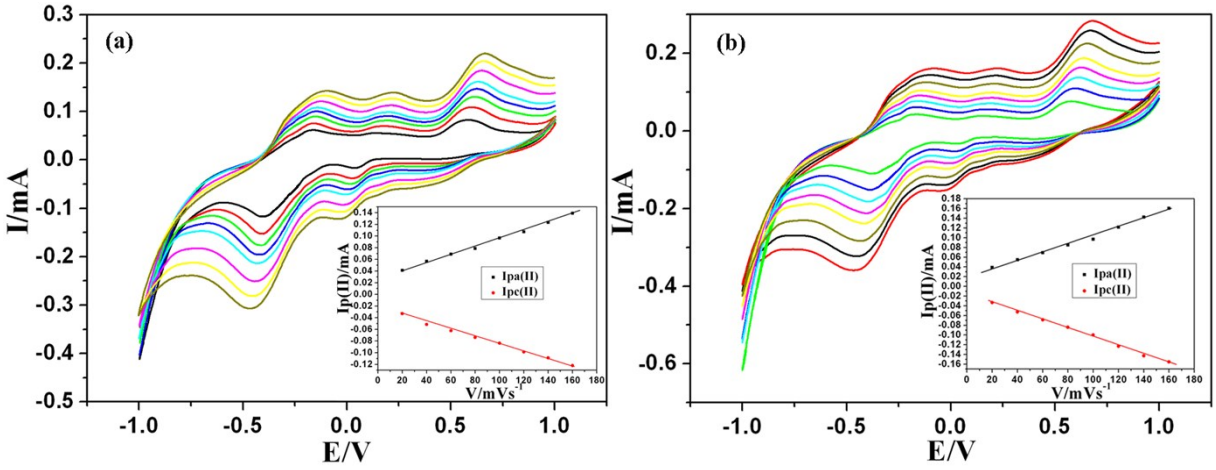

Fig. S9 Cyclic voltammograms of (a) **1-CPE** and (b) **2-CPE** in the 1 M H_2SO_4 solution at different scan rate. scan rates (from inner to outer: 20, 40, 60, 80, 100, 120,140, and 160 mV s^{-1}). Potentials vs. SCE. (Insert plots: The dependence of anodic and cathodic peak II current on scan rates.)

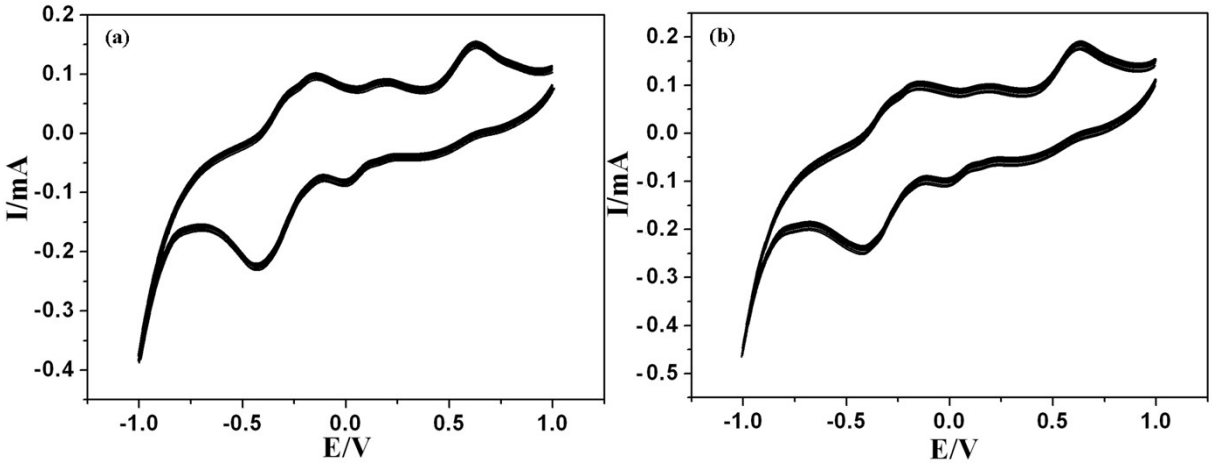

Fig. S10 Consecutive CVs (40 cycles) of (a) **1**-CPE and (b) **2**-CPE in 1M H_2SO_4 solutions at the scan rate of 100 $mV \cdot s^{-1}$ (Potentials vs. SCE).

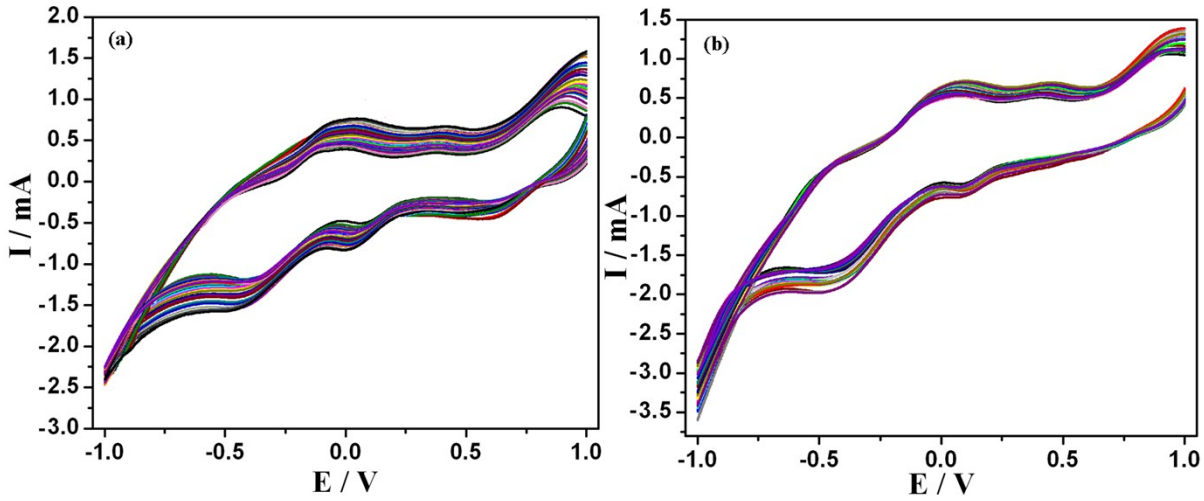

Fig. S11 Consecutive CVs (40 cycles) of (a) **1**-CPE and (b) **2**-CPE for reduction of NO_2^- in 1M H_2SO_4 solutions with concentration of 2.0 mM NO_2^- at the scan rate of 100 $mV \cdot s^{-1}$ (Potentials vs. SCE).

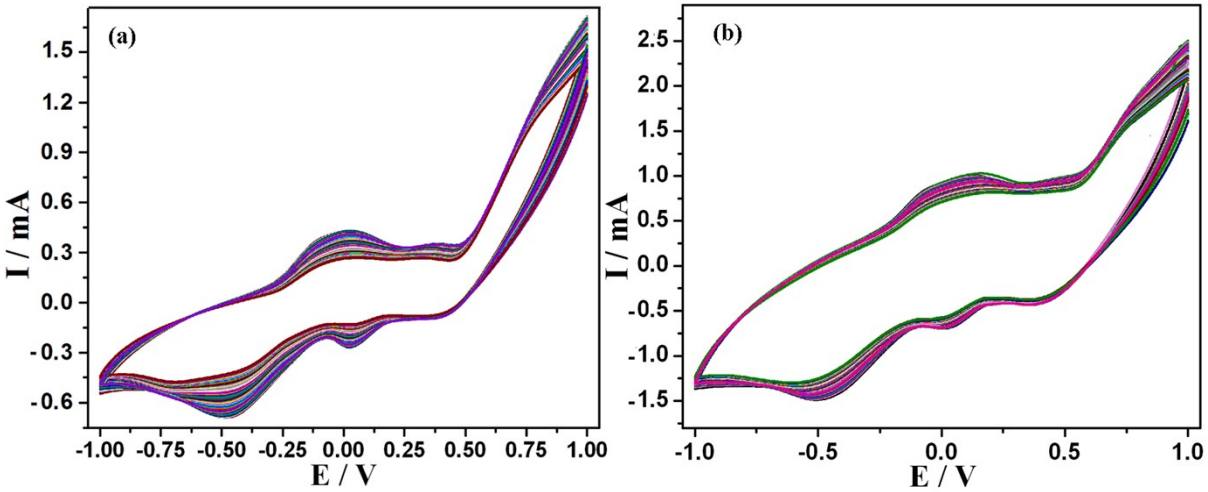

Fig. S12 Consecutive CVs (40 cycles) of (a) **1**-CPE and (b) **2**-CPE for oxidation of DA in 1M H_2SO_4 solutions with concentration of 2.0 mM DA at the scan rate of 100 $mV \cdot s^{-1}$ (Potentials vs. SCE).

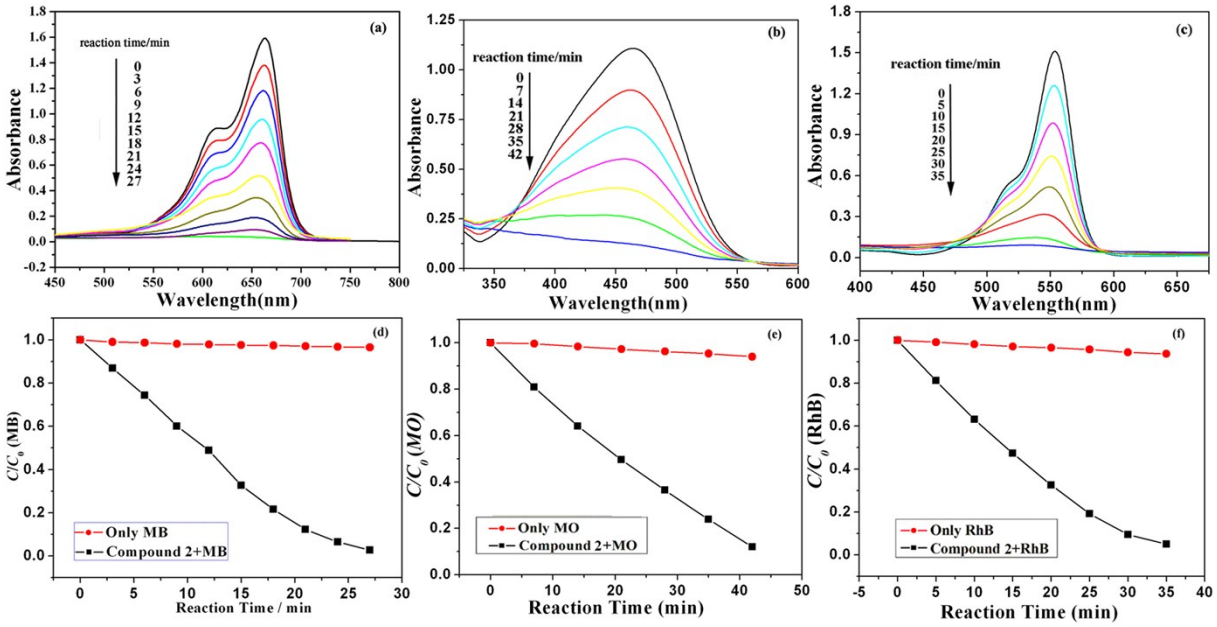

Fig. S13 UV-vis absorption spectra of (a) MB, (b) MO, (c) RhB solution during the decomposition reaction under UV irradiation in the presence of compound 2; Plot of irradiation time versus concentration for (d) MB, (e) MO, and (f) RhB in the presence of compound 2 under UV irradiation.

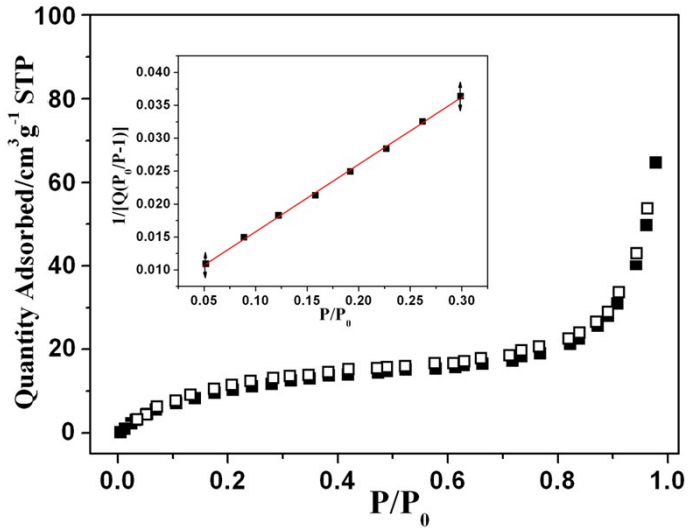

Fig. S14 N_2 sorption isotherm of compound **1** at 77 K (P_0 = 1 atm). Inset: Plot of the linear region for the BET equation.

Table 4. The quantum yields of degradation of MB, RhB, and MO in the presence of compound **1** under 280 nm monochromatic irradiation.

Substrates	**MB**	**RhB**	**MO**
Photointensity, I (Einstein $l^{-1}min^{-1}$)	1.80×10^{-5}	1.80×10^{-5}	1.80×10^{-5}
Molar absorptivity of substrstes, ε_λ ($cm^{-1}M^{-1}$)	2.38×10^{4}	2.26×10^{4}	2.01×10^{4}
Photocatalysis rate constant, k (min^{-1})	0.0930	0.0690	0.0541
Cell path length	2.4	2.4	2.4
Photocatalysis quantum yield, Φ	0.0393	0.0307	0.0271

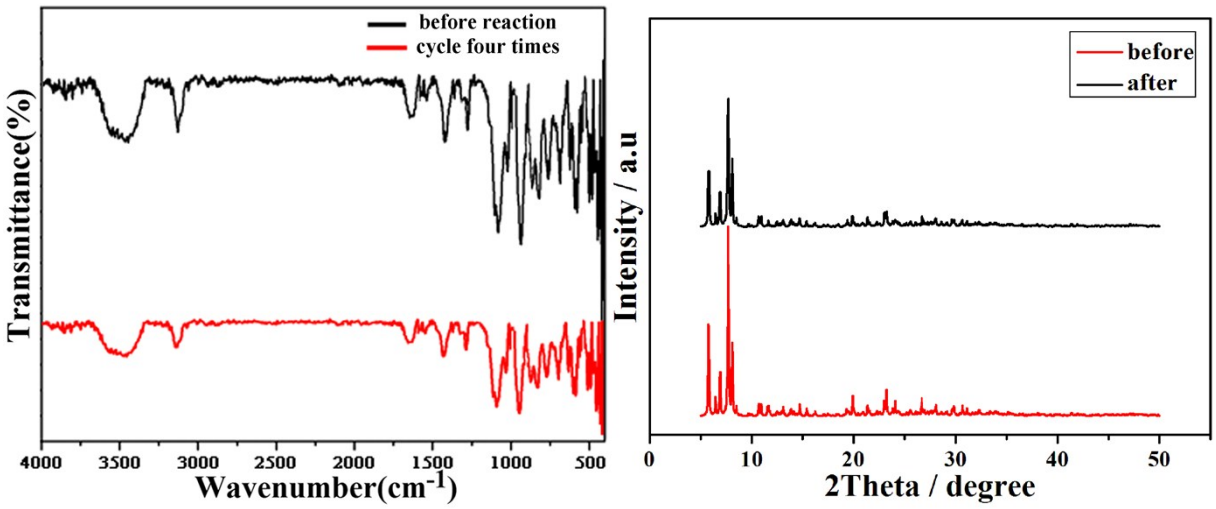

Fig. S15 The IR and XRD patterns of catalyst **1** before and after cycle four time.