Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting information

Influence of pH and organic ligand on the supramolecular network based on molybdenum phosphate/ strontium chemistry

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1. Structural figures

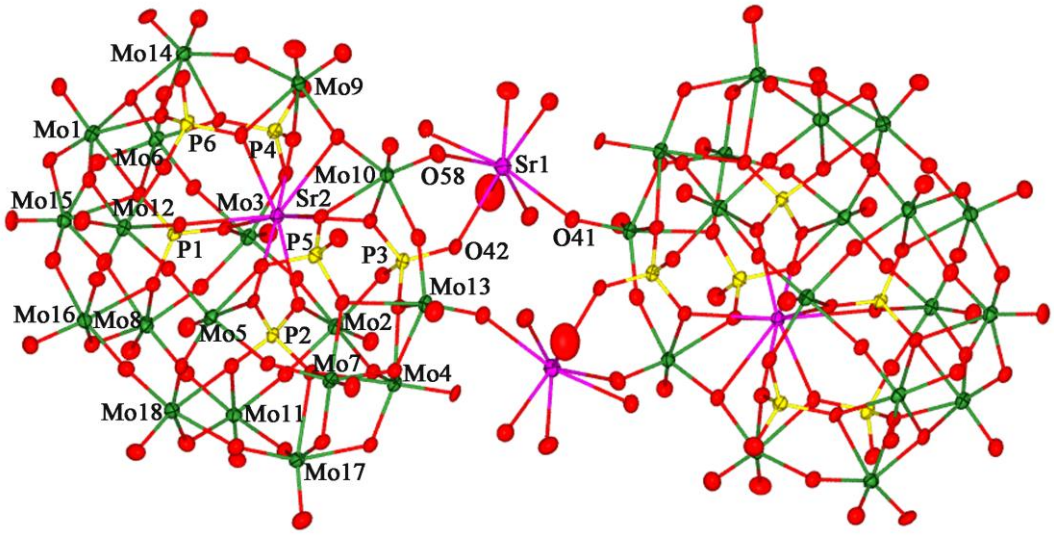


Fig. S1 ORTEP view of the basic units in compound **1** with 50% thermal ellipsoids.

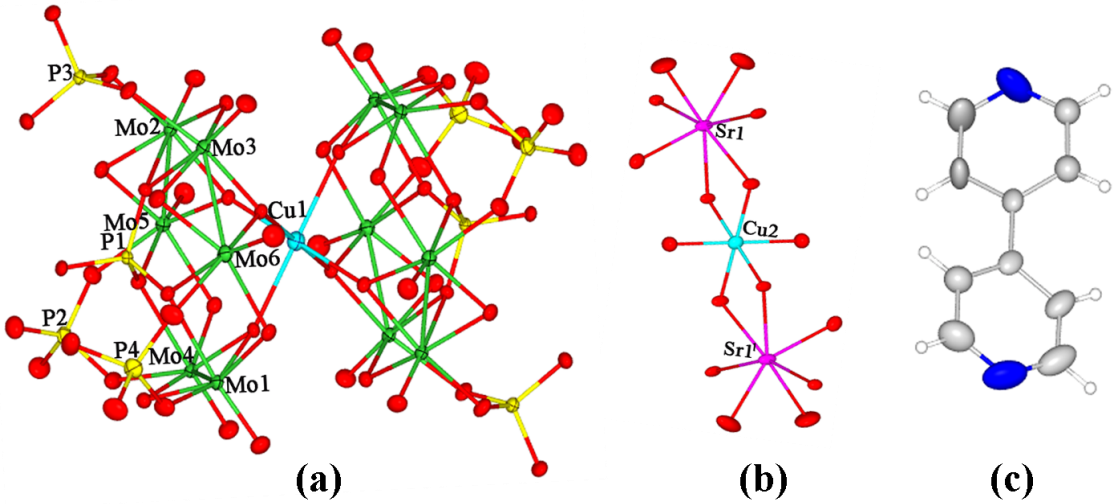


Fig. S2 ORTEP view of the basic units in compound **2** with 50% thermal ellipsoids: **(a)** the sandwich-type $\{Cu(P_4Mo_6)_2\}$ unit; **(b)** the trinuclear $\{Sr_2Cu\}$ linker; **(c)** the bpy ligand.

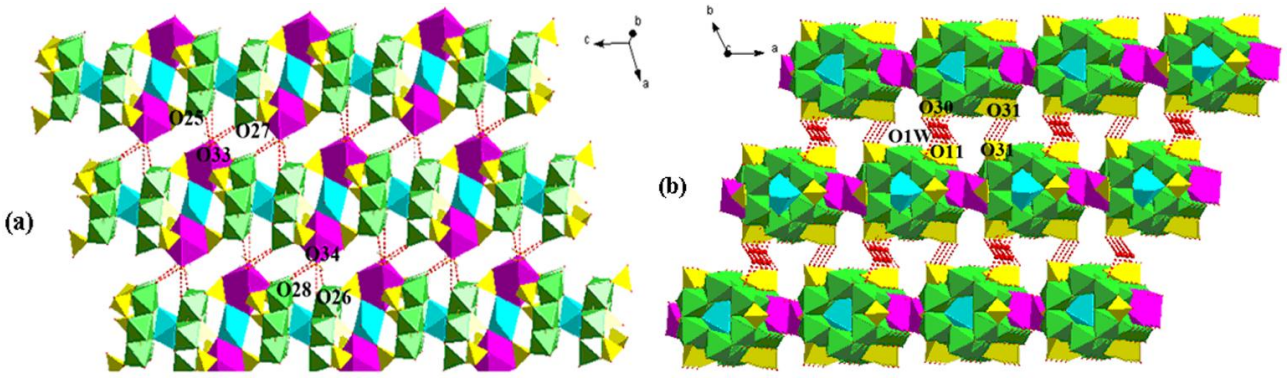


Figure S3 (a) The 2D supramolecular sheet of **2** along the b axis. (b) The 3D supramolecular framework along the c axis of **2**. The broken lines represent the hydrogen bonding interactions. Other isolated organic ligands and water molecules are omitted for clarity.

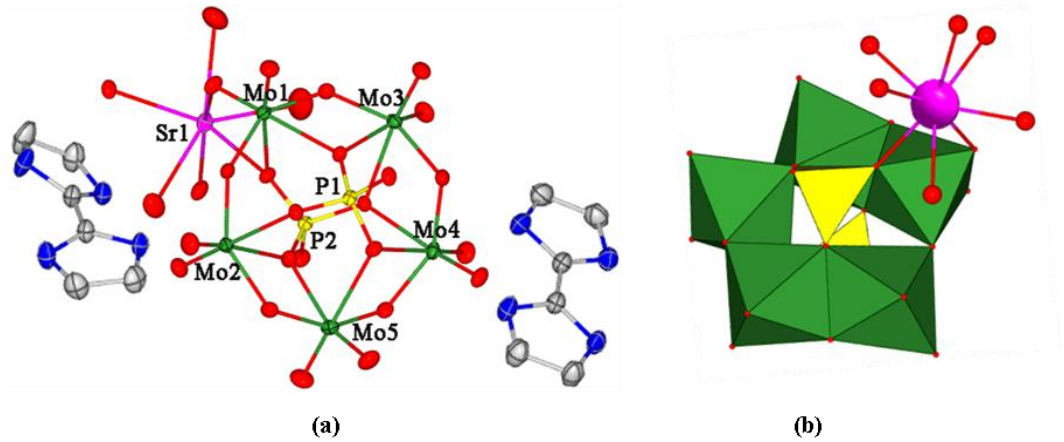


Fig. S4 (a) ORTEP view of the basic units in compound **3** with 50% thermal ellipsoids; **(b)** the Polyhedral representation of the $[Mo_5P_2]$ cluster.

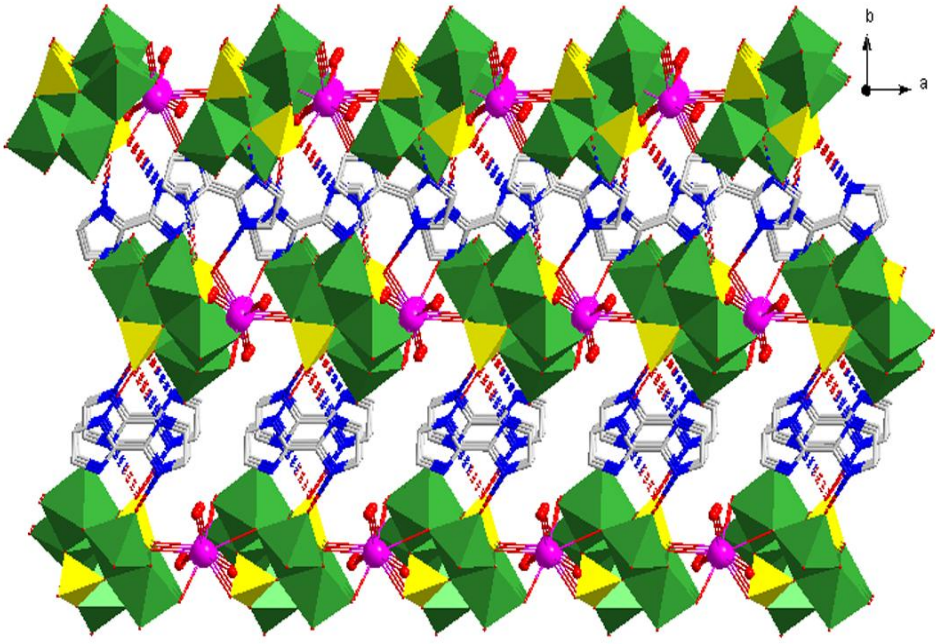


Figure S5 (b) The 3D supramolecular framework along the c axis of **3**. The broken lines represent the hydrogen bonding interactions. Other isolated organic ligands and water molecules are omitted for clarity.

2. Structural data

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

Mo(1)-O(54)	1.674(8)	Mo(3)-O(67)	1.670(9)	Mo(5)-O(46)	1.687(8)
Mo(1)-O(11)	1.787(8)	Mo(3)-O(1)	1.871(8)	Mo(5)-O(4)	1.868(8)
Mo(1)-O(51)	1.805(8)	Mo(3)-O(15)	1.890(8)	Mo(5)-O(22)	1.877(8)
Mo(1)-O(20)	2.057(8)	Mo(3)-O(37)	2.045(8)	Mo(5)-O(17)	2.037(8)
Mo(1)-O(38)	2.132(8)	Mo(3)-O(56)	2.071(8)	Mo(5)-O(29)	2.077(8)
Mo(1)-O(2)	2.431(8)	Mo(3)-O(18)	2.193(8)	Mo(5)-O(6)	2.216(8)
Mo(2)-O(55)	1.692(8)	Mo(4)-O(19)	1.693(7)	Mo(6)-O(25)	1.699(8)
Mo(2)-O(1)	1.859(8)	Mo(4)-O(34)	1.951(3)	Mo(6)-O(68)	1.780(8)
Mo(2)-O(35)	1.781(8)	Mo(4)-O(60)’	1.808(8)	Mo(6)-O(37	1.782(8)
Mo(2)-O(27)	2.039(8)	Mo(4)-O(13)	2.049(8)	Mo(6)-O(20)	2.045(8)
Mo(2)-O(34)	2.043(8)	Mo(4)-O(32)	2.114(8)	Mo(6)-O(36)	2.153(8)
Mo(2)-O(14)	2.219(8)	Mo(4)-O(21)	2.410(8)	Mo(6)-O(2)	2.373(8)
Mo(7)-O(62	1.674(8)	Mo(9)-O(70)	1.692(8)	Mo(11)-O(59)	1.700(8)
Mo(7)-O(17)	1.792(8)	Mo(9)-O(72)	1.711(9)	Mo(11)-O(35)	1.879(8)
Mo(7)-O(40)	1.802(8)	Mo(9)-O(8)	1.923(8)	Mo(11)-O(5)	1.889(8)
Mo(7)-O(13)	2.037(8)	Mo(9)-O(39)	1.967(8)	Mo(11)-O(45)	1.942(9)
Mo(7)-O(33)	2.142(8)	Mo(9)-O(9)	2.233(8)	Mo(11)-O(47)	2.094(8)
Mo(7)-O(21)	2.414(8)	Mo(9)-O(7)	2.278(8)	Mo(11)-O(16)	2.313(8)
Mo(8)-O(74)	1.686(8)	Mo(10)-O(58)	1.695(8)	Mo(12)-O(69)	1.686(9)
Mo(8)-O(5)	1.873(8)	Mo(10)-O(30)	1.705(8)	Mo(12)-O(4)	1.877(8)
Mo(8)-O(15)	1.882(8)	Mo(10)-O(8)	1.890(8)	Mo(12)-O(26)	1.878(8)
Mo(8)-O(43)	1.913(8)	Mo(10)-O(44)	2.005(8)	Mo(12)-O(11)	2.024(8)
Mo(8)-O(24	2.093(8)	Mo(10)-O(12)	2.224(8)	Mo(12)-O(28)	2.046(8)
Mo(8)-O(3)	2.288(8)	Mo(10)-O(23)	2.267(8)	Mo(12)-O(31)	2.218(8)
Mo(13)-O(49)	1.703(9)	Mo(15)-O(65)	1.694(8)	Mo(17)-O(48)	1.663(9)
Mo(13)-O(41)	1.735(8)	Mo(15)-O(53)	1.801(9)	Mo(17)-O(57)	1.805(8)
Mo(13)-O(44)	1.826(8)	Mo(15)-O(24)	1.808(8)	Mo(17)-O(47)	1.814(8)
Mo(13)-O(13)	2.052(8)	Mo(15)-O(51)	2.051(8)	Mo(17)-O(40)	2.073(8)
Mo(13)-O(33)	2.306(8)	Mo(15)-O(68)	2.122(9)	Mo(17)-O(60)	2.074(8)
Mo(13)-O(32)	2.343(8)	Mo(15)-O(2)	2.423(8)	Mo(17)-O(21)	2.429(8)
Mo(14)-O(52)	1.690(8)	Mo(16)-O(73)	1.670(9)	Mo(18)-O(61)	1.658(9)
Mo(14)-O(63)	1.715(9)	Mo(16)-O(10)	1.872(8)	Mo(18)-O(10)	1.874(8)
Mo(14)-O(39)	1.852(8)	Mo(16)-O(26)	1.882(8)	Mo(18)-O(22)	1.885(8)
Mo(14)-O(20)	2.042(8)	Mo(16)-O(43)	1.954(8)	Mo(18)-O(45)	1.957(8)
Mo(14)-O(38)	2.345(8)	Mo(16)-O(53)	2.100(8)	Mo(18)-O(57)	2.123(8)
Mo(14)-O(36)	2.366(8)	Mo(16)-O(3)	2.308(8)	Mo(18)-O(16)	2.282(8)
Sr(1)-O(41)	2.545(8)	Sr(1)-O(64)	2.603(9)	Sr(1)-O(58)#1	2.665(9)
Sr(1)-O(42)#1	2.554(8)	Sr(1)-O(63)#2	2.620(9)	Sr(1)-O(77)	2.694(12)
Sr(1)-O(75)	2.588(11)	Sr(1)-O(76)	2.660(12)	Sr(1)-O(19)	2.959(8)
Sr(2)-O(23	2.557(8)	Sr(2)-O(12)	2.609(8)	Sr(2)-O(14)	2.683(8)
Sr(2)-O(9)	2.586(8)	Sr(2)-O(6)	2.673(8)	Sr(2)-O(18)	2.688(8)
Sr(2)-O(7)	2.587(8)	Sr(2)-O(31	2.678(8)	Sr(2)-O(8)	2.860(8)
P(1)-O(31)	1.519(8)	P(2)-O(14)	1.510(9)	P(3)-O(42)	1.501(8)
P(1)-O(18)	1.525(8)	P(2)-O(6)	1.515(8)	P(3)-O(23)	1.529(8)
P(1)-O(3)	1.536(8)	P(2)-O(16)	1.530(8)	P(3)-O(27)	1.549(9)
P(1)-O(2)	1.581(8)	P(2)-O(21)	1.580(8)	P(3)-O(32)	1.581(8)
P(4)-O(7)	1.518(9)	P(5)-O(12)	1.508(8)	P(6)-O(50)	1.524(8)
P(4)-O(56)	1.518(8)	P(5)-O(71)	1.521(9)	P(6)-O(28)	1.532(9)
P(4)-O(66)	1.538(10)	P(5)-O(29)	1.536(8)	P(6)-O(9)	1.533(8)
P(4)-O(36)	1.550(8)	P(5)-O(33)	1.574(8)	P(6)-O(38)	1.571(9)
O(54)-Mo(1)-O(11)	104.9(4)	O(62)-Mo(7)-O(17)	102.9(4)	O(49)-Mo(13)-O(41)	102.7(4)
O(54)-Mo(1)-O(38)	98.9(4)	O(62)-Mo(7)-O(40)	103.5(4)	O(49)-Mo(13)-O(44)	104.0(4)
O(54)-Mo(1)-O(51)	101.2(4)	O(62)-Mo(7)-O(13)	99.4(4)	O(49)-Mo(13)-O(13)	98.6(4)

O(54)-Mo(1)-O(20)	99.7(4)	O(62)-Mo(7)-O(33)	97.1(4)	O(49)-Mo(13)-O(33)	88.0(4)
O(54)-Mo(1)-O(2)	170.3(4)	O(62)-Mo(7)-O(21)	172.0(3)	O(49)-Mo(13)-O(32)	166.4(4)
O(55)-Mo(2)-O(1)	98.9(4)	O(74)-Mo(8)-O(5)	100.8(4)	O(52)-Mo(14)-O(63)	103.2(4)
O(55)-Mo(2)-O(35)	101.7(4)	O(74)-Mo(8)-O(15)	100.8(4)	O(52)-Mo(14)-O(39)	103.6(4)
O(55)-Mo(2)-O(27)	96.0(4)	O(74)-Mo(8)-O(43)	100.9(4)	O(52)-Mo(14)-O(20)	99.1(4)
O(55)-Mo(2)-O(34)	92.9(4)	O(74)-Mo(8)-O(24)	93.5(4)	O(52)-Mo(14)-O(38)	86.4(4)
O(55)-Mo(2)-O(14)	172.9(3)	O(74)-Mo(8)-O(3)	169.5(4)	O(52)-Mo(14)-O(36)	166.0(4)
O(67)-Mo(3)-O(1)	98.8(4)	O(70)-Mo(9)-O(72)	102.2(5)	O(65)-Mo(15)-O(53)	104.3(4)
O(67)-Mo(3)-O(15)	103.3(4)	O(70)-Mo(9)-O(8)	99.9(4)	O(65)-Mo(15)-O(24)	104.5(4)
O(67)-Mo(3)-O(37)	92.9(4)	O(70)-Mo(9)-O(39)	96.9(4)	O(65)-Mo(15)-O(51)	97.4(4)
O(67)-Mo(3)-O(56)	93.2(4)	O(70)-Mo(9)-O(9)	92.4(4)	O(65)-Mo(15)-O(68)	95.6(4)
O(67)-Mo(3)-O(18)	170.0(4)	O(70)-Mo(9)-O(7)	168.7(4)	O(65)-Mo(15)-O(2)	163.1(4)
O(19)-Mo(4)-O(34)	102.9(4)	O(58)-Mo(10)-O(30)	102.1(4)	O(73)-Mo(16)-O(10)	99.9(4)
O(19)-Mo(4)-O(60)	103.3(4)	O(58)-Mo(10)-O(8)	101.3(4)	O(73)-Mo(16)-O(26)	102.6(4)
O(19)-Mo(4)-O(13)	99.4(4)	O(58)-Mo(10)-O(44)	94.5(4)	O(73)-Mo(16)-O(43)	100.4(4)
O(19)-Mo(4)-O(32)	96.8(4)	O(58)-Mo(10)-O(12)	165.2(4)	O(73)-Mo(16)-O(53)	93.4(4)
O(19)-Mo(4)-O(21)	171.8(3)	O(58)-Mo(10)-O(23)	88.7(4)	O(73)-Mo(16)-O(3)	169.4(4)
O(46)-Mo(5)-O(4)	99.2(4)	O(59)-Mo(11)-O(35)	101.0(4)	O(48)-Mo(17)-O(57)	104.3(4)
O(46)-Mo(5)-O(22)	102.7(4)	O(59)-Mo(11)-O(5)	100.6(4)	O(48)-Mo(17)-O(47)	103.1(4)
O(46)-Mo(5)-O(17)	92.0(4)	O(59)-Mo(11)-O(45)	100.7(4)	O(48)-Mo(17)-O(40)	98.2(4)
O(46)-Mo(5)-O(29)	94.1(4)	O(59)-Mo(11)-O(47)	92.7(4)	O(48)-Mo(17)-O(60)	97.3(4)
O(46)-Mo(5)-O(6)	171.2(4)	O(59)-Mo(11)-O(16)	169.3(4)	O(48)-Mo(17)-O(21)	164.7(4)
O(25)-Mo(6)-O(68)	102.1(4)	O(69)-Mo(12)-O(4)	99.2(4)	O(61)-Mo(18)-O(10)	101.6(4)
O(25)-Mo(6)-O(37)	103.5(4)	O(69)-Mo(12)-O(26)	102.1(4)	O(61)-Mo(18)-O(22)	101.9(4)
O(25)-Mo(6)-O(20)	98.4(4)	O(69)-Mo(12)-O(11)	93.1(4)	O(61)-Mo(18)-O(45)	99.9(4)
O(25)-Mo(6)-O(36)	95.3(4)	O(69)-Mo(12)-O(28)	95.5(4)	O(61)-Mo(18)-O(57)	92.0(4)
O(25)-Mo(6)-O(2)	171.7(3)	O(69)-Mo(12)-O(31)	171.6(4)	O(61)-Mo(18)-O(16)	168.7(4)
O(41)-Sr(1)-O(42)#1	85.4(3)	O(41)-Sr(1)-O(75)	128.5(3)	O(41)-Sr(1)-O(64)	77.4(3)
O(41)-Sr(1)-O(63)#2	79.9(3)	O(41)-Sr(1)-O(76)	136.4(3)	O(41)-Sr(1)-O(58)#1	146.3(3)
O(23)-Sr(2)-O(7)	81.3(3)	O(23)-Sr(2)-O(12)	65.4(3)	O(23)-Sr(2)-O(6)	102.4(2)
O(23)-Sr(2)-O(31)	169.9(2)	O(23)-Sr(2)-O(14)	73.7(2)	O(23)-Sr(2)-O(18)	118.7(3)
O(23)-Sr(2)-O(8)	58.7(2)	O(6)-Sr(2)-O(14)	54.3(2)		
O(31)-P(1)-O(18)	108.3(4)	O(31)-P(1)-O(3)	111.6(5)	O(31)-P(1)-O(2)	109.6(4)
O(14)-P(2)-O(6)	107.7(4)	O(14)-P(2)-O(16)	111.5(5)	O(14)-P(2)-O(21)	110.1(4)
O(42)-P(3)-O(23)	113.2(5)	O(42)-P(3)-O(27)	109.7(5)	O(42)-P(3)-O(32)	109.1(5)
O(7)-P(4)-O(56)	111.3(5)	O(7)-P(4)-O(66)	111.5(5)	O(7)-P(4)-O(36)	109.6(5)
O(12)-P(5)-O(71)	110.8(5)	O(12)-P(5)-O(29)	110.4(5)	O(12)-P(5)-O(33)	108.3(5)
O(50)-P(6)-O(28)	108.0(5)	O(50)-P(6)-O(9)	111.3(5)	O(50)-P(6)-O(38)	110.3(5)

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

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

Mo(1)-O(28)	1.675(3)	Mo(3)-O(25)	1.675(3)	Mo(5)-O(17)	1.673(3)
Mo(1)-O(6)	1.943(3)	Mo(3)-O(16)	1.929(3)	Mo(5)-O(15)	1.936(3)
Mo(1)-O(2)	1.983(3)	Mo(3)-O(1	1.985(3)	Mo(5)-O(5)	1.984(3)
Mo(1)-O(18)	2.066(3)	Mo(3)-O(9)#1	2.062(3)	Mo(5)-O(21)	2.049(3)
Mo(1)-O(13)	2.094(3)	Mo(3)-O(10)	2.113(3)	Mo(5)-O(11)	2.116(3)
Mo(1)-O(3)	2.266(3)	Mo(3)-O(8)	2.270(3)	Mo(5)-O(4)	2.296(3)
Mo(2)-O(26)	1.682(3)	Mo(4)-O(27)	1.669(3)	Mo(6)-O(20)	1.672(3)
Mo(2)-O(15)	1.927(3)	Mo(4)-O(6)	1.940(3)	Mo(6)-O(16)	1.934(3)
Mo(2)-O(5)	1.980(3)	Mo(4)-O(2)	1.983(3)	Mo(6)-O(1)	1.985(3)
Mo(2)-O(14)#	2.032(3)	Mo(4)-O(12)	2.052(3)	Mo(6)-O(22)	2.066(3)
Mo(2)-O(10)	2.103(3)	Mo(4)-O(11)	2.094(3)	Mo(6)-O(13)	2.101(3)
Mo(2)-O(8)	2.295(3)	Mo(4)-O(4)	2.326(3)	Mo(6)-O(3)	2.277(3)
Mo(1)-Mo(4)	2.5958(5)	Mo(2)-Mo(5)	2.5770(5)	Mo(3)-Mo(6)	2.5863(5)
Sr(1)-O(34)	2.506(4)	Sr(1)-O(33)	2.574(4)	Sr(1)-O(7)	2.674(3)

Sr(1)-O(19)	2.558(3)	Sr(1)-O(6)	2.601(3)		
Sr(1)-O(29)	2.559(4)	Sr(1)-O(23	2.624(3)		
Cu(1)-O(5)#2	2.146(3)	Cu(2)-O(7)#1	2.072(3)	Cu(2)-O(24)	2.074(3)
Cu(1)-O(5)	2.146(3)	Cu(2)-O(7)	2.072(3)	Cu(2)-O(19)#1	2.264(3)
Cu(1)-O(1)	2.149(3)	Cu(2)-O(24)#1	2.074(3)	Cu(2)-O(19)	2.264(3)
Cu(1)-O(1)#2	2.149(3)	Cu(1)-O(2)	2.164(3)	Cu(1)-O(2)#2	2.164(3)
P(1)-O(7)	1.520(3)	P(2)-O(29)	1.510(4)	P(3)-O(19)	1.518(3)
P(1)-O(8)	1.535(3)	P(2)-O(21)	1.530(3)	P(3)-O(14)	1.538(3)
P(1)-O(4)	1.540(3)	P(2)-O(12)	1.538(3)	P(3)-O(9)	1.547(3)
P(1)-O(3)	1.546(3)	P(2)-O(30)	1.571(3)	P(3)-O(23)	1.553(3)
P(4)-O(31)	1.513(3)	P(4)-O(22)	1.516(4)		
P(4)-O(18)	1.523(4)	P(4)-O(32)	1.593(4)		
O(28)-Mo(1)-O(6)	106.93(15)	O(26)-Mo(2)-O(15)	105.74(15)	O(25)-Mo(3)-O(16)	105.68(16)
O(6)-Mo(1)-O(2)	94.85(13)	O(26)-Mo(2)-O(5)	101.57(14)	O(25)-Mo(3)-O(1)	102.45(15)
O(6)-Mo(1)-O(18)	84.35(13)	O(26)-Mo(2)-O(14)#1	97.39(15)	O(25)-Mo(3)-O(9)#1	96.47(15)
O(6)-Mo(1)-O(13)	154.27(13)	O(26)-Mo(2)-O(10)	98.33(14)	O(25)-Mo(3)-O(10)	96.51(15)
O(6)-Mo(1)-O(3)	82.99(12)	O(26)-Mo(2)-O(8)	171.23(14)	O(25)-Mo(3)-O(8)	168.94(14)
O(27)-Mo(4)-O(6)	107.17(15)	O(17)-Mo(5)-O(15)	105.47(15)	O(20)-Mo(6)-O(16)	105.86(16)
O(27)-Mo(4)-O(2)	102.96(15)	O(17)-Mo(5)-O(5	102.88(15)	O(20)-Mo(6)-O(1)	102.64(15)
O(27)-Mo(4)-O(12)	96.99(15)	O(17)-Mo(5)-O(21)	97.05(15)	O(20)-Mo(6)-O(22)	98.06(16)
O(27)-Mo(4)-O(11)	98.46(15)	O(17)-Mo(5)-O(11)	97.42(15)	O(20)-Mo(6)-O(13)	99.07(15)
O(27)-Mo(4)-O(4)	170.77(14)	O(17)-Mo(5)-O(4)	170.23(14)	O(20)-Mo(6)-O(3)	170.31(15)
O(34)-Sr(1)-O(19)	124.74(14)	O(34)-Sr(1)-O(29)	78.33(14)	O(34)-Sr(1)-O(33)	75.50(17)
O(34)-Sr(1)-O(6)	84.54(14)	O(34)-Sr(1)-O(23)	77.02(14)	O(34)-Sr(1)-O(7)	154.66(14)
O(5)-Cu(1)-O(1)	96.43(11)	O(5)-Cu(1)-O(1)#2	83.57(11)	O(5)-Cu(1)-O(2)	95.42(11)
O(5)-Cu(1)-O(2)#2	84.58(11)	O(7)-Cu(2)-O(24)#1	92.68(14)	O(7)-Cu(2)-O(24)	87.33(14)
O(7)-Cu(2)-O(19)#1	99.63(12)	O(7)-Cu(2)-O(19)	89.20(13)		

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(4)	1.693(2)	Mo(1)-O(15)	1.721(2)	Mo(1)-O(10)#2	1.888(2)
Mo(1)-O(1)	1.963(2)	Mo(1)-O(2)#2	2.2890(18)	Mo(1)-O(8)	2.3287(19)
Mo(2)-O(22)	1.690(2)	Mo(2)-O(17)	1.730(2)	Mo(2)-O(10)	1.916(2)
Mo(2)-O(14)	1.933(2)	Mo(2)-O(7)	2.2400(18)	Mo(2)-O(16)#3	2.4477(19)
Mo(3)-O(21)	1.704(2)	Mo(3)-O(19)	1.741(2)	Mo(3)-O(1)	1.878(2)
Mo(3)-O(6)#2	1.967(2)	Mo(3)-O(2)#2	2.2169(18)	Mo(3)-O(11)	2.2988(19)
Mo(4)-O(20)	1.708(2)	Mo(4)-O(13)	1.734(2)	Mo(4)-O(12)	1.895(2)
Mo(4)-O(6)	1.922(2)	Mo(4)-O(11)#3	2.2547(19)	Mo(4)-O(3)	2.3535(19)
Mo(5)-O(23)	1.707(2)	Mo(5)-O(9)	1.718(2)	Mo(5)-O(14)	1.927(2)
Mo(5)-O(12)	1.951(2)	Mo(5)-O(16)#3	2.202(2)	Mo(5)-O(3)	2.335(2)
Sr(1)-O(5)	2.5541(19)	Sr(1)-O(15)	2.556(2)	Sr(1)-O(8)	2.5816(19)
Sr(1)-O(26)	2.589(3)	Sr(1)-O(25)	2.593(3)	Sr(1)-O(13)	2.615(2)
Sr(1)-O(24)	2.626(3)	Sr(1)-O(6)	2.833(2)	Sr(1)-O(3)	3.191(2)
Cu(1)-O(5)#2	2.146(3)	Cu(2)-O(7)#1	2.072(3)	Cu(2)-O(24)	2.074(3)
Cu(1)-O(5)	2.146(3)	Cu(2)-O(7)	2.072(3)	Cu(2)-O(19)#1	2.264(3)
Cu(1)-O(1)	2.149(3)	Cu(2)-O(24)#1	2.074(3)	Cu(2)-O(19)	2.264(3)
Cu(1)-O(1)#2	2.149(3)	Cu(1)-O(2)	2.164(3)	Cu(1)-O(2)#2	2.164(3)
P(1)-O(5)	1.5172(19)	P(1)-O(7)	1.530(2)	P(1)-O(3)	1.549(2)
P(1)-O(2)	1.557(2)	P(2)-O(8)	1.516(2)	P(2)-O(18)	1.528(2)
P(2)-O(16)	1.555(2)	P(2)-O(11)	1.5581(19)		
O(4)-Mo(1)-O(15)	103.25(10)	O(4)-Mo(1)-O(10)#2	101.23(10)	O(4)-Mo(1)-O(1)	100.25(9)
O(4)-Mo(1)-O(2)#2	86.80(9)	O(4)-Mo(1)-O(8)	172.86(9)	O(22)-Mo(2)-O(17)	102.03(11)
O(22)-Mo(2)-O(10)	103.56(10)	O(22)-Mo(2)-O(14)	102.06(10)	O(22)-Mo(2)-O(7)	88.06(9)
O(22)-Mo(2)-O(16)#	169.88(9)	O(21)-Mo(3)-O(19)	104.45(10)	O(21)-Mo(3)-O(1)	100.17(10)
O(21)-Mo(3)-O(6)#2	99.17(10)	O(21)-Mo(3)-O(2)#2	159.98(9)	O(21)-Mo(3)-O(11)	87.58(9)
O(20)-Mo(4)-O(13)	103.79(11)	O(20)-Mo(4)-O(12)	100.46(10)	O(20)-Mo(4)-O(6)	104.11(10)

O(20)-Mo(4)-O(11)#	91.29(9)	O(20)-Mo(4)-O(3)	169.81(9)	O(23)-Mo(5)-O(9)	104.07(12)
O(23)-Mo(5)-O(14)	99.23(10)	O(23)-Mo(5)-O(12)	95.08(10)	O(23)-Mo(5)-O(16)#3	98.20(10)
O(23)-Mo(5)-O(3)	166.01(10)	O(14)-Mo(5)-O(3)	89.68(8)	O(12)-Mo(5)-O(3)	72.68(7)
O(5)-Sr(1)-O(15)	78.57(6)	O(5)-Sr(1)-O(8)	128.09(6)	O(5)-Sr(1)-O(26)	149.49(9)
O(5)-Sr(1)-O(25)	77.99(8)	O(5)-Sr(1)-O(13)	106.89(6)	O(5)-Sr(1)-O(24)	74.53(7)
O(5)-Sr(1)-O(6)	73.62(6)	O(5)-Sr(1)-O(3)	50.39(5)	O(15)-Sr(1)-O(3)	123.67(6)
O(5)-P(1)-O(7)	110.66(11)	O(5)-P(1)-O(3)	110.08(11)	O(5)-P(1)-O(2)	109.91(11)
O(8)-P(2)-O(18)	111.60(11)	O(8)-P(2)-O(16)	107.49(11)	O(8)-P(2)-O(11)	109.88(11)

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

Table S4 Hydrogen Bond Lengths (Å) and Bond Angles (°) of compound 1

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA	Symmetry
N10- H10···O45	0.86	2.30	3.06(2)	148.7	—
O1W-H1WA···O3W	0.85	2.20	2.97(2)	150.7	—
O3W- H3WA ··· O4W	0.85	2.30	2.88(2)	126.5	—
O6W- H6WA··· O66	0.85	1.73	2.278(9)	120.3	—
O4W- H4WA··· O5W	0.85	2.22	2.713(16)	116.8	—
N1- H1A··· O55	0.86	2.51	3.12(2)	128.4	—
N8- H8··· O57	0.86	2.11	2.93(2)	160.3	-x, -y+1, -z+1
N8- H8 ··· O40	0.86	2.58	3.20(2)	129.8	-x, -y+1, -z+1
O8W - H8WA ··· O77	0.85	2.54	3.29(3)	146.7	x, y, z-1
O8W - H8WA ··· O49	0.85	2.61	3.10(2)	118.3	x, y, z-1
O8W - H8WB ··· O2W	0.85	2.09	2.93(3)	173.6	x-1, y, z-1
O7W - H7WA ··· O76	0.85	2.22	2.78(2)	123.4	x, y, z-1
O7W - H7WB ··· O77	0.85	2.12	2.87(2)	146.9	x, y, z-1
O1W-H1WB···O72	0.85	2.62	3.102(17)	116.9	-x+1, -y+1, -z+2
O3W-H3WB···O71	0.85	2.14	2.599(17)	113.7	x+1, y, z
O2W - H2WA ··· O71	0.85	2.17	2.825(17)	133.9	x+1, y, z
O2W-H2WB···O8W	0.85	2.36	2.93(3)	125.7	x+1, y, z+1
O6W-H6WB···O76	0.85	1.81	2.388(12)	124.1	-x+1, -y+1, -z+2
O4W-H4WB···O62	0.85	2.22	3.017(15)	156.6	x+1, y, z
O5W-H5WA···N7	0.85	2.61	3.25(3)	133.5	-x+1, -y+1, -z+1
O76-H76A···O72	0.85	2.73	3.242(15)	120.4	-x+1, -y+1, -z+2
N6-H6···O62	0.85	2.61	3.107(18)	118.3	x+1, y+1, z
N4-H4A···O28	0.85	2.62	3.28(3)	134.2	x+1, y, z

Table S5 Hydrogen Bond Lengths (Å) and Bond Angles (°) of compound 2

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA	Symmetry
O2W - H2WB ··· O16	0.85	1.98	2.802(8)	161.4	x+1, y+1, z+1
O31 - H31 ··· O31	0.82	1.71	2.455(7)	149.6	-x, -y-1, -z
O30 - H30 ··· O1W	0.82	1.84	2.658(6)	176.3	-x+1, -y+1, -z+1
O33 - H33A ··· O27	0.85	2.18	2.979(6)	156.2	-x+1, -y, -z+1
O33 - H33B ·· O25	0.85	2.57	3.018(5)	114.2	x+1, y, z
O34 - H34A ··· O28	0.85	2.22	2.969(6)	146.9	-x+1, -y, -z+1
O34 - H34B ··· O26	0.85	2.50	2.933(5)	112.8	x+1, y, z
O34 - H34B ··· O14	0.85	2.59	3.403(6)	161.2	-x+1, -y, -z
O1W - H1WB ·· O11	0.85	2.05	2.822(5)	151.7	—
O1W - H1WA ··· O2W	0.85	2.26	2.851(9)	126.7	—
O32 - H32 ··· O3	0.82	2.42	2.930(5)	121.6	—

O32- H32··· O7	0.82	2.10	2.786(5)	141.7	—
O24- H24A·· O29	0.85	2.00	2.817(5)	160.8	—

Table S6 Hydrogen Bond Lengths (Å) and Bond Angles (°) of compound 3

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠DHA	Symmetry
O24- H24B ··· O9	0.85	2.14	2.984(3)	169.9	—
O26 - H26A ··· O1	0.82	2.65	3.257(4)	129.7	—
O1W - H1WA ··· O21	0.82	2.40	2.968(5)	124.7	—
O24 - H24A··· O17	0.85	2.22	3.020(3)	157.5	x+1, y, z
O2W - H2WA ·· O18	0.85	2.32	2.952(3)	131.8	x-1, y, z-1
O2W - H2WA ··· O16	0.85	2.37	3.109(3)	146.4	x-1, y, z-1
O2W - H2WB··· N5	0.85	1.97	2.749(4)	151.1	x-1, y, z
O2W - H2WB ··· O21	0.85	2.54	2.947(3)	110.2	x-1, y, z
O25 - H25A ·· O14	0.85	2.39	2.887(3)	117.8	x, y, z-1
O25 - H25B ··· O19	0.85	2.09	2.842(4)	147.5	x-1, y, z

Table S7 Bond valence sum calculations for Mo atoms in **1**[1]

	Mo^{V}	Mo^{VI}	Average
Mo1	5.75	6.02	5.89
Mo2	5.54	5.80	5.67
Mo3	5.58	5.84	5.71
Mo4	5.74	6.01	5.88
Mo5	5.52	5.77	5.65
Mo6	5.78	6.05	5.92
Mo7	5.79	6.06	5.93
Mo8	5.66	5.93	5.80
Mo9	5.80	6.07	5.94
Mo10	5.83	6.11	5.97
Mo11	5.47	5.73	5.60
Mo12	5.57	5.83	5. 70
Mo13	5.63	5.89	5.76
Mo14	5.67	5.93	5.80
Mo15	5.63	5.90	5.77
Mo16	5.61	5.87	5.74
Mo17	5.78	6.05	5.92
Mo18	5.65	5.91	5.78
Sum	5.67	5.93	**5.80**

[1] ref: I. D. Brown, D. Altermatt, *Acta Crystallogr.*, 1985, **B41**, 244–247.

3. Physical characterization

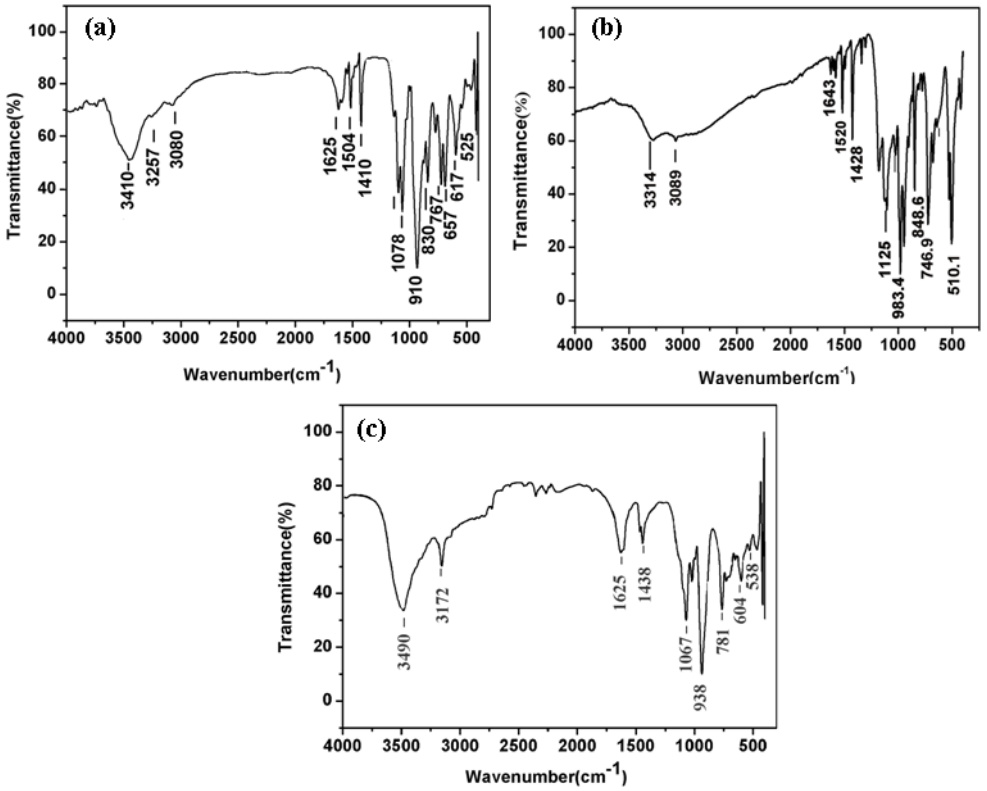


Fig. S6 IR spectra of **(a)** compound **1**, **(b)** compound **2** and **(c)** compound **(3).**

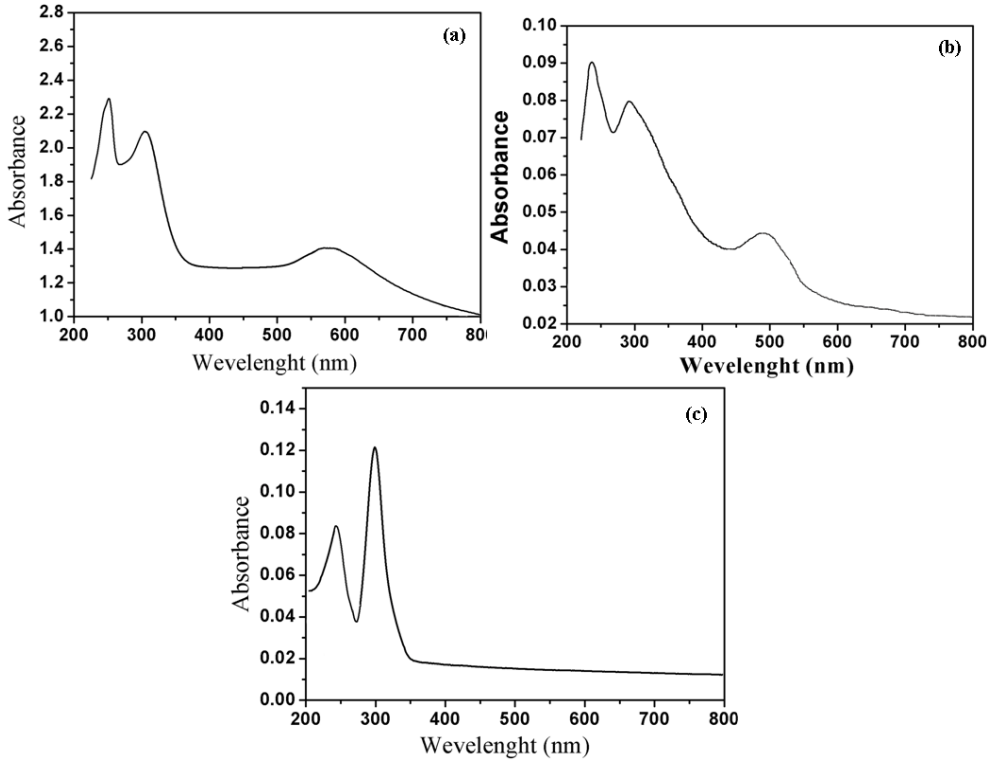


Fig. S7 Solid state UV-vis spectra of **(a)** compound **1**, **(b)** compound **2** and **(c)** compound **3.**

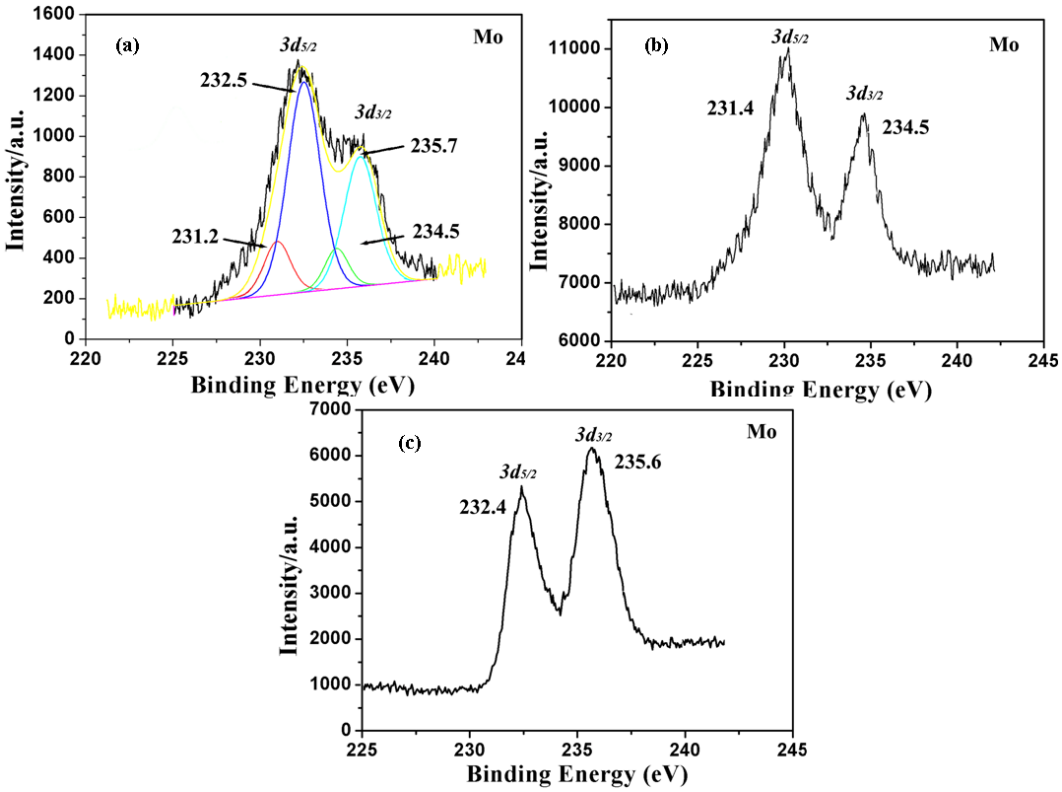


Fig. S8 The XPS spectrum of **(a)** compound **1**, **(b)** compound **2** and **(c)** compound **3.**

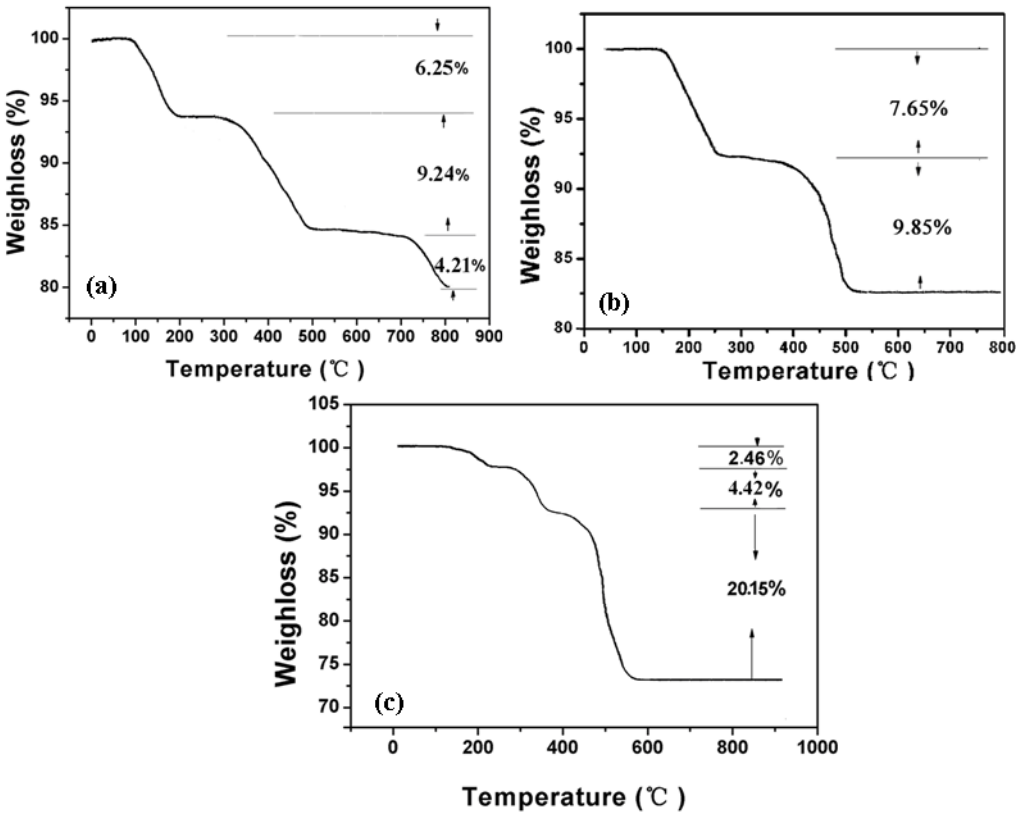


Fig. S9 TG of **(a)** compound **1**, **(b)** compound **2** and **(c)** compound **3.**

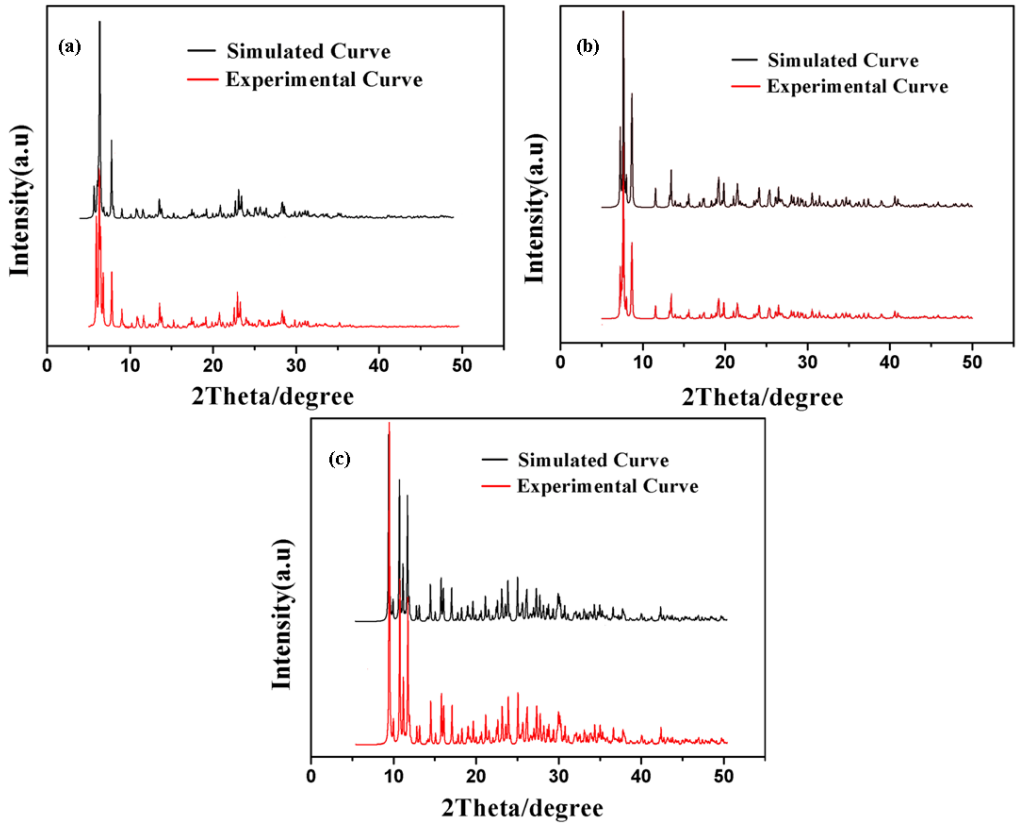
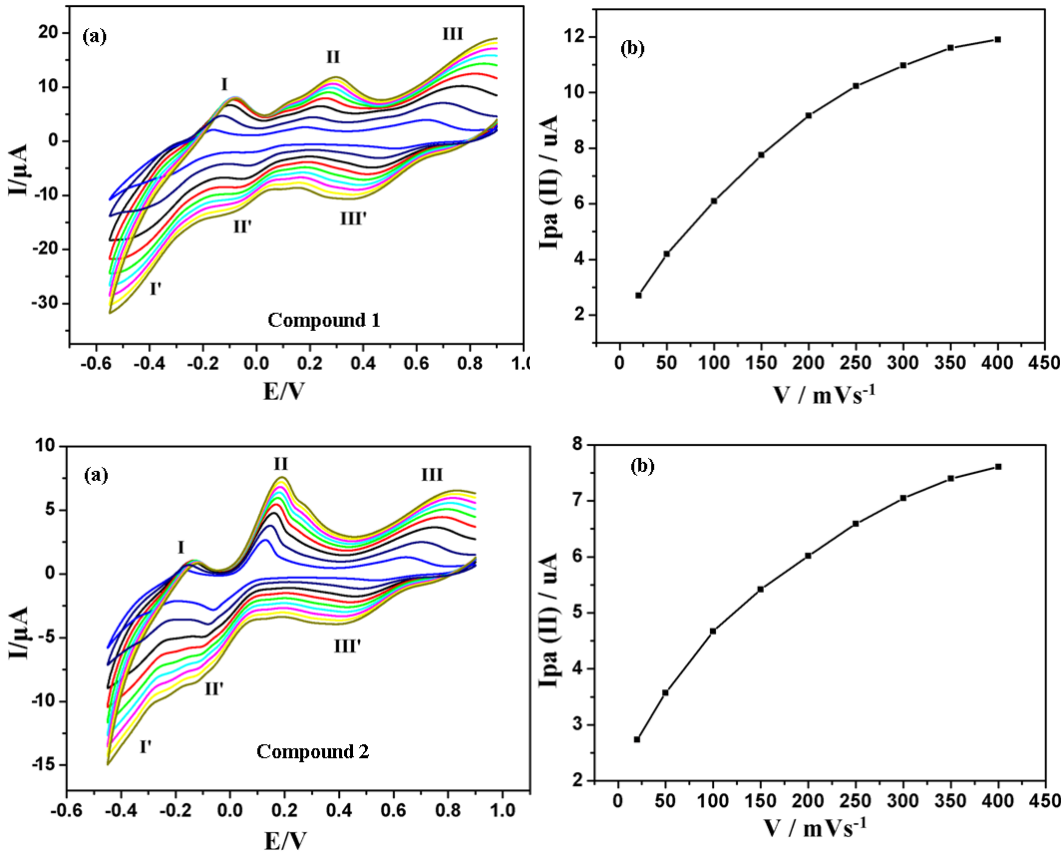


Figure S10. The XPRD contrast curves of **(a)** compound **1**, **(b)** compound **2** and **(c)** compound **3.**



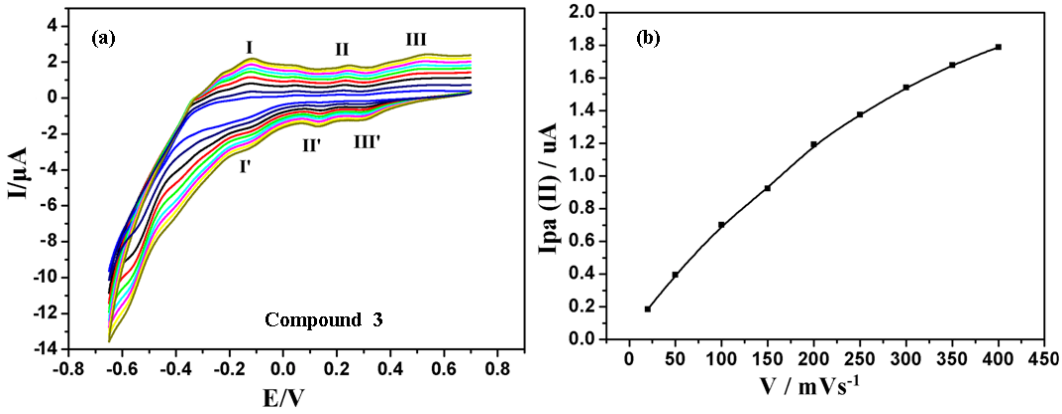


Fig. S11 (a) Cyclic voltammograms of **1-CPE, 2-CPE, and 3-CPE** in the 1.0 M H_2SO_4 solution at different scan rates (from inner to outer: 20, 50, 100, 150, 200, 250, 300, 350, 400 mV s^{-1}). **(b)** The dependence of anodic peak II current on scan rates.