Support Information

1,4-Bis(imidazole)butane Ligand and Strontium(II) Directed 1-D chains Based on Basket-type Molybdophosphates and Transition Metal (TM) Linkers

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1. Structural figures

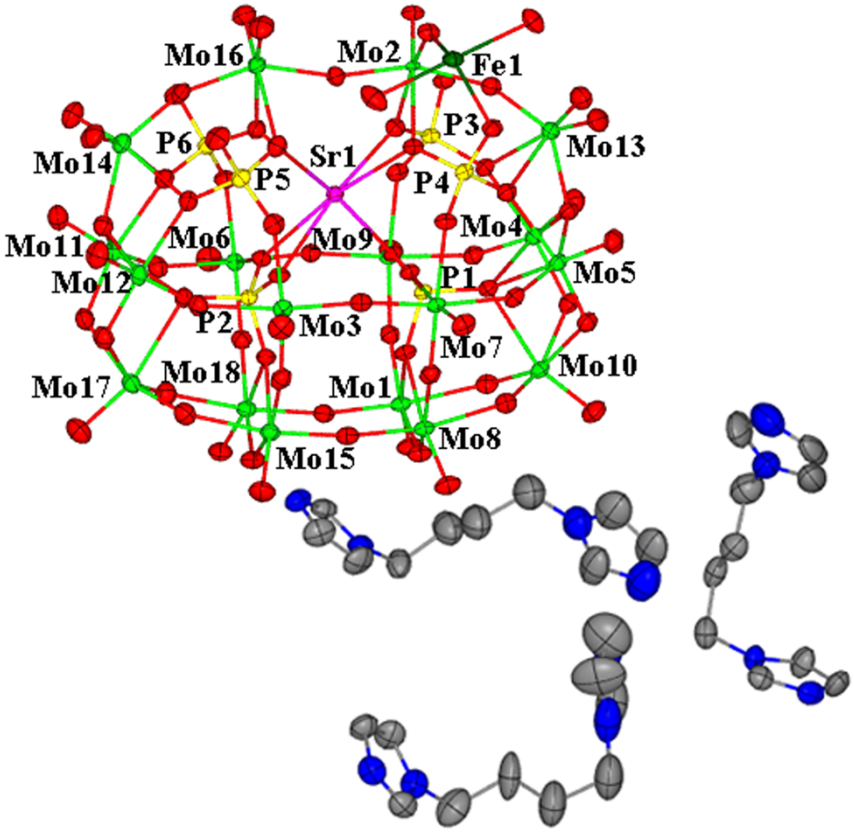

Figure S1 ORTEP view of the basic units in compound **1** with 50% thermal ellipsoid.

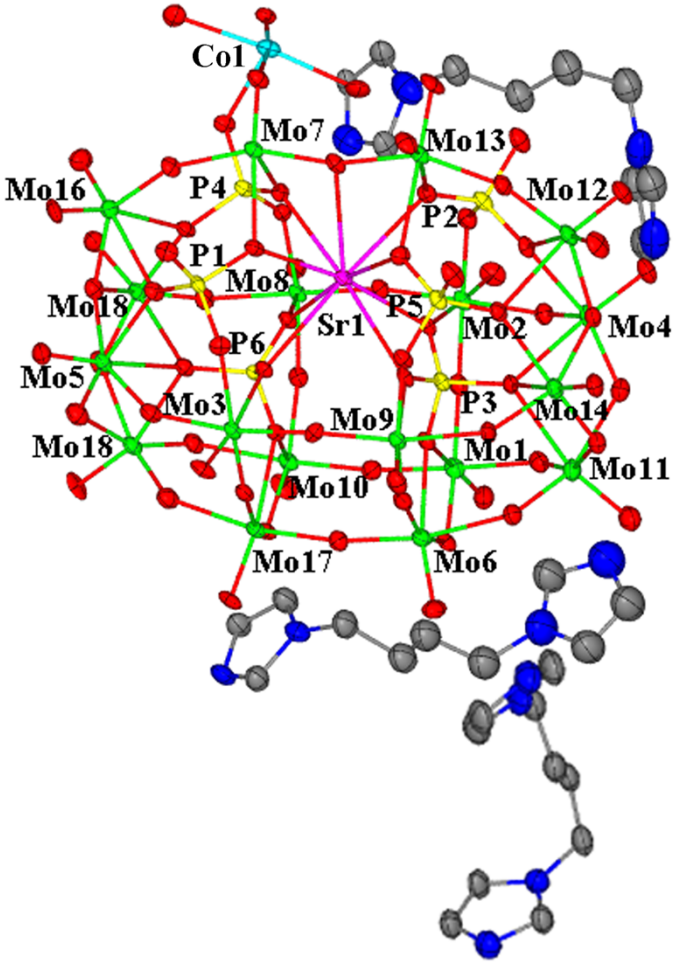

Figure S2 ORTEP view of the basic units in compound **2** with 50% thermal ellipsoid.

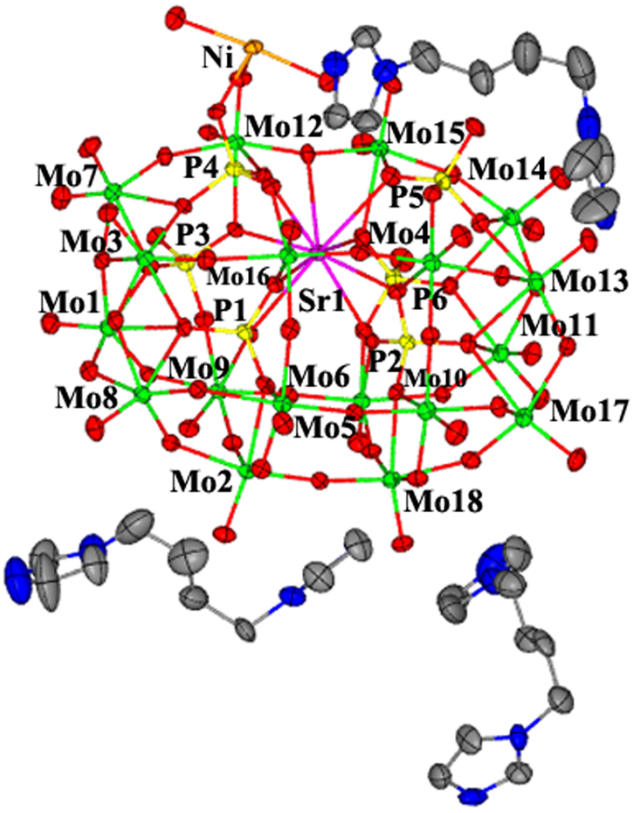

Figure S3 ORTEP view of the basic units in compound **3** with 50% thermal ellipsoid.

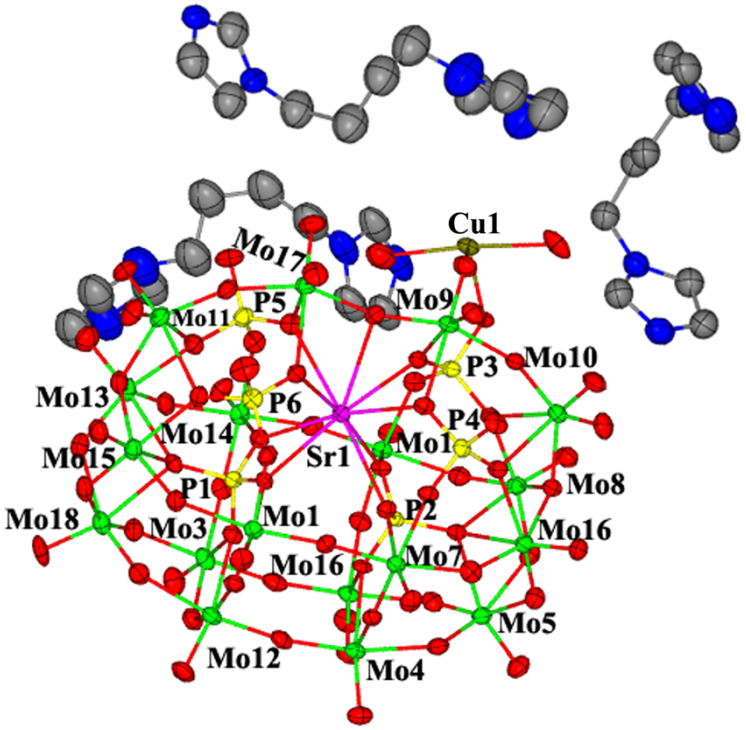

Figure S4 ORTEP view of the basic units in compound **4** with 50% thermal ellipsoid.

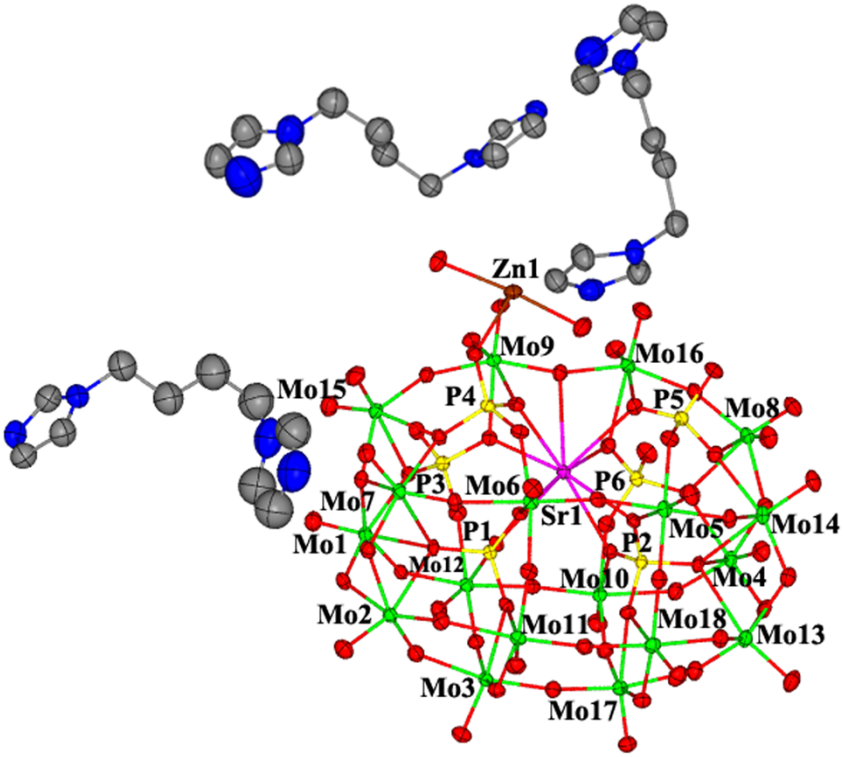

Figure S5 ORTEP view of the basic units in compound **5** with 50% thermal ellipsoid.

2. Structural data

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

Mo(1)-O(35)	1.671(8)	Mo(1)-O(34)	1.867(7)	Mo(1)-O(23)	1.872(7)
Mo(1)-O(74)	1.954(7)	Mo(1)-O(28)	2.083(7)	Mo(1)-O(20)	2.287(7)
Mo(2)-O(11)	1.667(7)	Mo(2)-O(50)	1.873(7)	Mo(2)-O(34)	1.895(7)
Mo(2)-O(40)	2.017(7)	Mo(2)-O(72)	2.062(7)	Mo(2)-O(42)	2.220(7)
Mo(3)-O(26)	1.675(7)	Mo(3)-O(31)	1.876(7)	Mo(3)-O(39)	1.878(7)
Mo(3)-O(10)	2.023(8)	Mo(3)-O(69)	2.068(7)	Mo(3)-O(16)	2.206(7)
Mo(4)-O(15)	1.675(7)	Mo(4)-O(64)	1.784(8)	Mo(4)-O(40)	1.792(7)
Mo(4)-O(75)	2.051(7)	Mo(4)-O(46)	2.146(7)	Mo(4)-O(63)	2.385(7)
Mo(5)-O(24)	1.656(8)	Mo(5)-O(10)	1.782(8)	Mo(5)-O(70)	1.814(7)
Mo(5)-O(61)	2.062(7)	Mo(5)-O(22)	2.123(7)	Mo(5)-O(29)	2.429(7)
Mo(6)-O(55)	1.665(7)	Mo(6)-O(65)	1.887(7)	Mo(6)-O(74)	1.939(7)
Mo(6)-O(32)	2.090(7)	Mo(6)-O(20)	2.281(7)	Mo(6) -O(9)	1.887(7)
Mo(7)-O(73)	1.716(7)	Mo(7)-O(52)#1	1.723(7)	Mo(7)-O(14)	1.853(7)
Mo(7)-O(17)	1.980(7)	Mo(7)-O(58)	2.197(7)	Mo(7)-O(53)	2.214(7)
Mo(8)-O(21)	1.681(7)	Mo(8)-O(50)	1.857(7)	Mo(8)-O(47)	1.876(7)
Mo(8)-O(36)	2.013(7)	Mo(8)-O(18)	2.049(7)	Mo(8)-O(19)	2.222(7)
Mo(9)-O(37)	1.678(7)	Mo(9)-O(39)	1.852(7)	Mo(9)-O(65)	1.869(7)
Mo(9)-O(30)	2.009(7)	Mo(9)-O(51)	2.020(7)	Mo(9)-O(43)	2.237(7)
Mo(10)-O(4)	1.663(7)	Mo(10)-O(23)	1.867(7)	Mo(10)-O(54)	1.894(7)
Mo(10)-O(47)	1.898(7)	Mo(10)-O(41)	2.118(8)	Mo(10)-O(27)	2.295(7)
Mo(11)-O(57)	1.674(8)	Mo(11)-O(32)	1.787(7)	Mo(11)-O(28)	1.788(7)
Mo(11)-O(64)	2.078(7)	Mo(11)-O(67)	2.104(7)	Mo(11)-O(63)	2.407(7)
Mo(12)-O(68)	1.694(7)	Mo(12)-O(59)	1.699(7)	Mo(12)-O(1)	1.830(7)
Mo(12)-O(75)	2.047(7)	Mo(12)-O(66)	2.351(7)	Mo(12)-O(46)	2.377(7)
Mo(13)-O(48)	1.685(7)	Mo(13)-O(49)	1.701(7)	Mo(13)-O(14)	1.948(7)
Mo(13)-O(1)	1.950(7)	Mo(13)-O(56)	2.294(7)	Mo(13)-O(33)	2.299(7)
Mo(14)-O(45)	1.680(7)	Mo(14)-O(67)	1.780(8)	Mo(14)-O(30)	1.793(7)
Mo(14)-O(75)	2.041(7)	Mo(14)-O(66)	2.125(7)	Mo(14)-O(63)	2.438(7)
Mo(15)-O(6)	1.690(7)	Mo(15)-O(62)	1.789(8)	Mo(15)-O(41)	1.796(7)
Mo(15)-O(70)	2.059(8)	Mo(15)-O(60)	2.073(8)	Mo(15)-O(29)	2.376(7)
Mo(16)-O(71)	1.700(8)	Mo(16)-O(8)	1.703(8)	Mo(16)-O(17)	1.815(7)
Mo(16)-O(61)	2.034(7)	Mo(16)-O(38)	2.352(7)	Mo(16)-O(22)	2.377(7)
Mo(17)-O(7)	1.683(7)	Mo(17)-O(31)	1.885(7)	Mo(17)-O(54)	1.925(7)
Mo(17)-O(62)	2.116(8)	Mo(17)-O(27)	2.296(7)	Mo(17) -O(9)	1.857(7)
Mo(18)-O(12)	1.682(7)	Mo(18)-O(18)	1.775(7)	Mo(18)-O(60)	1.822(7)
Mo(18)-O(61)	2.049(7)	Mo(18)-O(38)	2.109(7)	Mo(18)-O(29)	2.426(7)
P(1)-O(44)	1.508(7)	P(2)-O(33)	1.505(7)	P(3)-O(43)	1.510(7)
P(1)-O(69)	1.523(7)	P(2)-O(72)	1.527(7)	P(3)-O(42)	1.529(7)
P(1)-O(53)	1.562(7)	P(2)-O(46)	1.529(7)	P(3)-O(20)	1.541(7)
P(1)-O(22)	1.568(7)	P(2)-O(5)	1.564(8)	P(3)-O(63)	1.554(7)
P(4)-O(25)	1.512(7)	P(5)-O(56)	1.514(7)	P(6)-O(19)	1.508(7)
P(4)-O(58)	1.534(7)	P(5)-O(51)	1.531(7)	P(6)-O(27)	1.510(7)
P(4)-O(36)	1.531(7)	P(5)-O(2)	1.547(8)	P(6)-O(16)	1.518(7)
P(4)-O(38)	1.571(7)	P(5)-O(66)	1.556(8)	P(6)-O(29)	1.567(8)
Sr(1)-O(53)	2.505(7)	Sr(1)-O(58)	2.522(7)	Sr(1)-O(56)	2.589(7)
Sr(1)-O(42)	2.622(7)	Sr(1)-O(33)	2.623(7)	Sr(1)-O(43)	2.637(7)
Sr(1)-O(19)	2.654(7)	Sr(1)-O(16)	2.663(7)	Sr(1)-O(14)	2.840(7)
Fe(1)-O(44)#2	2.033(7)	Fe(1)-O(25)	2.059(7)	Fe(1)-O(52)	2.099(7)
Fe(1)-O(73)	2.119(7)	Fe(1)-O(13)	2.151(8)	Fe(1)-O(3)	2.201(8)
O(35)-Mo(1)-O(34)	101.7(4)	O(11)-Mo(2)-O(50)	98.9(3)	O(26)-Mo(3)-O(31)	101.1(3)
O(35)-Mo(1)-O(23)	100.3(3)	O(11)-Mo(2)-O(34)	101.6(3)	O(26)-Mo(3)-O(39)	97.4(3)
O(35)-Mo(1)-O(74)	100.0(3)	O(11)-Mo(2)-O(40)	94.1(3)	O(26)-Mo(3)-O(10)	94.3(3)

O(35)-Mo(1)-O(28)	93.1(3)	O(11)-Mo(2)-O(72)	95.1(3)	O(26)-Mo(3)-O(69)	95.4(3)
O(35)-Mo(1)-O(20)	168.9(3)	O(11)-Mo(2)-O(42)	173.1(3)	O(26)-Mo(3)-O(16)	172.6(3)
O(15)-Mo(4)-O(64)	102.0(4)	O(24)-Mo(5)-O(10)	105.5(4)	O(55)-Mo(6)-O(65)	101.0(3)
O(15)-Mo(4)-O(40)	104.1(3)	O(24)-Mo(5)-O(70)	102.3(3)	O(55)-Mo(6)-O(9)	101.4(3)
O(15)-Mo(4)-O(75)	97.8(3)	O(24)-Mo(5)-O(61)	99.4(3)	O(55)-Mo(6)-O(74)	100.7(3)
O(15)-Mo(4)-O(46)	96.8(3)	O(24)-Mo(5)-O(22)	96.2(3)	O(55)-Mo(6)-O(32)	91.3(3)
O(15)-Mo(4)-O(63)	170.1(3)	O(24)-Mo(5)-O(29)	170.5(3)	O(55)-Mo(6)-O(20)	167.2(3)
O(73)-Mo(7)-O(52)#1	104.3(3)	O(21)-Mo(8)-O(50)	100.9(3)	O(37)-Mo(9)-O(39)	98.3(3)
O(73)-Mo(7)-O(14)	99.7(3)	O(21)-Mo(8)-O(47)	99.5(3)	O(37)-Mo(9)-O(65)	101.1(3)
O(73)-Mo(7)-O(17)	94.9(3)	O(21)-Mo(8)-O(36)	97.5(3)	O(37)-Mo(9)-O(30)	94.5(3)
O(73)-Mo(7)-O(58)	90.6(3)	O(21)-Mo(8)-O(18)	91.4(3)	O(37)-Mo(9)-O(51)	96.2(3)
O(73)-Mo(7)-O(53)	166.0(3)	O(21)-Mo(8)-O(19)	172.6(3)	O(37)-Mo(9)-O(43)	173.4(3)
O(4)-Mo(10)-O(23)	100.5(4)	O(57)-Mo(11)-O(32)	105.1(4)	O(68)-Mo(12)-O(59)	103.4(4)
O(4)-Mo(10)-O(54)	102.2(3)	O(57)-Mo(11)-O(28)	104.0(4)	O(68)-Mo(12)-O(1)	106.1(4)
O(4)-Mo(10)-O(47)	99.9(3)	O(57)-Mo(11)-O(64)	97.5(3)	O(68)-Mo(12)-O(75)	96.9(3)
O(4)-Mo(10)-O(41)	92.8(3)	O(57)-Mo(11)-O(67)	96.5(3)	O(68)-Mo(12)-O(66)	163.2(3)
O(4)-Mo(10)-O(27)	169.4(3)	O(57)-Mo(11)-O(63)	164.0(3)	O(68)-Mo(12)-O(46)	84.8(3)
O(48)-Mo(13)-O(49)	103.3(4)	O(45)-Mo(14)-O(67)	101.6(4)	O(6)-Mo(15)-O(62)	105.0(3)
O(48)-Mo(13)-O(14)	98.5(3)	O(45)-Mo(14)-O(30)	105.2(3)	O(6)-Mo(15)-O(41)	105.5(3)
O(48)-Mo(13)-O(1)	100.3(3)	O(45)-Mo(14)-O(75)	99.2(3)	O(6)-Mo(15)-O(70)	94.2(3)
O(48)-Mo(13)-O(56)	168.4(3)	O(45)-Mo(14)-O(66)	97.4(3)	O(6)-Mo(15)-O(60)	93.5(3)
O(48)-Mo(13)-O(33)	90.7(3)	O(45)-Mo(14)-O(63)	170.4(3)	O(6)-Mo(15)-O(29)	161.5(3)
O(71)-Mo(16)-O(8)	102.9(4)	O(7)-Mo(17)-O(9)	100.0(3)	O(12)-Mo(18)-O(18)	105.0(3)
O(71)-Mo(16)-O(17)	103.6(3)	O(7)-Mo(17)-O(31)	100.9(3)	O(12)-Mo(18)-O(60)	101.4(3)
O(71)-Mo(16)-O(61)	101.0(3)	O(7)-Mo(17)-O(54)	101.6(3)	O(12)-Mo(18)-O(61)	98.7(3)
O(71)-Mo(16)-O(38)	167.8(3)	O(7)-Mo(17)-O(62)	92.1(3)	O(12)-Mo(18)-O(38)	97.7(3)
O(71)-Mo(16)-O(22)	85.7(3)	O(7)-Mo(17)-O(27)	168.6(3)	O(12)-Mo(18)-O(29)	170.2(3)
O(44)-P(1)-O(69)	109.1(4)	O(44)-P(1)-O(53)	111.4(4)	O(44)-P(1)-O(22)	111.0(4)
O(33)-P(2)-O(72)	111.2(4)	O(33)-P(2)-O(46)	110.3(4)	O(33)-P(2)-O(5)	110.2(4)
O(43)-P(3)-O(42)	108.4(4)	O(43)-P(3)-O(20)	110.5(4)	O(43)-P(3)-O(63)	110.0(4)
O(25)-P(4)-O(58)	110.5(4)	O(25)-P(4)-O(36)	110.4(4)	O(25)-P(4)-O(38)	108.6(4)
O(56)-P(5)-O(51)	110.7(4)	O(56)-P(5)-O(2)	111.7(4)	O(56)-P(5)-O(66)	108.3(4)
O(19)-P(6)-O(27)	111.4(4)	O(19)-P(6)-O(16)	108.1(4)	O(19)-P(6)-O(29)	110.1(4)
O(53)-Sr(1)-O(58)	64.9(2)	O(53)-Sr(1)-O(56)	81.1(2)	O(53)-Sr(1)-O(42)	171.0(2)
O(53)-Sr(1)-O(33)	114.5(2)	O(53)-Sr(1)-O(43)	119.5(2)	O(53)-Sr(1)-O(19)	100.9(2)
O(53)-Sr(1)-O(16)	72.1(2)	O(53)-Sr(1)-O(14)	57.4(2)		
O(44)#2-Fe(1)-O(25)	176.1(3)	O(44)#2-Fe(1)-O(52)	90.4(3)	O(44)#2-Fe(1)-O(73)	91.8(3)
O(44)#2-Fe(1)-O(13)	86.0(3)	O(44)#2-Fe(1)-O(3)	97.9(3)		

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(60)	1.726(5)	Mo(2)-O(14)	1.769(5)	Mo(3)-O(69)	1.717(5)
Mo(1)-O(4)	1.927(5)	Mo(2)-O(39)	1.770(5)	Mo(3)-O(9)	1.935(5)
Mo(1)-O(45)	1.937(5)	Mo(2)-O(1)	1.926(5)	Mo(3)-O(5)	1.935(6)
Mo(1)-O(13)	1.983(5)	Mo(2)-O(30)	2.026(5)	Mo(3)-O(51)	2.087(5)
Mo(1)-O(56)	2.175(5)	Mo(2)-O(11)	2.262(5)	Mo(3)-O(57)	2.120(5)
Mo(1)-O(25)	2.344(5)	Mo(2)-O(22	2.264(5)	Mo(3)-O(16)	2.281(5)
Mo(4)-O(49)	1.727(5)	Mo(5)-O(27)	1.730(5)	Mo(6)-O(50)	1.728(5)
Mo(4)-O(17)	1.833(5)	Mo(5)-O(18)	1.823(5)	Mo(6)-O(12)	1.916(5)
Mo(4)-O(31)	1.859(5)	Mo(5)-O(19)	1.852(5)	Mo(6)-O(34)	1.927(5)
Mo(4)-O(47)	2.114(5)	Mo(5)-O(47)	2.122(5)	Mo(6)-O(28)	2.091(5)
Mo(4)-O(41)	2.180(5)	Mo(5)-O(63)	2.161(5)	Mo(6)-O(32)	2.101(5)
Mo(4)-O(33)	2.505(5)	Mo(5)-O(33)	2.483(5)	Mo(6)-O(3)	2.294(5)
Mo(7)-O(65)	1.729(5)	Mo(8)-O(58)	1.720(5)	Mo(9)-O(24)	1.726(5)
Mo(7)-O(9)	1.913(5)	Mo(8)-O(2)	1.918(5)	Mo(9)-O(45)	1.925(5)
Mo(7)-O(29)	1.924(5)	Mo(8)-O(29)	1.949(5)	Mo(9)-O(12)	1.932(5)

Mo(7)-O(8)	2.082(5)	Mo(8)-O(13)	1.955(5)	Mo(9)-O(17)	2.089(5)
Mo(7)-O(18)	2.113(5)	Mo(8)-O(53)	2.189(5)	Mo(9)-O(37)	2.117(5)
Mo(7)-O(20)	2.277(5)	Mo(8)-O(25)	2.360(5)	Mo(9)-O(38)	2.271(5)
Mo(10)-O(54)	1.735(5)	Mo(11)-O(48)	1.734(6)	Mo(12)-O(67)	1.733(6)
Mo(10)-O(53)	1.837(5)	Mo(11)-O(32)	1.830(5)	Mo(12)-O(51)	1.833(5)
Mo(10)-O(56)	1.838(5)	Mo(11)-O(55)	1.848(5)	Mo(12)-O(62)	1.859(6)
Mo(10)-O(31)	2.134(5)	Mo(11)-O(43)	2.110(5)	Mo(12)-O(43)	2.106(5)
Mo(10)-O(19)	2.144(5)	Mo(11)-O(40)	2.195(5)	Mo(12)-O(61)	2.189(5)
Mo(10)-O(33)	2.435(5)	Mo(11)-O(6)	2.495(5)	Mo(12)-O(6)	2.450(5)
Mo(13)-O(71)	1.750(6)	Mo(14)-O(74)	1.748(6)	Mo(15)-O(75)	1.726(6)
Mo(13)-O(59)	1.755(6)	Mo(14)-O(73)	1.751(6)	Mo(15)-O(5)	1.931(6)
Mo(13)-O(30)	1.882(5)	Mo(14)-O(36)	1.899(5)	Mo(15)-O(2)	1.941(5)
Mo(13)-O(47)	2.078(5)	Mo(14)-O(43)	2.097(5)	Mo(15)-O(15)	2.010(5)
Mo(13)-O(63)	2.406(5)	Mo(14)-O(40)	2.400(5)	Mo(15)-O(52)	2.143(6)
Mo(13)-O(41)	2.450(5)	Mo(14)-O(61)	2.439(5)	Mo(15)-O(7)	2.354(5)
Mo(16)-O(68)	1.747(6)	Mo(17)-O(72)	1.739(6)	Mo(18)-O(23)	1.720(5)
Mo(16)-O(64)	1.755(6)	Mo(17)-O(26)	1.842(5)	Mo(18)-O(34)	1.932(5)
Mo(16)-O(1)	1.998(5)	Mo(17)-O(52)	1.843(6)	Mo(18)-O(4)	1.941(5)
Mo(16)-O(36)	2.003(5)	Mo(17)-O(62)	2.127(5)	Mo(18)-O(15)	1.991(5)
Mo(16)-O(44)	2.344(5)	Mo(17)-O(55)	2.140(5)	Mo(18)-O(26)	2.157(5)
Mo(16)-O(10)	2.354(5)	Mo(17)-O(6)	2.476(5)	Mo(18)-O(7)	2.363(5)
P(1)-O(38)	1.558(5)	P(2)-O(7)	1.562(5)	P(3)-O(42)	1.537(5)
P(1)-O(20)	1.563(5)	P(2)-O(3)	1.564(5)	P(3)-O(22)	1.578(5)
P(1)-O(25)	1.570(5)	P(2)-O(16)	1.569(5)	P(3)-O(37)	1.583(5)
P(1)-O(33)	1.623(5)	P(2)-O(6)	1.618(5)	P(3)-O(41)	1.612(5)
P(4)-O(21)	1.546(5)	P(5)-O(10)	1.549(5)	P(6)-O(28)	1.559(5)
P(4)-O(8)	1.574(5)	P(5)-O(57)	1.565(6)	P(6)-O(44)	1.562(5)
P(4)-O(11)	1.580(5)	P(5)-O(61)	1.599(5)	P(6)-O(46)	1.587(6)
P(4)-O(63)	1.621(5)	P(5)-O(66)	1.607(5)	P(6)-O(40)	1.603(5)
Sr(1)-O(11)	2.602(5)	Sr(1)-O(22)	2.616(5)	Sr(1)-O(44)	2.654(5)
Sr(1)-O(10)	2.704(5)	Sr(1)-O(16)	2.705(5)	Sr(1)-O(3)	2.709(5)
Sr(1)-O(20)	2.726(5)	Sr(1)-O(38)	2.732(5)	Sr(1)-O(1)	2.934(5)
Co(1)-O(42)#1	2.093(5)	Co(1)-O(21)	2.106(5)	Co(1)-O(39)#1	2.163(5)
Co(1)-O(14)	2.169(5)	Co(1)-O(70)	2.181(6)	Co(1)-O(35)	2.220(5)
O(60)-Mo(1)-O(4)	100.5(2)	O(14)-Mo(2)-O(39)	103.6(2)	O(69)-Mo(3)-O(9)	98.5(2)
O(60)-Mo(1)-O(45)	101.5(2)	O(14)-Mo(2)-O(1)	99.7(2)	O(69)-Mo(3)-O(5)	101.4(2)
O(60)-Mo(1)-O(13)	100.9(2)	O(14)-Mo(2)-O(30)	94.2(2)	O(69)-Mo(3)-O(51)	94.2(2)
O(60)-Mo(1)-O(56)	91.9(2)	O(14)-Mo(2)-O(11)	90.1(2)	O(69)-Mo(3)-O(57)	95.6(2)
O(60)-Mo(1)-O(25)	168.2(2)	O(14)-Mo(2)-O(22)	166.0(2)	O(69)-Mo(3)-O(16)	173.3(2)
O(49)-Mo(4)-O(17)	104.8(2)	O(27)-Mo(5)-O(18)	104.7(3)	O(50)-Mo(6)-O(12)	99.5(2)
O(49)-Mo(4)-O(31)	101.6(2)	O(27)-Mo(5)-O(19)	100.9(2)	O(50)-Mo(6)-O(34)	101.1(2)
O(49)-Mo(4)-O(47)	99.6(2)	O(27)-Mo(5)-O(47)	98.5(2)	O(50)-Mo(6)-O(28)	96.1(2)
O(49)-Mo(4)-O(41)	97.1(2)	O(27)-Mo(5)-O(63)	98.2(2)	O(50)-Mo(6)-O(32)	93.3(2)
O(49)-Mo(4)-O(33)	170.6(2)	O(27)-Mo(5)-O(33)	170.0(2)	O(50)-Mo(6)-O(3)	172.8(2)
O(65)-Mo(7)-O(9)	99.9(2)	O(58)-Mo(8)-O(2)	100.2(2)	O(24)-Mo(9)-O(45)	101.7(2)
O(65)-Mo(7)-O(29)	100.3(2)	O(58)-Mo(8)-O(29)	100.4(2)	O(24)-Mo(9)-O(12)	98.5(2)
O(65)-Mo(7)-O(8)	97.1(2)	O(58)-Mo(8)-O(13)	102.1(2)	O(24)-Mo(9)-O(17)	93.2(2)
O(65)-Mo(7)-O(18)	91.8(2)	O(58)-Mo(8)-O(53)	93.0(2)	O(24)-Mo(9)-O(37)	94.7(2)
O(65)-Mo(7)-O(20)	172.9(2)	O(58)-Mo(8)-O(25)	169.5(2)	O(24)-Mo(9)-O(38)	172.0(2)
O(54)-Mo(10)-O(53)	105.6(3)	O(48)-Mo(11)-O(32)	104.4(3)	O(67)-Mo(12)-O(51)	104.5(3)
O(54)-Mo(10)-O(56)	105.0(3)	O(48)-Mo(11)-O(55)	102.2(3)	O(67)-Mo(12)-O(62)	101.7(3)
O(54)-Mo(10)-O(31)	93.7(2)	O(48)-Mo(11)-O(43)	99.1(2)	O(67)-Mo(12)-O(43)	97.4(2)
O(54)-Mo(10)-O(19)	94.0(2)	O(48)-Mo(11)-O(40)	96.9(2)	O(67)-Mo(12)-O(61)	97.1(2)
O(54)-Mo(10)-O(33)	161.3(2)	O(48)-Mo(11)-O(6)	170.4(2)	O(67)-Mo(12)-O(6)	169.7(2)
O(71)-Mo(13)-O(59)	102.6(3)	O(74)-Mo(14)-O(73)	103.1(3)	O(75)-Mo(15)-O(5)	101.9(3)
O(71)-Mo(13)-O(30)	104.3(3)	O(74)-Mo(14)-O(36)	104.6(3)	O(75)-Mo(15)-O(2)	100.5(2)
O(71)-Mo(13)-O(47)	99.3(2)	O(74)-Mo(14)-O(43)	99.1(2)	O(75)-Mo(15)-O(15)	100.1(3)

O(71)-Mo(13)-O(63)	85.7(2)	O(74)-Mo(14)-O(40)	87.1(2)	O(75)-Mo(15)-O(52)	92.9(2)
O(71)-Mo(13)-O(41)	166.7(2)	O(74)-Mo(14)-O(61)	166.4(2)	O(75)-Mo(15)-O(7)	169.1(2)
O(68)-Mo(16)-O(64)	103.5(3)	O(72)-Mo(17)-O(26)	104.7(3)	O(23)-Mo(18)-O(34)	101.1(2)
O(68)-Mo(16)-O(1)	99.2(2)	O(72)-Mo(17)-O(52)	104.9(3)	O(23)-Mo(18)-O(4)	101.3(2)
O(68)-Mo(16)-O(36)	99.0(2)	O(72)-Mo(17)-O(62)	96.7(3)	O(23)-Mo(18)-O(15)	100.7(2)
O(68)-Mo(16)-O(44)	168.8(2)	O(72)-Mo(17)-O(55)	95.7(3)	O(23)-Mo(18)-O(26)	91.4(2)
O(68)-Mo(16)-O(10)	91.2(2)	O(72)-Mo(17)-O(6)	163.3(2)	O(23)-Mo(18)-O(7)	167.6(2)
O(38)-P(1)-O(20)	108.0(3)	O(7)-P(2)-O(3)	111.1(3)	O(42)-P(3)-O(22)	110.8(3)
O(38)-P(1)-O(25)	110.9(3)	O(7)-P(2)-O(16)	111.1(3)	O(42)-P(3)-O(37)	109.1(3)
O(38)-P(1)-O(33)	109.6(3)	O(7)-P(2)-O(6)	107.6(3)	O(42)-P(3)-O(41)	111.7(3)
O(21)-P(4)-O(8)	110.4(3)	O(10)-P(5)-O(57)	111.1(3)	O(28)-P(6)-O(44)	111.0(3)
O(21)-P(4)-O(11)	110.3(3)	O(10)-P(5)-O(61)	109.8(3)	O(28)-P(6)-O(46)	104.5(3)
O(21)-P(4)-O(63)	109.3(3)	O(10)-P(5)-O(66)	110.8(3)	O(28)-P(6)-O(40)	112.2(3)
O(11)-Sr(1)-O(22)	64.57(15)	O(11)-Sr(1)-O(44)	115.98(16)	O(11)-Sr(1)-O(10)	79.99(16)
O(11)-Sr(1)-O(16)	118.81(15)	O(11)-Sr(1)-O(3)	170.91(15)	O(11)-Sr(1)-O(20)	72.52(15)
O(11)-Sr(1)-O(38)	100.96(15)	O(11)-Sr(1)-O(1)	58.18(14)		
O(42)#1-Co(1)-O(21)	176.6(2)	O(42)#1-Co(1)-O(39)#1	90.11(19)	O(42)#1-Co(1)-O(14)	91.66(19)
O(42)#1-Co(1)-O(70)	84.8(2)	O(42)#1-Co(1)-O(35)	98.0(2)		

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

Table S3 Selected bond lengths (Å) and bond angles (º) of compound **3**

Mo(1)-O(59)	1.675(6)	Mo(1)-O(39)	1.775(5)	Mo(1)-O(17)	1.800(6)
Mo(1)-O(31)	2.040(5)	Mo(1)-O(27)	2.123(5)	Mo(1)-O(20)	2.431(5)
Mo(2)-O(69)	1.676(6)	Mo(2)-O(3)	1.861(5)	Mo(2)-O(42)	1.873(5)
Mo(2)-O(6)	1.921(5)	Mo(2)-O(29)	2.101(6)	Mo(2)-O(24)	2.266(5)
Mo(3)-O(26)	1.663(5)	Mo(3)-O(44)	1.770(6)	Mo(3)-O(35)	1.807(5)
Mo(3)-O(31)	2.053(5)	Mo(3)-O(46)	2.095(5)	Mo(3)-O(20)	2.394(5)
Mo(4)-O(62)	1.669(6)	Mo(4)-O(5)	1.875(6)	Mo(4)-O(7)	1.880(5)
Mo(4)-O(43)	2.023(5)	Mo(4)-O(28)	2.048(6)	Mo(4)-O(32)	2.217(5)
Mo(5)-O(74)	1.674(6)	Mo(5)-O(4)	1.856(5)	Mo(5)-O(41)	1.871(5)
Mo(5)-O(14	2.021(5)	Mo(5)-O(36)	2.023(6)	Mo(5)-O(16)	2.223(5)
Mo(6)-O(66)	1.676(6)	Mo(6)-O(2)	1.854(5)	Mo(6)-O(19)	1.884(6)
Mo(6)-O(6)	1.895(6)	Mo(6)-O(30)	2.123(6)	Mo(6)-O(24)	2.291(5)
Mo(7)-O(63)	1.686(6)	Mo(7)-O(67)	1.695(6)	Mo(7)-O(8)	1.814(5)
Mo(7)-O(31)	2.027(6)	Mo(7)-O(46)	2.335(5)	Mo(7)-O(27)	2.367(5)
Mo(8)-O(40)	1.673(6)	Mo(8)-O(30)	1.778(6)	Mo(8)-O(29)	1.779(6)
Mo(8)-O(17)	2.065(6)	Mo(8)-O(35)	2.068(5)	Mo(8)-O(20)	2.367(5)
Mo(9)-O(54)	1.679(5)	Mo(9)-O(4)	1.854(5)	Mo(9)-O(42)	1.873(5)
Mo(9)-O(39)	2.015(5)	Mo(9)-O(23)	2.049(5)	Mo(9)-O(49)	2.193(5)
Mo(10)-O(72)	1.672(6)	Mo(10)-O(5)	1.870(6)	Mo(10)-O(2)	1.872(5)
Mo(10)-O(50)	1.950(6)	Mo(10)-O(10)	2.074(6)	Mo(10)-O(21)	2.277(5)
Mo(11)-O(53)	1.670(6)	Mo(11)-O(14)	1.783(5)	Mo(11)-O(61)	1.796(6)
Mo(11)-O(38)	2.044(5)	Mo(11)-O(25)	2.134(5)	Mo(11)-O(18)	2.416(5)
Mo(12)-O(55)	1.708(5)	Mo(12)-O(45)	1.722(5)	Mo(12)-O(1)	1.864(5)
Mo(12)-O(8)	1.960(5)	Mo(12)-O(12)	2.191(5)	Mo(12)-O(22)	2.197(5)
Mo(13)-O(65)	1.674(6)	Mo(13)-O(43)	1.771(5)	Mo(13)-O(51)	1.807(6)
Mo(13)-O(38)	2.046(5)	Mo(13)-O(58)	2.124(6)	Mo(13)-O(18)	2.353(5)
Mo(14)-O(71)	1.685(6)	Mo(14)-O(52)	1.689(6)	Mo(14)-O(11)	1.838(6)
Mo(14)-O(38)	2.029(6)	Mo(14)-O(25)	2.303(6)		
Mo(15)-O(48)	1.683(6)	Mo(15)-O(70)	1.687(6)	Mo(15)-O(1)	1.923(5)
Mo(15)-O(11)	1.932(6)	Mo(15)-O(15)	2.271(6)	Mo(15)-O(60)	2.274(6)
Mo(16)-O(73)	1.674(6)	Mo(16)-O(7)	1.834(5)	Mo(16)-O(19)	1.875(6)
Mo(16)-O(34)	2.020(5)	Mo(16)-O(44)	2.037(6)	Mo(16)-O(33)	2.205(5)
Mo(17)-O(64)	1.691(6)	Mo(17)-O(9)	1.779(6)	Mo(17)-O(10)	1.783(6)
Mo(17)-O(61)	2.070(6)	Mo(17)-O(51)	2.070(6)	Mo(17)-O(18)	2.405(6)
Mo(18)-O(37)	1.658(6)	Mo(18)-O(41)	1.869(5)	Mo(18)-O(3)	1.869(5)

Mo(18)-O(50)	1.926(6)	Mo(18)-O(9)	2.085(6)	Mo(18)-O(21)	2.278(5)
P(1)-O(33)	1.505(5)	P(2)-O(32)	1.505(5)	P(3)-O(56)	1.497(5)
P(1)-O(49)	1.507(5)	P(2)-O(16)	1.508(6)	P(3)-O(22)	1.528(5)
P(1)-O(24)	1.523(6)	P(2)-O(21)	1.532(6)	P(3)-O(23)	1.536(6)
P(1)-O(20)	1.564(5)	P(2)-O(18)	1.565(6)	P(3)-O(27)	1.552(5)
P(4)-O(13)	1.503(5)	P(5)-O(28)	1.507(6)	P(6)-O(60)	1.508(6)
P(4)-O(34)	1.521(5)	P(5)-O(15)	1.514(6)	P(6)-O(36)	1.514(6)
P(4)-O(12)	1.522(5)	P(5)-O(57)	1.546(6)	P(6)-O(68)	1.538(6)
P(4)-O(46)	1.565(5)	P(5)-O(41)	1.560(6)	P(6)-O(25)	1.561(6)
Sr(1)-O(12)	2.519(5)	Sr(1)-O(15)	2.613(6)	Sr(1)-O(33)	2.638(5)
Sr(1)-O(22)	2.522(5)	Sr(1)-O(32)	2.612(5)	Sr(1)-O(49)	2.648(5)
Sr(1)-O(60)	2.569(5)	Sr(1)-O(16)	2.630(5)	Sr(1)-O(1)	2.852(6)
Ni(1)-O(56)#1	2.017(5)	Ni(1)-O(13)	2.031(5)	Ni(1)-O(45)#1	2.063(5)
Ni(1)-O(55)	2.088(5)	Ni(1)-O(75)	2.051(6)	Ni(1)-O(47)	2.066(6)
O(59)-Mo(1)-O(39)	105.1(3)	O(69)-Mo(2)-O(3)	100.9(3)	O(26)-Mo(3)-O(44)	104.5(3)
O(59)-Mo(1)-O(17)	102.1(3)	O(69)-Mo(2)-O(42)	101.7(3)	O(26)-Mo(3)-O(35)	101.3(3)
O(59)-Mo(1)-O(31)	99.4(3)	O(69)-Mo(2)-O(6)	100.5(3)	O(26)-Mo(3)-O(31)	98.1(3)
O(59)-Mo(1)-O(27)	96.4(3)	O(69)-Mo(2)-O(29)	91.9(3)	O(26)-Mo(3)-O(46)	97.9(3)
O(59)-Mo(1)-O(20)	170.4(2)	O(69)-Mo(2)-O(24)	168.4(2)	O(26)-Mo(3)-O(20)	169.9(2)
O(62)-Mo(4)-O(5)	101.4(3)	O(74)-Mo(5)-O(4)	99.8(3)	O(66)-Mo(6)-O(2)	100.2(3)
O(62)-Mo(4)-O(7)	98.4(3)	O(74)-Mo(5)-O(41)	100.6(3)	O(66)-Mo(6)-O(19)	100.6(3)
O(62)-Mo(4)-O(43)	93.7(3)	O(74)-Mo(5)-O(14)	92.9(3)	O(66)-Mo(6)-O(6)	101.6(3)
O(62)-Mo(4)-O(28)	95.8(3)	O(74)-Mo(5)-O(36)	96.9(3)	O(66)-Mo(6)-O(30)	92.8(3)
O(62)-Mo(4)-O(32)	173.4(2)	O(74)-Mo(5)-O(16)	173.2(3)	O(66)-Mo(6)-O(24)	169.4(2)
O(63)-Mo(7)-O(67)	102.8(3)	O(40)-Mo(8)-O(30)	105.6(3)	O(54)-Mo(9)-O(4)	98.3(3)
O(63)-Mo(7)-O(8)	104.4(3)	O(40)-Mo(8)-O(29)	104.8(3)	O(54)-Mo(9)-O(42)	101.8(3)
O(63)-Mo(7)-O(31)	99.1(3)	O(40)-Mo(8)-O(17)	93.5(3)	O(54)-Mo(9)-O(39)	93.3(2)
O(63)-Mo(7)-O(46)	85.9(3)	O(40)-Mo(8)-O(35)	93.7(3)	O(54)-Mo(9)-O(23)	94.8(2)
O(63)-Mo(7)-O(27)	166.9(2)	O(40)-Mo(8)-O(20)	160.7(3)	O(54)-Mo(9)-O(49)	171.8(2)
O(72)-Mo(10)-O(5)	102.2(3)	O(53)-Mo(11)-O(14)	104.6(3)	O(55)-Mo(12)-O(45)	103.8(3)
O(72)-Mo(10)-O(2)	100.5(3)	O(53)-Mo(11)-O(61)	102.5(3)	O(55)-Mo(12)-O(1)	99.3(2)
O(72)-Mo(10)-O(50)	100.1(3)	O(53)-Mo(11)-O(38)	98.8(3)	O(55)-Mo(12)-O(8)	94.8(2)
O(72)-Mo(10)-O(10)	92.9(3)	O(53)-Mo(11)-O(25)	96.4(3)	O(55)-Mo(12)-O(12)	90.0(2)
O(72)-Mo(10)-O(21)	169.3(3)	O(53)-Mo(11)-O(18)	170.0(2)	O(55)-Mo(12)-O(22)	165.7(2)
O(65)-Mo(13)-O(43)	104.5(3)	O(71)-Mo(14)-O(52)	102.8(3)	O(48)-Mo(15)-O(70)	103.8(3)
O(65)-Mo(13)-O(51)	101.2(3)	O(71)-Mo(14)-O(11)	105.7(3)	O(48)-Mo(15)-O(1)	98.5(3)
O(65)-Mo(13)-O(38)	96.4(3)	O(71)-Mo(14)-O(38)	96.7(3)	O(48)-Mo(15)-O(11)	99.7(3)
O(65)-Mo(13)-O(58)	96.7(3)	O(71)-Mo(14)-O(25)	164.0(3)	O(48)-Mo(15)-O(15)	91.4(3)
O(65)-Mo(13)-O(18)	169.0(2)			O(48)-Mo(15)-O(60)	168.7(3)
O(73)-Mo(16)-O(7)	99.7(3)	O(64)-Mo(17)-O(9)	104.2(3)	O(37)-Mo(18)-O(41)	101.6(3)
O(73)-Mo(16)-O(19)	100.0(3)	O(64)-Mo(17)-O(10)	104.6(3)	O(37)-Mo(18)-O(3)	102.2(3)
O(73)-Mo(16)-O(34)	97.4(2)	O(64)-Mo(17)-O(61)	95.7(3)	O(37)-Mo(18)-O(50)	100.0(3)
O(73)-Mo(16)-O(44)	91.5(3)	O(64)-Mo(17)-O(51)	96.7(3)	O(37)-Mo(18)-O(9)	90.7(3)
O(73)-Mo(16)-O(33)	172.9(2)	O(64)-Mo(17)-O(18)	163.1(3)	O(37)-Mo(18)-O(21)	167.1(2)
O(33)-P(1)-O(49)	108.2(3)	O(33)-P(1)-O(24)	111.6(3)	O(33)-P(1)-O(20)	109.2(3)
O(32)-P(2)-O(16)	108.0(3)	O(32)-P(2)-O(21)	111.1(3)	O(32)-P(2)-O(18)	109.0(3)
O(56)-P(3)-O(22)	110.2(3)	O(56)-P(3)-O(23)	109.8(3)	O(56)-P(3)-O(27)	111.4(3)
O(13)-P(4)-O(34)	110.9(3)	O(13)-P(4)-O(12)	110.0(3)	O(13)-P(4)-O(46)	109.1(3)
O(28)-P(5)-O(15)	111.9(3)	O(28)-P(5)-O(58)	111.3(3)	O(28)-P(5)-O(57)	108.2(3)
O(60)-P(6)-O(36)	111.4(3)	O(60)-P(6)-O(68)	111.9(3)	O(60)-P(6)-O(25)	108.4(3)
O(12)-Sr(1)-O(22)	64.62(17)	O(12)-Sr(1)-O(32)	119.24(17)	O(12)-Sr(1)-O(49)	101.33(16)
O(12)-Sr(1)-O(60)	115.76(18)	O(12)-Sr(1)-O(16)	170.77(17)	O(12)-Sr(1)-O(1)	58.08(16)
O(12)-Sr(1)-O(15)	79.46(17)	O(12)-Sr(1)-O(33)	72.83(17)	O(56)#1-Ni(1)-O(55)	90.8(2)
O(56)#1-Ni(1)-O(13)	177.2(2)	O(56)#1-Ni(1)-O(75)	85.1(2)	O(56)#1-Ni(1)-O(45)#1	90.5(2)
O(56)#1-Ni(1)-O(47)	97.4(2)				

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

Table S4 Selected bond lengths (Å) and bond angles (º) of compound **4**

Mo(1)-O(45)	1.670(9)	Mo(2)-O(55)	1.679(9)	Mo(3)-O(66)	1.678(10)
Mo(1)-O(8)	1.865(9)	Mo(2)-O(2)	1.860(9)	Mo(3)-O(7)	1.869(10)
Mo(1)-O(15)	1.883(9)	Mo(2)-O(44)	1.876(9)	Mo(3)-O(56)	1.889(10)
Mo(1)-O(10)	2.038(9)	Mo(2)-O(23)	2.037(9)	Mo(3)-O(49)	1.941(10)
Mo(1)-O(12)	2.054(9)	Mo(2)-O(52)	2.071(9)	Mo(3)-O(41)	2.101(9)
Mo(1)-O(27)	2.226(8)	Mo(2)-O(1)	2.222(8)	Mo(3)-O(9)	2.285(8)
Mo(4)-O(68)	1.674(9)	Mo(5)-O(20)	2.917(19)	Mo(6)-O(58)	1.676(9)
Mo(4)-O(18)	1.869(9)	Mo(5)-O(70)	1.782(10)	Mo(6)-O(17)	1.782(9)
Mo(4)-O(5)	1.869(9)	Mo(5)-O(16)	1.794(9)	Mo(6)-O(30)	1.810(10)
Mo(4)-O(19)	1.922(9)	Mo(5)-O(30)	2.078(9)	Mo(6)-O(25)	2.068(9)
Mo(4)-O(70)	2.123(10)	Mo(5)-O(28)	2.086(10)	Mo(6)-O(26)	2.121(9)
Mo(4)-O(70)	2.290(8)	Mo(5)-O(13)	2.398(8)	Mo(6)-O(13)	2.429(9)
Mo(7)-O(48)	1.688(9)	Mo(8)-O(42)	1.681(9)	Mo(9)-O(64)	1.709(10)
Mo(7)-O(2)	1.876(9)	Mo(8)-O(10)	1.782(9)	Mo(9)-O(65)	1.713(10)
Mo(7)-O(5)	1.896(9)	Mo(8)-O(28)	1.796(9)	Mo(9)-O(4)	1.876(9)
Mo(7)-O(17)	2.029(9)	Mo(8)-O(25)	2.056(9)	Mo(9)-O(14)	1.989(9)
Mo(7)-O(24)	2.075(8)	Mo(8)-O(22)	2.121(9)	Mo(9)-O(11)	2.212(9)
Mo(7)-O(36)	2.211(8)	Mo(8)-O(13)	2.409(9)	Mo(9)-O(33)	2.214(8)
Mo(10)-O(63)	1.696(11)	Mo(11)-O(74)	1.697(10)	Mo(12)-O(61)	1.680(9)
Mo(10)-O(71)	1.693(10)	Mo(11)-O(73)	1.704(10)	Mo(12)-O(18)	1.885(10)
Mo(10)-O(14)	1.818(9)	Mo(11)-O(32)	1.848(10)	Mo(12)-O(44)	1.888(9)
Mo(10)-O(25)	2.033(9)	Mo(11)-O(43)	2.045(10)	Mo(12)-O(49)	1.945(10)
Mo(10)-O(22)	2.328(8)	Mo(11)-O(34)	2.338(9)	Mo(12)-O(62) (3)#16	2.109(10)
Mo(10)-O(26)	2.408(9)	Mo(11)-O(53)	2.342(9)	Mo(12)-O(9)	2.308(9)
Mo(13)-O(67)	1.677(10)	Mo(14)-O(54)	1.684(9)	Mo(15)-O(46)	1.688(10)
Mo(13)-O(29)	1.772(10)	Mo(14)-O(8)	1.870(9)	Mo(15)-O(52)	1.762(9)
Mo(13)-O(39)	1.824(10)	Mo(14)-O(56)	1.896(9)	Mo(15)-O(60)	1.807(10)
Mo(13)-O(43)	2.055(10)	Mo(14)-O(29)	2.041(10)	Mo(15)-O(43)	2.058(10)
Mo(13)-O(53)	2.127(9)	Mo(14)-O(59)	2.060(9)	Mo(15)-O(34)	2.129(9)
Mo(13)-O(21)	2.393(9)	Mo(14)-O(35)	2.222(9)	Mo(15)-O(21)	2.429(9)
Mo(16)-O(50)	1.668(9)	Mo(17)-O(51)	1.692(10)	Mo(18)-O(57)	1.684(9)
Mo(16)-O(7)	1.879(10)	Mo(17)-O(72)	1.698(10)	Mo(18)-O(41)	1.770(10)
Mo(16)-O(15)	1.892(9)	Mo(17)-O(4)	1.936(9)	Mo(18)-O(62)	1.784(10)
Mo(16)-O(19)	1.912(9)	Mo(17)-O(32)	1.945(9)	Mo(18)-O(39)	2.073(10)
Mo(16)-O(16)	2.116(9)	Mo(17)-O(37)	2.272(9)	Mo(18)-O(60)	2.073(10)
Mo(16)-O(38)	2.312(8)	Mo(17)-O(6)	2.281(9)	Mo(18)-O(21)	2.415(8)
P(1)-O(35)	1.513(9)	P(2)-O(36)	1.518(9)	P(3)-O(31)	1.516(9)
P(1)-O(9)	1.522(9)	P(2)-O(27)	1.522(8)	P(3)-O(12)	1.517(9)
P(1)-O(1)	1.523(9)	P(2)-O(38)	1.528(8)	P(3)-O(11)	1.526(9)
P(1)-O(21)	1.572(9)	P(2)-O(13)	1.579(9)	P(3)-O(22)	1.572(9)
P(4)-O(40)	1.513(9)	P(5)-O(59)	1.516(10)	P(6)-O(23)	1.518(9)
P(4)-O(33)	1.532(9)	P(5)-O(6)	1.519(10)	P(6)-O(37)	1.527(9)
P(4)-O(24)	1.539(9)	P(5)-O(69)	1.534(10)	P(6)-O(47)	1.544(10)
P(4)-O(26)	1.555(9)	P(5)-O(53)	1.566(10)	P(6)-O(34)	1.574(9)
Sr(1)-O(11)	2.543(9)	Sr(1)-O(6)	2.600(9)	Sr(1)-O(27)	2.645(8)
Sr(1)-O(33)	2.555(9)	Sr(1)-O(35)	2.628(9)	Sr(1)-O(36)	2.659(9)
Sr(1)-O(37)	2.577(9)	Sr(1)-O(1)	2.641(8)	Sr(1)-O(4)	2.856(9)
Cu(1)-O(40)#1	1.935(9)	Cu(1)-O(64)#1	2.124(11)	Cu(1)-O(76)	2.195(12)
Cu(1)-O(31)	1.954(9)	Cu(1)-O(65)	2.157(10)	Cu(1)-O(75)	2.241(11)
O(45)-Mo(1)-O(8)	99.6(4)	O(55)-Mo(2)-O(2)	99.8(4)	O(66)-Mo(3)-O(7))	99.9(5)
O(45)-Mo(1)-O(15)	100.4(4)	O(55)-Mo(2)-O(44)	101.6(4)	O(66)-Mo(3)-O(56)	102.1(5)
O(45)-Mo(1)-O(10)	92.1(4)	O(55)-Mo(2)-O(23)	95.5(4)	O(66)-Mo(3)-O(49)	99.5(5)
O(45)-Mo(1)-O(12)	96.9(4)	O(55)-Mo(2)-O(52)	93.2(4)	O(66)-Mo(3)-O(41)	92.6(4)
O(45)-Mo(1)-O(27)	172.7(4)	O(55)-Mo(2)-O(1)	172.4(4)	O(66)-Mo(3)-O(9)	168.3(4)
O(68)-Mo(4)-O(18)	100.5(4)	O(20)-Mo(5)-O(70)	104.9(5)	O(58)-Mo(6)-O(17)	104.8(4)

O(68)-Mo(4)-O(5)	101.9(4)	O(20)-Mo(5)-O(16)	104.5(4)	O(58)-Mo(6)-O(30)	101.6(4)
O(68)-Mo(4)-O(19)	100.6(4)	O(20)-Mo(5)-O(30)	95.6(4)	O(58)-Mo(6)-O(25)	99.4(4)
O(68)-Mo(4)-O(70)	91.5(4)	O(20)-Mo(5)-O(28)	95.5(4)	O(58)-Mo(6)-O(26)	96.7(4)
O(68)-Mo(4)-O(38)	167.8(4)	O(20)-Mo(5)-O(13)	162.7(4)	O(58)-Mo(6)-O(13)	170.3(4)
O(48)-Mo(7)-O(2)	99.1(4)	O(42)-Mo(8)-O(10)	104.6(4)	O(64)-Mo(9)-O(65)	102.6(5)
O(48)-Mo(7)-O(5)	101.4(4)	O(42)-Mo(8)-O(28)	100.9(4)	O(64)-Mo(9)-O(4)	102.0(4)
O(48)-Mo(7)-O(17)	93.2(4)	O(42)-Mo(8)-O(25)	98.5(4)	O(64)-Mo(9)-O(14)	91.7(4)
O(48)-Mo(7)-O(24)	94.7(4)	O(42)-Mo(8)-O(22)	98.0(4)	O(64)-Mo(9)-O(11)	165.3(4)
O(48)-Mo(7)-O(36)	172.1(4)	O(42)-Mo(8)-O(13)	170.0(4)	O(64)-Mo(9)-O(33)	90.1(4)
O(63)-Mo(10)-O(71)	102.4(5)	O(74)-Mo(11)-O(73)	102.9(5)	O(61)-Mo(12)-O(18)	101.6(5)
O(63)-Mo(10)-O(14)	104.3(5)	O(74)-Mo(11)-O(32)	106.1(5)	O(61)-Mo(12)-O(44)	100.2(5)
O(63)-Mo(10)-O(25)	100.6(4)	O(74)-Mo(11)-O(43)	96.4(5)	O(61)-Mo(12)-O(49)	102.1(5)
O(63)-Mo(10)-O(22)	85.6(4)	O(74)-Mo(11)-O(34)	163.6(4)	O(61)-Mo(12)-O(62)	91.3(4)
O(63)-Mo(10)-O(26)	167.7(4)	O(74)-Mo(11)-O(53)	85.6(4)	O(61)-Mo(12)-O(9)	167.9(4)
O(67)-Mo(13)-O(29)	105.2(5)	O(54)-Mo(14)-O(8)	98.5(4)	O(46)-Mo(15)-O(52)	104.7(5)
O(67)-Mo(13)-O(39)	100.5(5)	O(54)-Mo(14)-O(56)	100.7(4)	O(46)-Mo(15)-O(60)	102.3(5)
O(67)-Mo(13)-O(43)	97.5(5)	O(54)-Mo(14)-O(29)	93.3(4)	O(46)-Mo(15)-O(43)	98.5(5)
O(67)-Mo(13)-O(53)	98.2(5)	O(54)-Mo(14)-O(59)	96.4(4)	O(46)-Mo(15)-O(34)	96.8(4)
O(67)-Mo(13)-O(21)	169.2(4)	O(54)-Mo(14)-O(35)	173.3(4)	O(46)-Mo(15)-O(21)	170.1(4)
O(50)-Mo(16)-O(7)	99.4(5)	O(51)-Mo(17)-O(72)	103.4(5)	O(57)-Mo(18)-O(41)	104.6(5)
O(50)-Mo(16)-O(15)	99.7(4)	O(51)-Mo(17)-O(4)	99.1(5)	O(57)-Mo(18)-O(62)	104.2(5)
O(50)-Mo(16)-O(19)	102.9(4)	O(51)-Mo(17)-O(32)	98.8(5)	O(57)-Mo(18)-O(39)	97.0(5)
O(50)-Mo(16)-O(16)	93.3(4)	O(51)-Mo(17)-O(37)	168.4(4)	O(57)-Mo(18)-O(60)	96.1(5)
O(50)-Mo(16)-O(38)	170.6(4)	O(51)-Mo(17)-O(6)	91.6(4)	O(57)-Mo(18)-O(21)	163.7(5)
O(35)-P(1)-O(9)	111.4(5)	O(36)-P(2)-O(27)	107.9(5)	O(31)-P(3)-O(12)	110.0(5)
O(35)-P(1)-O(1)	108.0(5)	O(36)-P(2)-O(38)	110.7(5)	O(31)-P(3)-O(11)	110.2(5)
O(35)-P(1)-O(21)	109.4(5)	O(36)-P(2)-O(13)	109.2(5)	O(31)-P(3)-O(22)	108.3(5)
O(40)-P(4)-O(33)	109.9(5)	O(59)-P(5)-O(6)	110.0(5)	O(23)-P(6)-O(37)	110.1(5)
O(40)-P(4)-O(24)	109.3(5)	O(59)-P(5)-O(69)	109.0(6)	O(23)-P(6)-O(47)	106.0(6)
O(40)-P(4)-O(26)	110.6(5)	O(59)-P(5)-O(53)	110.6(5)	O(23)-P(6)-O(34)	111.5(5)
O(11)-Sr(1)-O(33)	64.5(3)	O(11)-Sr(1)-O(1)	170.6(3)	O(31)-Cu(1)-O(64)#1	86.4(4)
O(11)-Sr(1)-O(37)	115.7(3)	O(11)-Sr(1)-O(27)	72.1(3)	O(31)-Cu(1)-O(65)	93.5(4)
O(11)-Sr(1)-O(6)	80.5(3)	O(11)-Sr(1)-O(36)	100.5(3)	O(31)-Cu(1)-O(76)	95.6(4)

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

Table S5 Selected bond lengths (Å) and bond angles (º) of compound **5**

Mo(1)-O(40)	1.691(5)	Mo(1)-O(50)	1.795(5)	Mo(1)-O(6)	1.830(5)
Mo(1)-O(33)	2.089(5)	Mo(1)-O(30)	2.145(5)	Mo(1)-O(21)	2.465(5)
Mo(2)-O(68)	1.713(5)	Mo(2)-O(17)	1.807(5)	Mo(2)-O(44)	1.809(5)
Mo(2)-O(6)	2.109(5)	Mo(2)-O(52)	2.111(5)	Mo(2)-O(21)	2.392(5)
Mo(3)-O(57)	1.699(5)	Mo(3)-O(3)	1.894(5)	Mo(3)-O(27)	1.910(5)
Mo(3)-O(7)	1.950(5)	Mo(3)-O(44)	2.135(5)	Mo(3)-O(20)	2.308(5)
Mo(4)-O(71)	1.696(5)	Mo(4)-O(39)	1.796(5)	Mo(4)-O(63)	1.816(5)
Mo(4)-O(51)	2.075(5)	Mo(4)-O(23)	2.163(5)	Mo(4)-O(18)	2.461(5)
Mo(5)-O(70)	1.688(6)	Mo(5)-O(32)	1.902(5)	Mo(5)-O(5)	1.916(5)
Mo(5)-O(37)	2.056(5)	Mo(5)-O(31)	2.086(5)	Mo(5)-O(43)	2.257(5)
Mo(6)-O(54)	1.705(6)	Mo(6)-O(32)	1.873(5)	Mo(6)-O(9)	1.897(5)
Mo(6)-O(29)	2.048(5)	Mo(6)-O(25)	2.072(5)	Mo(6)-O(8)	2.242(5)
Mo(7)-O(66)	1.694(5)	Mo(7)-O(25)	1.791(5)	Mo(7)-O(52)	1.832(5)
Mo(7)-O(33)	2.085(5)	Mo(7)-O(64)	2.132(5)	Mo(7)-O(21)	2.441(5)
Mo(8)-O(72)	1.710(6)	Mo(8)-O(69)	1.715(5)	Mo(8)-O(11)	1.868(5)
Mo(8)-O(51)	2.066(5)	Mo(8)-O(23)	2.362(5)	Mo(8)-O(60)	2.395(5)
Mo(9)-O(26)	1.738(5)	Mo(9)-O(35)	1.741(5)	Mo(9)-O(1)	1.888(5)
Mo(9)-O(12)	1.998(5)	Mo(9)-O(19)	2.233(5)	Mo(9)-O(13)	2.238(5)
Mo(10)-O(59)	1.700(6)	Mo(10)-O(4)	1.885(5)	Mo(10)-O(46)	1.899(5)
Mo(10)-O(39)	2.062(5)	Mo(10)-O(14)	2.065(5)	Mo(10)-O(15)	2.255(5)

Mo(11)-O(56)	1.688(5)	Mo(11)-O(2)	1.875(5)	Mo(11)-O(9)	1.920(5)
Mo(11)-O(7)	1.927(5)	Mo(11)-O(17)	2.151(5)	Mo(11)-O(20)	2.323(5)
Mo(12)-O(34)	1.687(5)	Mo(12)-O(4)	1.888(5)	Mo(12)-O(27)	1.900(5)
Mo(12)-O(50)	2.056(5)	Mo(12)-O(28)	2.084(5)	Mo(12)-O(41)	2.233(5)
Mo(13)-O(73)	1.713(5)	Mo(13)-O(62)	1.804(6)	Mo(13)-O(24)	1.807(5)
Mo(13)-O(42)	2.099(5)	Mo(13)-O(63)	2.111(5)	Mo(13)-O(18)	2.433(5)
Mo(14)-O(61)	1.701(5)	Mo(14)-O(37)	1.796(5)	Mo(14)-O(42)	1.824(5)
Mo(14)-O(51)	2.071(5)	Mo(14)-O(60)	2.160(5)	Mo(14)-O(18)	2.397(5)
Mo(15)-O(75)	1.717(6)	Mo(15)-O(67)	1.721(6)	Mo(15)-O(12)	1.840(5)
Mo(15)-O(33)	2.048(5)	Mo(15)-O(64)	2.372(5)	Mo(15)-O(20)	2.404(5)
Mo(16)-O(47)	1.709(5)	Mo(16)-O(55)	1.717(6)	Mo(16)-O(11)	1.963(5)
Mo(16)-O(1)	1.964(5)	Mo(16)-O(10)	2.315(5)	Mo(16)-O(36)	2.321(5)
Mo(17)-O(49)	1.689(5)	Mo(17)-O(3)	1.901(5)	Mo(17)-O(46)	1.906(5)
Mo(17)-O(22)	1.957(5)	Mo(17)-O(24)	2.120(5)	Mo(17)-O(58)	2.320(5)
Mo(18)-O(53)	1.699(5)	Mo(18)-O(5)	1.891(5	Mo(18)-O(2)	1.911(5)
Mo(18)-O(22)	1.984(5)	Mo(18)-O(62)	2.108(5)	Mo(18)-O(58)	2.317(5)
P(1)-O(41)	1.534(5)	P(1)-O(8)	1.535(5)	P(2)-O(43)	1.529(5)
P(1)-O(21)	1.594(5)	P(1)-O(20)	1.549(5)	P(2)-O(15)	1.537(5)
P(2)-O(58)	1.551(5)	P(3)-O(48)	1.524(5)	P(3)-O(28)	1.566(5)
P(2)-O(18)	1.590(5)	P(3)-O(13)	1.555(5)	P(3)-O(30)	1.584(5)
P(4)-O(16)	1.532(5)	P(4)-O(29)	1.553(5)	P(5)-O(31)	1.531(5)
P(4)-O(19)	1.553(5)	P(4)-O(64)	1.591(5)	P(5)-O(10)	1.536(5)
P(5)-O(60)	1.576(5)	P(6)-O(36)	1.531(5)	P(6)-O(38)	1.563(5)
P(5)-O(65)	1.591(5)	P(6)-O(14)	1.537(5)	P(6)-O(23)	1.572(5)
Sr(1)-O(19)	2.559(5)	Sr(1)-O(13)	2.562(5)	Sr(1)-O(36)	2.610(5)
Sr(1)-O(10)	2.657(5)	Sr(1)-O(43)	2.664(5)	Sr(1)-O(15)	2.664(5)
Sr(1)-O(8)	2.679(5)	Sr(1)-O(41)	2.681(5)	Sr(1)-O(1)	2.881(5)
Zn(1)-O(48)#1	2.043(5)	Zn(1)-O(16)	2.077(5)	Zn(1)-O(26)#1	2.135(6)
Zn(1)-O(74)	2.123(5)	Zn(1)-O(35)	2.158(5)	Zn(1)-O(45)	2.206(5)
O(40)-Mo(1)-O(50)	105.0(3)	O(68)-Mo(2)-O(17)	105.2(3)	O(57)-Mo(3)-O(3)	101.0(2)
O(40)-Mo(1)-O(6)	101.4(2)	O(68)-Mo(2)-O(44)	105.0(3)	O(57)-Mo(3)-O(27)	101.2(2)
O(40)-Mo(1)-O(33)	99.5(2)	O(68)-Mo(2)-O(6)	93.5(2)	O(57)-Mo(3)-O(7)	100.9(2)
O(40)-Mo(1)-O(30)	97.2(2)	O(68)-Mo(2)-O(52)	93.5(2)	O(57)-Mo(3)-O(44)	91.8(2)
O(40)-Mo(1)-O(21)	170.5(2)	O(68)-Mo(2)-O(21)	160.9(2)	O(57)-Mo(3)-O(20)	168.4(2)
O(71)-Mo(4)-O(39)	104.4(3)	O(70)-Mo(5)-O(32)	98.5(2)	O(54)-Mo(6)-O(32)	100.1(2)
O(71)-Mo(4)-O(63)	102.3(2)	O(70)-Mo(5)-O(5)	101.8(2)	O(54)-Mo(6)-O(9)	100.2(2)
O(71)-Mo(4)-O(51)	99.3(2)	O(70)-Mo(5)-O(37)	94.4(2)	O(54)-Mo(6)-O(29)	97.0(2)
O(71)-Mo(4)-O(23)	96.6(2)	O(70)-Mo(5)-O(31)	95.3(2)	O(54)-Mo(6)-O(25)	91.7(2)
O(71)-Mo(4)-O(18)	170.2(2)	O(70)-Mo(5)-O(43)	172.9(2)	O(54)-Mo(6)-O(8)	172.8(2)
O(66)-Mo(7)-O(25)	104.4(3)	O(72)-Mo(8)-O(69)	103.7(3)	O(26)-Mo(9)-O(35)	103.4(2)
O(66)-Mo(7)-O(52)	101.2(2)	O(72)-Mo(8)-O(11)	104.7(2)	O(26)-Mo(9)-O(1)	100.9(2)
O(66)-Mo(7)-O(33)	98.3(2)	O(72)-Mo(8)-O(51)	99.3(2)	O(26)-Mo(9)-O(12)	92.9(2)
O(66)-Mo(7)-O(64)	97.9(2)	O(72)-Mo(8)-O(23)	86.9(2)	O(26)-Mo(9)-O(19)	165.8(2)
O(66)-Mo(7)-O(21)	170.2(2)	O(72)-Mo(8)-O(60)	166.3(2)	O(26)-Mo(9)-O(13)	90.2(2)
O(59)-Mo(10)-O(4)	100.1(2)	O(56)-Mo(11)-O(2)	100.2(2)	O(34)-Mo(12)-O(4)	99.0(2)
O(59)-Mo(10)-O(46)	100.3(2)	O(56)-Mo(11)-O(9)	100.4(2)	O(34)-Mo(12)-O(27)	101.1(2)
O(59)-Mo(10)-O(39)	92.9(2)	O(56)-Mo(11)-O(7)	102.1(2)	O(34)-Mo(12)-O(50)	93.1(2)
O(59)-Mo(10)-O(14)	96.4(2)	O(56)-Mo(11)-O(17)	92.9(2)	O(34)-Mo(12)-O(28)	94.7(2)
O(59)-Mo(10)-O(15)	172.8(2)	O(56)-Mo(11)-O(20)	169.7(2)	O(34)-Mo(12)-O(41)	172.1(2)
O(73)-Mo(13)-O(62)	104.8(3)	O(61)-Mo(14)-O(37)	104.2(3)	O(75)-Mo(15)-O(67)	102.9(3)
O(73)-Mo(13)-O(24)	104.4(3)	O(61)-Mo(14)-O(42)	101.8(2)	O(75)-Mo(15)-O(12)	104.4(2)
O(73)-Mo(13)-O(42)	97.1(2)	O(61)-Mo(14)-O(51)	97.5(2)	O(75)-Mo(15)-O(33)	98.8(2)
O(73)-Mo(13)-O(63)	95.8(2)	O(61)-Mo(14)-O(60)	96.7(2)	O(75)-Mo(15)-O(64)	86.0(2)
O(73)-Mo(13)-O(18)	163.4(2)	O(61)-Mo(14)-O(18)	169.8(2)	O(75)-Mo(15)-O(30)	166.5(2)
O(47)-Mo(16)-O(55)	103.7(3)	O(49)-Mo(17)-O(3)	101.8(2)	O(53)-Mo(18)-O(5)	101.8(3)
O(47)-Mo(16)-O(11)	99.4(2)	O(49)-Mo(17)-O(46)	100.8(3)	O(53)-Mo(18)-O(2)	100.6(2)
O(47)-Mo(16)-O(1)	99.4(2)	O(49)-Mo(17)-O(22)	100.3(2)	O(53)-Mo(18)-O(22)	100.0(2)

O(47)-Mo(16)-O(10)	91.1(2)	O(49)-Mo(17)-O(24)	91.2(2)	O(53)-Mo(18)-O(62)	93.1(2)
O(47)-Mo(16)-O(36)	168.4(2)	O(49)-Mo(17)-O(58)	167.4(2)	O(53)-Mo(18)-O(58)	169.0(2)
O(41)-P(1)-O(8)	107.8(3)	O(43)-P(2)-O(15)	108.3(3)	O(48)-P(3)-O(13)	110.9(3)
O(41)-P(1)-O(20)	110.6(3)	O(43)-P(2)-O(58)	111.3(3)	O(48)-P(3)-O(28)	109.1(3)
O(41)-P(1)-O(21)	109.7(3)	O(43)-P(2)-O(18)	109.3(3)	O(48)-P(3)-O(30)	111.4(3)
O(16)-P(4)-O(19)	110.4(3)	O(31)-P(5)-O(10)	111.8(3)	O(36)-P(6)-O(14)	111.0(3)
O(16)-P(4)-O(29)	109.7(3)	O(31)-P(5)-O(60)	111.9(3)	O(36)-P(6)-O(38)	111.9(3)
O(16)-P(4)-O(64)	109.7(3)	O(31)-P(5)-O(65)	107.7(3)	O(36)-P(6)-O(23)	108.7(3)
O(19)-Sr(1)-O(13)	64.94(16)	O(19)-Sr(1)-O(36)	115.81(15)	O(19)-Sr(1)-O(10)	79.13(15)
O(19)-Sr(1)-O(43)	118.74(16)	O(19)-Sr(1)-O(15)	170.92(15)	O(19)-Sr(1)-O(8)	72.92(15)
O(19)-Sr(1)-O(41)	101.80(15)	O(19)-Sr(1)-O(1)	58.04(15)	O(48)#1-Zn(1)-O(16)	175.9(2)
O(48)#1-Zn(1)-O(26)#1	90.9(2)	O(48)#1-Zn(1)-O(74)	86.0(2)	O(48)#1-Zn(1)-O(35)	91.6(2)
O(48)#1-Zn(1)-O(45)	97.82(19)				

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

Table S6 Selected Hydrogen Bond Lengths ( ) and Bond Angles (°) of complexes **1-5**

	D-H...A	d(D-H)	d(H...A)	<D-H...A	d(D...A)	Symmetry
1	O13- H13B...O33	0.85	2.38	152.8	3.164(10)	
	O13- H13B...O58	0.85	2.45	121.1	2.978(10)	
	N7- H7A...O21	0.86	2.57	125.5	3.145(15)	
	N10- H10A...O67	0.86	2.57	132.0	3.21(2)	
	N12-H12...O15	0.86	2.43	125.7	3.011(19)	
	O3- H3C...O56	0.85	2.26	148.1	3.011(10)	[-x, y-1/2, -z+1/2]
	O3- H3C...O53	0.85	2.44	121.3	2.968(10)	[-x, y-1/2, -z+1/2]
	O3- H3C...O14	0.85	2.59	133.0	3.228(10)	[-x, y-1/2, -z+1/2]
	O13-H13C...O3W	0.85	2.39	122.7	2.941(12)	[x-1, y, z]
	N2-H2...O25	0.86	2.14	139.1	2.845(13)	[-x+1,y+1/2,-z+1/2]
	N5-H5...O74	0.86	1.94	168.4	2.786(11)	[-x+1, y+1/2, -z+1/2]
	N7- H7A...O26	0.86	2.60	136.5	3.274(16)	[x, y-1, z]
	O3W-H3WB.. .O5	0.85	2.28	119.2	2.799(13)	[x+1, y, z]
	O1W-H1WA...N12	0.85	2.15	158.6	2.96(2)	[x, -y+1/2, z+1/2]
	O1W-H1WB...O64	0.85	2.47	123.3	3.011(19)	[x,-y+1/2, z+1/2]
	O4W-H4WA...O2	0.85	2.07	123.1	2.636(12)	[x+1, y, z]
	O4W-H4WB...O5	0.85	2.58	127.1	3.169(12)	[-x+1, -y+1, -z]
2	O35-H35A...O14	0.85	2.96	85.0	3.004(7)	
	O70-H70A...O10	0.85	2.50	155.5	3.297(8)	
	O70-H70A...O11	0.85	2.55	118.1	3.040(8)	
	N9-H9... O15	0.86	2.03	167.2	2.870(9)	
	O35-H35B...O44	0.85	2.36	146.8	3.105(7)	[-x, y-1/2, -z+1/2]
	O35-H35B...O22	0.85	2.53	117.5	3.022(8)	[-x, y-1/2, -z+1/2]
	O35-H35B...O1	0.85	2.58	141.3	3.282(8)	[-x, y-1/2, -z+1/2]
	O70-H70B...O2W	0.85	2.55	115.4	3.012(11)	[x-1, y, z]
	N7-H7...O37	0.86	2.26	162.7	3.087(10)	[-x+1, y-1/2, -z+1/2]
	N4-H4...O21	0.86	2.22	138.8	2.924(9)	[-x+1, -y, -z+1]
	N1-H1...O5W	0.86	2.04	158.1	2.86(3)	[x, y-1, z]
	N5-H5A...O4W	0.86	2.33	151.4	3.12(2)	[-x+1, -y+1, -z+1]
	N5-H5A...O67	0.86	2.60	120.4	3.13(2)	[-x+1, y+1/2, -z+1/2]
	O1W-H1WA...O73	0.85	2.47	115.2	2.936(11)	[-x+1, -y+1, -z]

	O1W-H1WB...O46	0.85	2.17	118.5	2.678(10)	[x+1, y, z]
	O4W-H4WA...O62	0.85	2.58	114.4	3.034(11)	[x, -y+1/2, z+1/2]
	O4W-H4WB...N5	0.85	2.40	142.6	3.12(2)	[-x+1, -y+1, -z+1]
	O3W-H3WA...O56	0.85	2.90	85.8	2.964(11)	[-x+1, y-1/2, -z+1/2]
	O5W-H5WB...O26	0.85	2.53	171.0	3.37(3)	[x, -y+3/2, z+1/2]
	O2W-H2WA...O66	0.85	2.10	148.6	2.861(11)	[x+1, y, z]
	O2W-H2WB...O59	0.85	2.44	123.6	2.994(11)	[-x+1, y-1/2, -z+1/2]
3	O47-H47A ...O55	0.85	2.73	89.6	2.857(8)	
	O75-H75A...O15	0.85	2.47	148.5	3.229(8)	
	N4-H4...O50	0.86	1.92	166.7	2.766(10)	
	O4W-H4WA...O69	0.85	2.49	145.1	3.228(12)	
	N8-H8A...O3W	0.86	1.88	161.9	2.71(2)	
	O3W-H3WB...O64	0.85	2.78	94.8	2.974(18)	
	O5W-H5WA..O7W	0.85	1.83	130.3	2.47(3)	
	N10-H10A...O65	0.86	2.49	120.2	3.02(2)	
	O47-H47B...O70	0.85	2.34	129.3	2.955(8)	[-x, y+1/2, -z+1/2]
	O47-H47B...O60	0.85	2.36	133.4	3.006(8)	[-x, y+1/2, -z+1/2]
	O47-H47B...O1	0.85	2.38	151.5	3.149(8))	[-x, y+1/2, -z+1/2]
	O75-H75B... O45	0.85	2.97	86.3	3.040(8)	[-x, y+1/2, -z+1/2]
	O2W-H2WA...O57	0.85	2.04	140.6	2.755(10)	[x+1, y, z]
	O2W-H2WA...O48	0.85	2.34	111.5	2.768(10)	[x+1, y, z]
	O2W-H2WB...O67	0.85	2.39	115.3	2.862(10)	[-x+1,y+1/2,-z+1/2]
	O1W-H1WA...O71	0.85	2.34	119.6	2.858(11)	[-x+1, -y+1, -z]
	O1W-H1WB...O68	0.85	2.24	106.0	2.609(10)	[x+1, y, z]
	N6-H6...O13	0.86	2.12	137.4	2.809(10)	[-x+1,y-1/2, -z+1/2]
	N12-H12...O23	0.86	2.15	158.6	2.966(10)	[x, y+1, z]
	O6W-H6WB...O51	0.85	2.26	133.4	2.906(11)	[x, -y+3/2, z+1/2]
	O4W-H4WA...O72	0.85	2.28	131.2	2.911(12)	[-x+1,y-1/2, -z+1/2]
	O4W-H4WB...O5W	0.85	2.16	116.3	2.65(3)	[x, -y+1/2, z-1/2]
	N1-H1...O17	0.86	2.19	149.4	2.962(17)	[-x+1, -y+1, -z+1]
	N1-H1...O40	0.86	2.33	136.2	3.014(16)	[-x+1, -y+1, -z+1]
	O5W-H5WB...O3W	0.85	1.94	126.5	2.54(3)	[x, y, z+1]
	N10-H10A...O6W	0.86	2.21	149.0	2.98(2)	[x, -y+3/2, z-1/2]
4	O75- H75A... O65	0.85	2.85	2.946(14)	88.2	
	O76- H76A... O6	0.85	2.43	3.209(15)	152.7 .	
	O75- H75B... O37	0.85	2.31	3.064(13)	147.5	[-x+1, y+1/2, -z+1/2]
	O75- H75B... O4	0.85	2.53	3.275(14)	146.8	[-x+1, y+1/2, -z+1/2]
	O75- H75B... O72	0.85	2.58	3.105(16)	120.6	[-x+1, y+1/2, -z+1/2]
	O1W- H1WB... O74	0.85	2.24	2.91(2)	134.9	[-x+1, -y+1, -z+1]
	O1W- H1WB... O72	0.85	2.43	2.91(2)	116.4	[x, y+1, z]
	O3W- H3WA... O70	0.85	2.24	2.96(2)	143.1	[x, y+1, z]
	O3W- H3WB... O66	0.85	2.77	3.01(3)	97.9	[-x, y+1/2, -z+1/2]
	O2W- H2WB... O39	0.85	2.50	3.026(19)	121.2	[-x+1, -y+1, -z+1]
	O4W- H4WB... O73	0.85	2.52	2.85(4)	103.9	[x, -y+1/2, z-1/2]
	O4W- H4WB... O46	0.85	2.68	3.17(4)	118.3	[x, -y+1/2, z-1/2]

5	O5W-H5WA...O73	0.85	2.92	92.2	3.071(18)	
	O45-H45A...O35	0.85	2.82	90.0	2.946(7)	
	O74-H74A...O10	0.85	2.42	153.4	3.206(8)	
	O74-H74A...O19	0.85	2.44	120.4	2.967(8)	
	O74-H74B...O1W	0.85	2.40	119.5	2.912(9)	
	N10-H10...O3W	0.86	2.37	144.0	3.106(17)	
	O1W-H1WA...O65	0.85	2.56	96.9	2.796(9)	
	O7W-H7WA...O4W	0.85	2.24	112.5	2.69(3)	[-x+1, -y+1, -z+1]
	O7W-H7WB...O5W	0.85	2.22	106.7	2.60(3)	[-x+1, y+1/2, -z+1/2]
	O6W-H6WA...O53	0.85	2.56	158.6	3.37(2)	[-x+1, y-1/2, -z+1/2]
	O6W-H6WB...O3W	0.85	2.28	105.4	2.64(2)	[-x+1, -y+1, -z+1]
	O45-H45B...O55	0.85	2.39	131.7	3.018(8)	[-x+1, y+1/2, -z+1/2]
	O45-H45B...O36	0.85	2.39	134.6	3.051(7)	[-x+1, y+1/2, -z+1/2]
	O45-H45B...O1	0.85	2.47	149.5	3.231(8)	[-x+1, y+1/2, -z+1/2]
	O4W-H4WA...O53	0.85	2.33	132.2	2.966(11)	[-x+2, y-1/2, -z+1/2]
	O3W-H3WA...O42	0.85	2.49	118.5	2.987(11)	[x, -y+3/2, z+1/2]
	O1W-H1WB...O72	0.85	2.91	103.7	3.214(9)	[-x+1, -y+1, -z]
	O2W-H2WA...O69	0.85	2.15	151.2	2.925(10)	[-x+1, -y+1, -z]
	O2W-H2WB...O75	0.85	3.15	85.7	3.202(10)	[-x+1, y-1/2, -z+1/2]
	N1-H1...O22	0.86	1.96	167.4	2.808(9)	[x-1, y, z]
	N4-H4...O28	0.86	2.20	161.5	3.029(10)	[x, -y+1/2, z+1/2]
	N6-H6...O16	0.86	2.17	137.9	2.871(9)	[-x+1, y-1/2, -z+1/2]
	N9-H9...O17	0.86	2.25	160.4	3.070(13)	[-x+1, y-1/2, -z+1/2]
	N10-H10...O61	0.86	2.45	126.3	3.041(16)	[x, -y+3/2, z+1/2]
	O2W-H2WB...O66	0.85	2.48	118.6	2.985(11)	[-x+1, y-1/2, -z]
	O1W-H1WB...O67	0.85	2.12	168.1	2.961(12)	[-x+1, y+1/2, -z]

3. Physical characterization

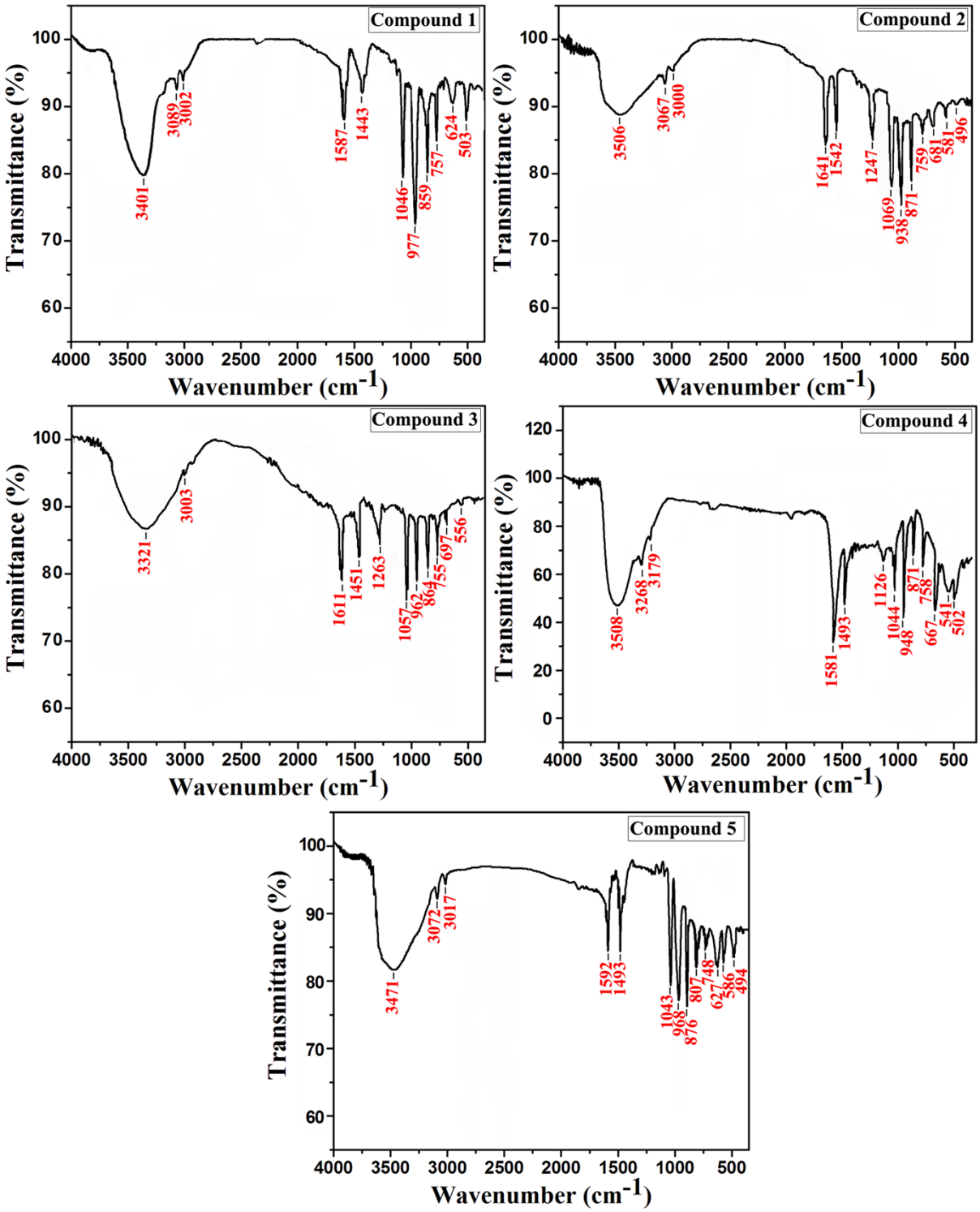

Fig. S6 IR spectra of compounds **1-5.**

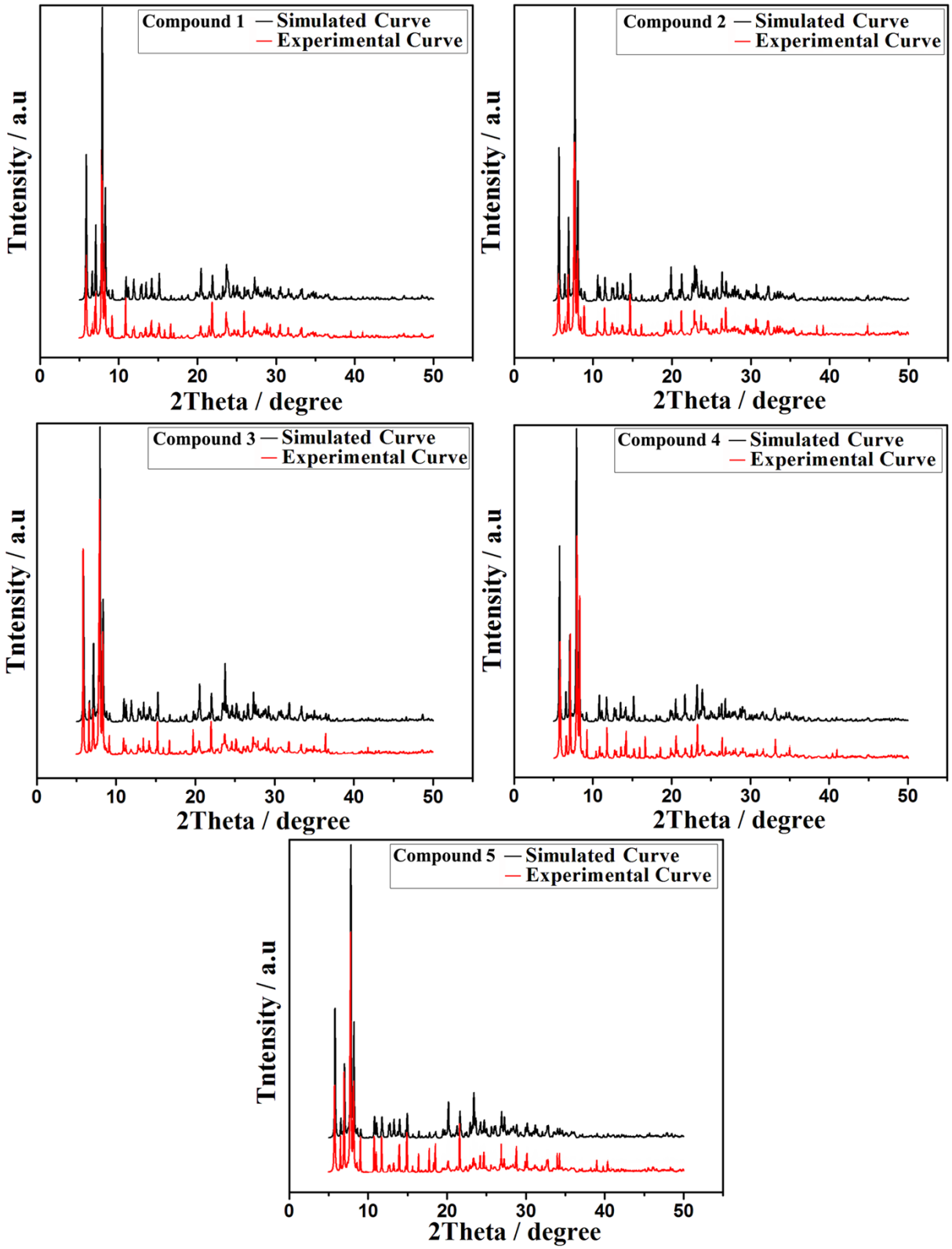

Fig. S7 The PXRD contrast curves of compounds **1-5**.

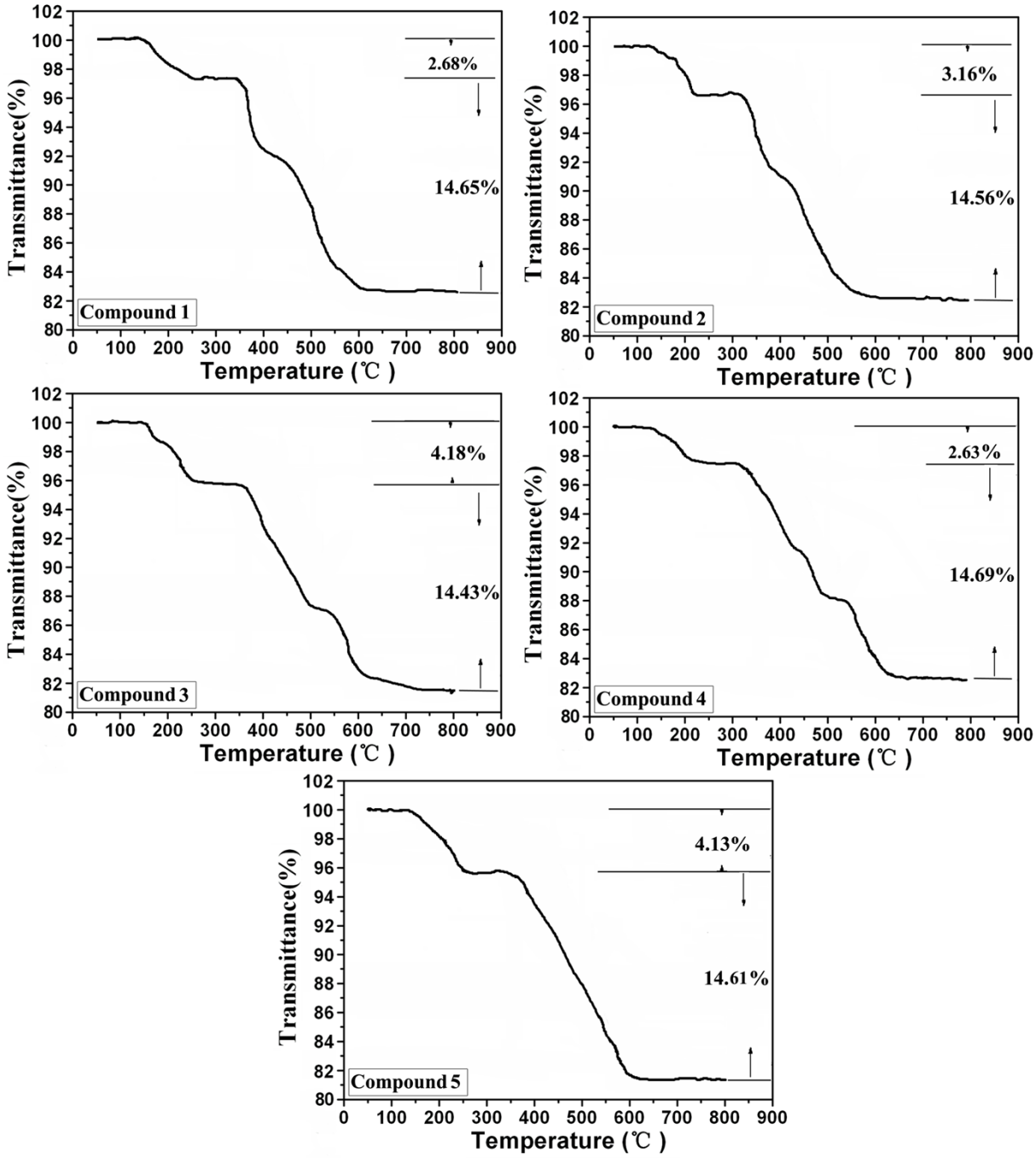

Fig. S8 TG curves of compounds **1-5.**

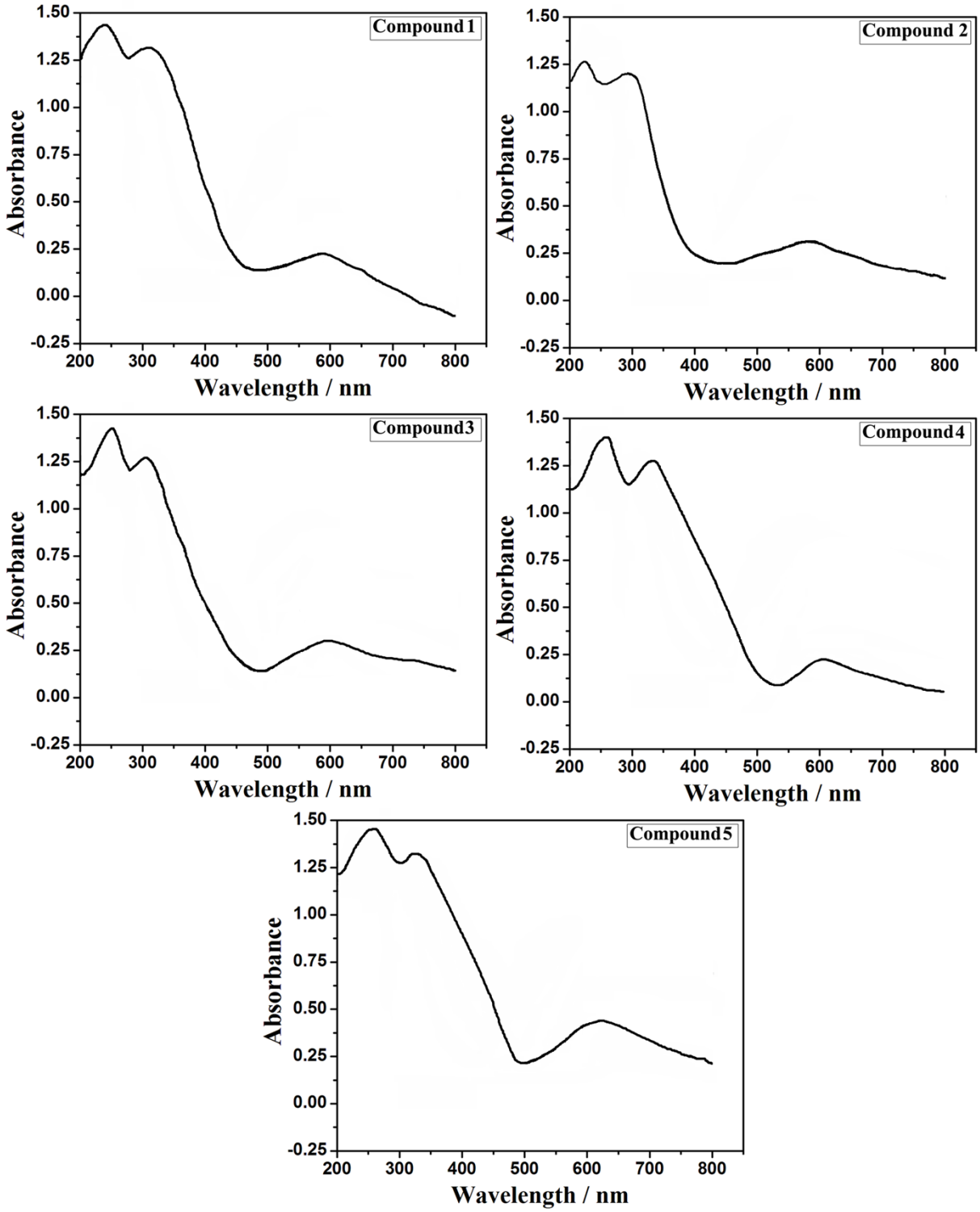

Fig. S9 The UV-vis spectra of compounds **1-5** in solid state at room temperature**.**

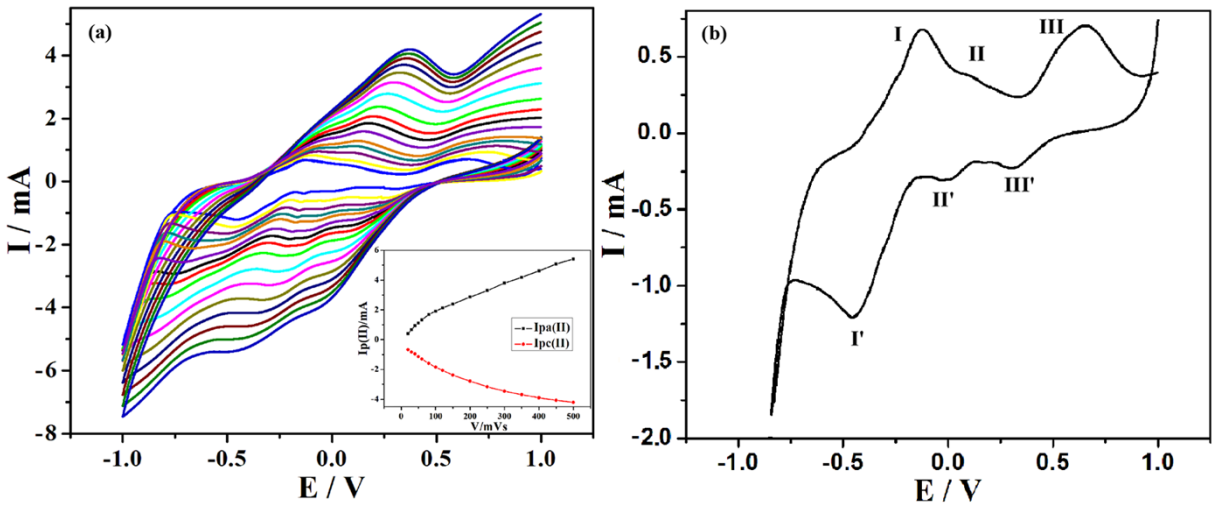

Fig. S10 (a) Cyclic voltammograms of **2-CPE** in the 1.0 M H_2SO_4 solution at different scan rate. rates (from inner to outer: 20, 30, 40, 60, 80, 100, 120, 150, 200, 250, 300, 350, 400, 450, 500 mV s^{-1}; Insert plots: The dependence of anodic and cathodic peak II current on scan rates.) **(b)** Cyclic voltammograms of **2-CPE** in the 1.0 M H_2SO_4 solution at at scan rate of 20 mV s^{-1}; Potentials vs. SCE.

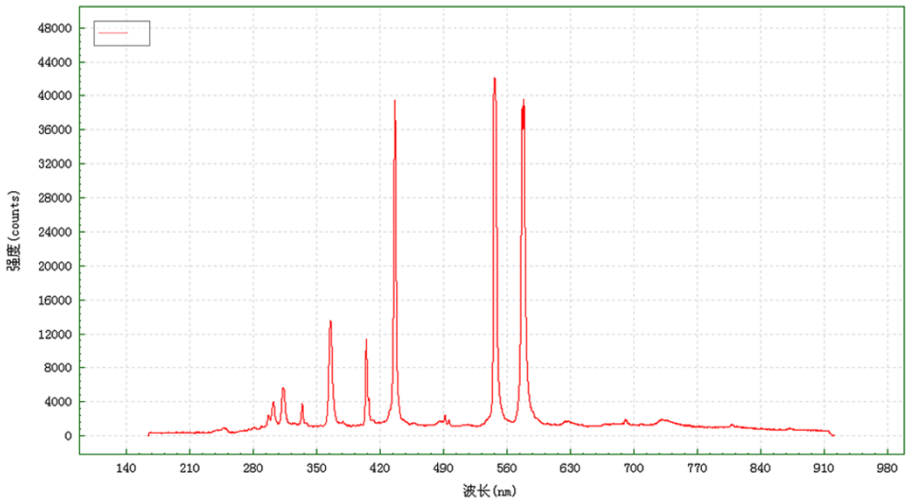

Figure S11 The light spectrum of for the photocatalytic reaction

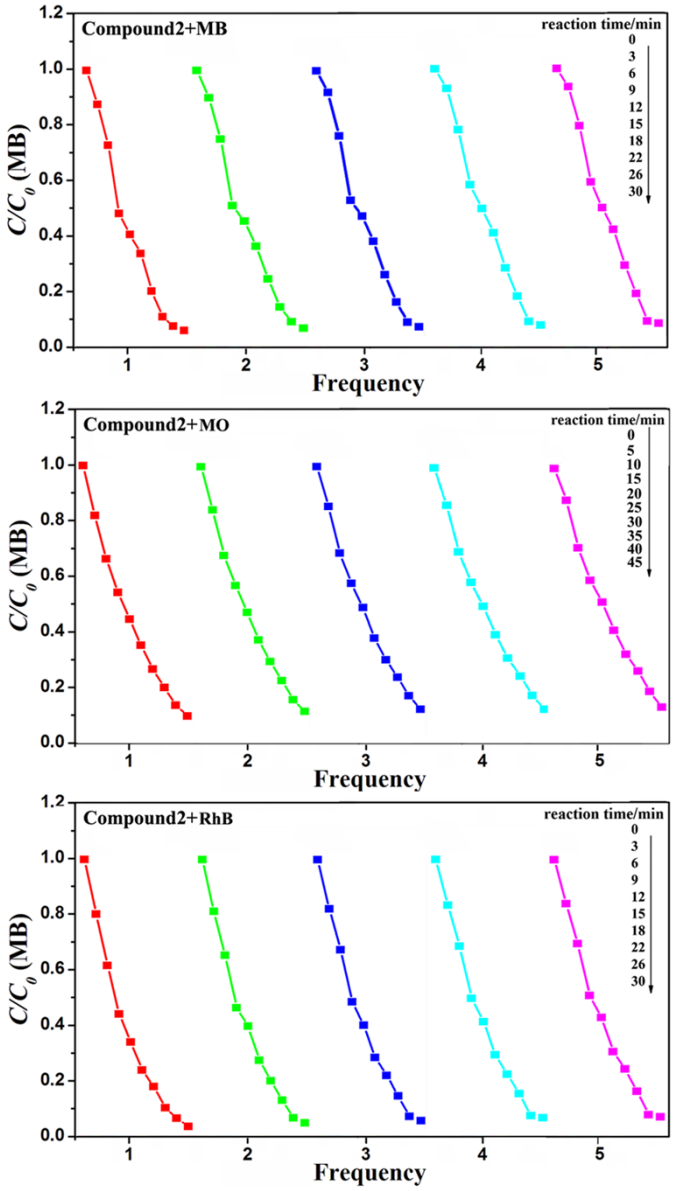

Fig.S12 Changes of concentration for MB, MO, and RhB under different irradiation time in the presence of the compound **2** with repeating the reactions.

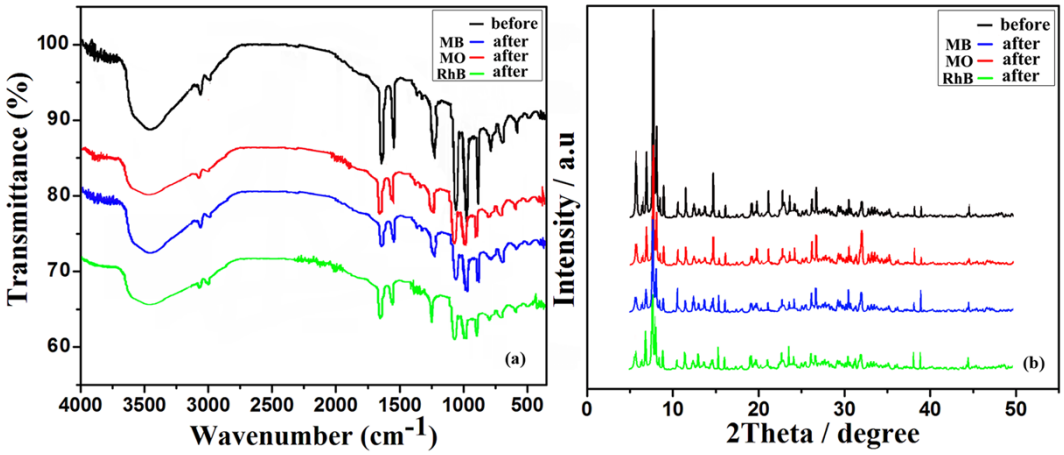

Fig.S13 (a) The IR spectra of compound **2** before and after cycle reaction; (b) The XRD patterns of compound **2** before and after cycle five time.