

Support Information

Two extended Wells–Dawson arsenomolybdate architectures directed by Na(I) and/or Cu(I) organic complex linkers

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1. Structural figures

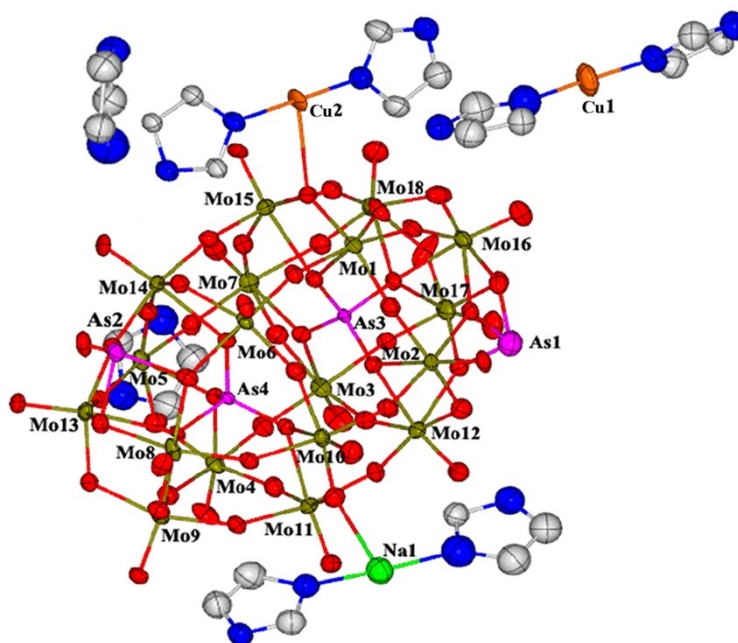


Figure S1 ORTEP view of the basic units in compound **1** with 50% thermal ellipsoid.

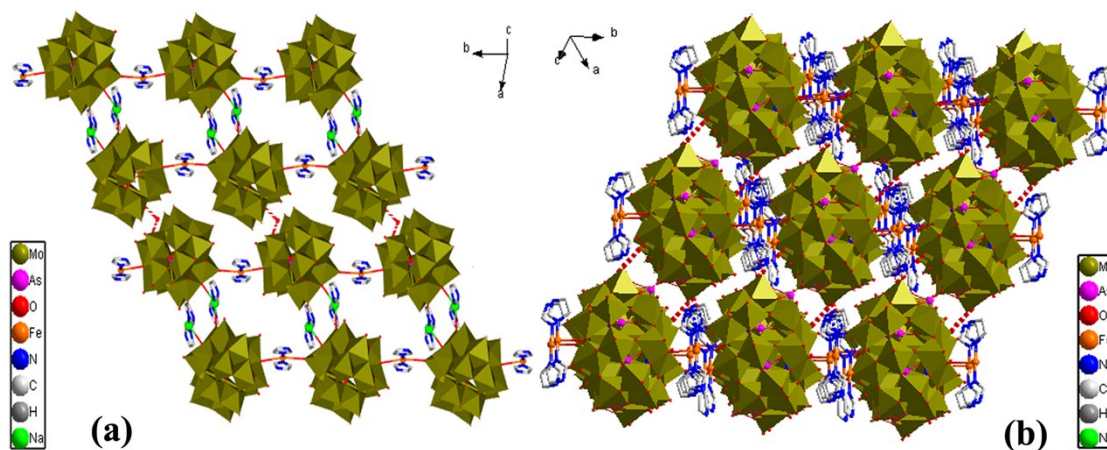


Figure S2 (a) The 2-D supramolecular layer of compound **1**; (b) The 3-D supramolecular network of compound **1**.

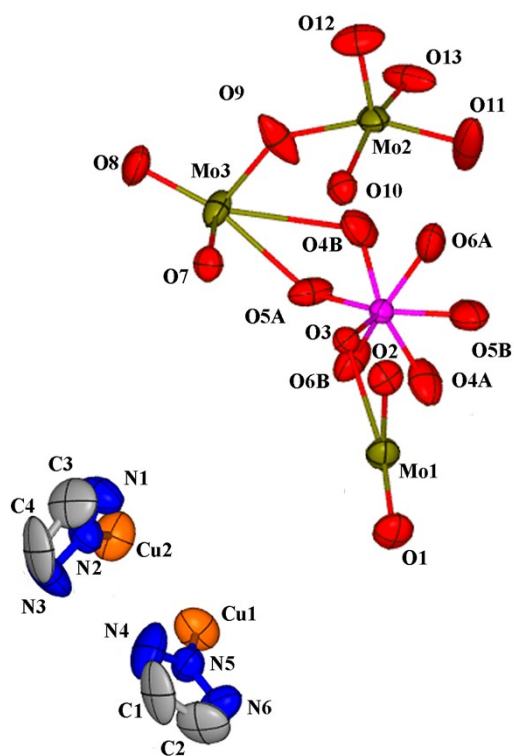


Figure S3 ORTEP view of the basic units in compound **2** with 50% thermal ellipsoid.

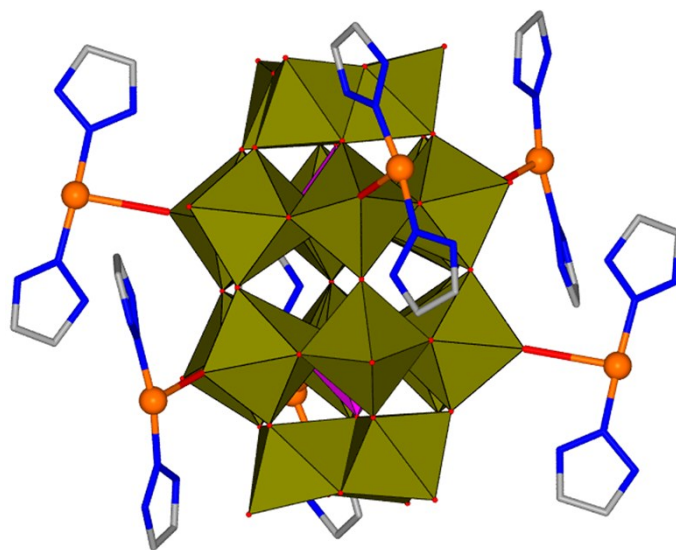


Figure S4 View of the coordinate modes of anions $\{\text{As}_2\text{Mo}_{18}\}$ in compound **2**

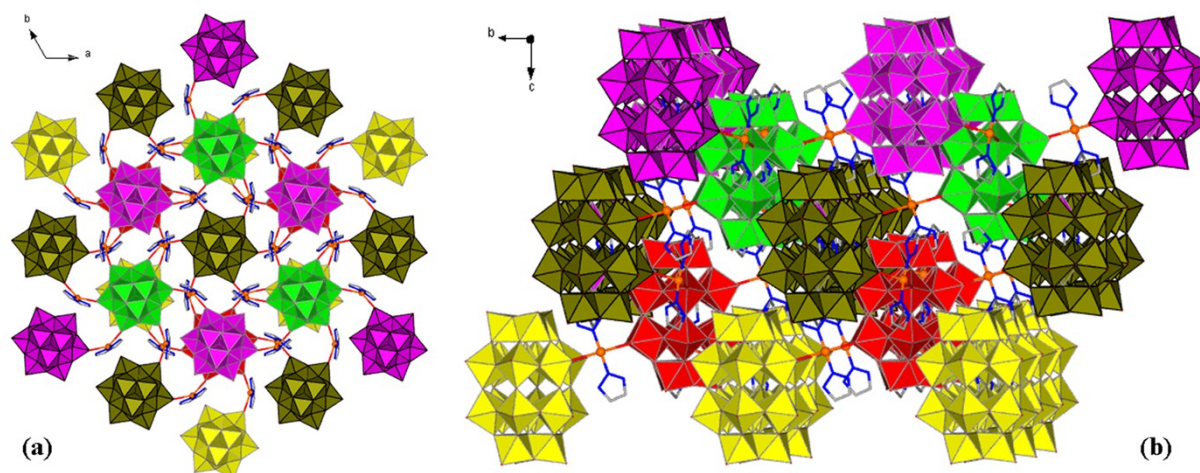


Figure S5 (a) The 6-connected 3D structure of compound **2** along *ab* plane; (b) The 3D structure of compound **2** along *bc* plane. (The middle plane is drawn in dark yellow polyhedra, two planes above the middle plane represented by green and purple polyhedra, other two sheets below the middle plane represented by red and yellow polyhedra.)

2. Structural data

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

Mo(1)-O(1)	1.671(11)	Mo(2)-O(11)	1.680(11)	Mo(3)-O(2)	1.663(12)
Mo(1)-O(44)	1.911(11)	Mo(2)-O(58)	1.824(11)	Mo(3)-O(17)	1.866(11)
Mo(1)-O(62)	1.917(11)	Mo(2)-O(62)	1.848(11)	Mo(3)-O(36)	1.910(11)
Mo(1)-O(34)	1.922(11)	Mo(2)-O(23)	1.980(12)	Mo(3)-O(22)	1.911(11)
Mo(1)-O(16)	2.006(11)	Mo(2)-O(7)	2.160(10)	Mo(3)-O(25)	2.049(11)
Mo(1)-O(37)	2.312(10)	Mo(2)-O(38)	2.293(11)	Mo(3)-O(29)	2.303(11)
Mo(4)-O(6)	1.681(12)	Mo(5)-O(3)	1.682(11)	Mo(6)-O(21)	1.673(11)
Mo(4)-O(17)	1.882(11)	Mo(5)-O(13)	1.863(11)	Mo(6)-O(44)	1.860(11)
Mo(4)-O(15)	1.915(12)	Mo(5)-O(5)	1.904(11)	Mo(6)-O(39)	1.882(11)
Mo(4)-O(26)	1.922(11)	Mo(5)-O(15)	1.924(12)	Mo(6)-O(40)	1.971(11)
Mo(4)-O(14)	2.063(11)	Mo(5)-O(9)	2.054(10)	Mo(6)-O(46)	2.093(11)
Mo(4)-O(33)	2.295(10)	Mo(5)-O(33)	2.316(10)	Mo(6)-O(12)	2.302(10)
Mo(7)-O(20)	1.683(11)	Mo(8)-O(4)	1.67(2)	Mo(9)-O(10)	1.684(11)
Mo(7)-O(13)	1.896(11)	Mo(8)-O(31)	1.873(11)	Mo(9)-O(14)	1.846(11)
Mo(7)-O(49)	1.898(11)	Mo(8)-O(61)	1.906(11)	Mo(9)-O(53)	1.902(11)
Mo(7)-O(36)	1.941(11)	Mo(8)-O(46)	1.972(11)	Mo(9)-O(28)	1.974(11)
Mo(7)-O(35)	2.067(11)	Mo(8)-O(50)	1.981(11)	Mo(9)-O(31)	1.988(11)
Mo(7)-O(29)	2.321(10)	Mo(8)-O(42)	2.355(10)	Mo(9)-O(42)	2.344(10)
Mo(10)-O(43)	1.664(12)	Mo(11)-O(57)	1.669(11)	Mo(12)-O(24)	1.690(11)
Mo(10)-O(39)	1.890(11)	Mo(11)-O(26)	1.851(11)	Mo(12)-O(22)	1.842(11)
Mo(10)-O(48)	1.918(12)	Mo(11)-O(48)	1.940(12)	Mo(12)-O(41)	1.847(11)
Mo(10)-O(61)	1.960(11)	Mo(11)-O(41)	1.975(11)	Mo(12)-O(23)	1.945(12)
Mo(10)-O(58)	1.998(11)	Mo(11)-O(53)	1.996(11)	Mo(12)-O(47)	2.170(11)
Mo(10)-O(54)	2.310(11)	Mo(11)-O(54)	2.289(11)	Mo(12)-O(38)	2.324(10)

Mo(13)-O(8)	1.688(11)	Mo(14)-O(19)	1.677(11)	Mo(15)-O(52)	1.671(11)
Mo(13)-O(9)	1.807(10)	Mo(14)-O(55)	1.853(11)	Mo(15)-O(49)	1.903(11)
Mo(13)-O(28)	1.906(11)	Mo(14)-O(5)	1.877(11)	Mo(15)-O(34)	1.912(11)
Mo(13)-O(56)	1.946(11)	Mo(14)-O(40)	1.930(11)	Mo(15)-O(55)	1.918(11)
Mo(13)-O(42)	2.361(10)	Mo(14)-O(56)	2.097(11)	Mo(15)-O(45)	2.014(11)
Mo(13)-O(50)	2.081(11)	Mo(14)-O(12)	2.304(10)	Mo(15)-O(37)	2.313(10)
Mo(16)-O(59)	1.684(13)	Mo(17)-O(18)	1.709(12)	Mo(18)-O(51)	1.712(12)
Mo(16)-O(60)	1.792(12)	Mo(17)-O(30)	1.733(12)	Mo(18)-O(35)	1.807(12)
Mo(16)-O(16)	1.822(11)	Mo(17)-O(25)	1.782(11)	Mo(18)-O(45)	1.830(11)
Mo(16)-O(7)	2.062(10)	Mo(17)-O(47)	2.075(11)	Mo(18)-O(60)	2.037(12)
Mo(16)-O(32)	2.076(12)	Mo(17)-O(32)	2.096(12)	Mo(18)-O(30)	2.050(11)
Mo(16)-O(27)	2.350(10)	Mo(17)-O(27)	2.370(10)	Mo(18)-O(27)	2.361(10)
As(1)-O(47)	1.780(12)	As(3)-O(37)	1.668(10)	As(4)-O(33)	1.673(10)
As(1)-O(32)	1.907(14)	As(3)-O(29)	1.668(11)	As(4)-O(54)	1.674(11)
As(1)-O(7)	1.849(12)	As(3)-O(27)	1.716(10)	As(4)-O(12)	1.679(10)
As(2)-O(56)	1.850(11)	As(3)-O(38)	1.674(10)	As(4)-O(42)	1.716(10)
As(2)-O(46)	1.928(12)	Na(1)-O(48)	2.653(14)	Cu(1)-N(9)	1.84(2)
As(2)-O(50)	1.993(12)	Na(1)#2-O(43)	2.597(14)	Cu(1)-N(11)	1.868(17)
Cu(2)-N(4)	1.866(15)	Cu(2)-N(2)	1.889(17)	Cu(1)-O21	2.781(2)
Cu(2)-O34	2.765(3)	Cu(2)-O57	2.645(3)	Cu(1)-O1	3.165
Na(1)-N(5)	2.05(3)	Na(1)-O(43)#2	2.597(14)	O(2)-Mo(3)-O(17)	100.6(6)
Na(1)-N(7)	2.09(3)	O(11)-Mo(2)-O(58)	100.7(5)	O(2)-Mo(3)-O(36)	101.2(6)
O(1)-Mo(1)-O(44)	99.3(5)	O(11)-Mo(2)-O(62)	103.7(6)	O(2)-Mo(3)-O(22)	102.0(6)
O(1)-Mo(1)-O(62)	105.2(6)	O(11)-Mo(2)-O(23)	98.5(6)	O(2)-Mo(3)-O(25)	90.9(5)
O(1)-Mo(1)-O(34)	100.0(6)	O(11)-Mo(2)-O(7)	92.6(5)	O(2)-Mo(3)-O(29)	170.3(5)
O(1)-Mo(1)-O(16)	94.1(5)	O(11)-Mo(2)-O(38)	167.5(5)	O(17)-Mo(3)-O(36)	95.4(5)
O(1)-Mo(1)-O(37)	170.2(5)	O(58)-Mo(2)-O(62)	95.5(5)	O(17)-Mo(3)-O(22)	89.0(5)
O(44)-Mo(1)-O(62)	89.7(5)	O(58)-Mo(2)-O(23)	95.1(5)	O(17)-Mo(3)-O(25)	167.1(5)
O(44)-Mo(1)-O(34)	91.7(5)	O(58)-Mo(2)-O(7)	166.0(5)	O(17)-Mo(3)-O(29)	87.6(4)
O(44)-Mo(1)-O(16)	165.8(5)	O(58)-Mo(2)-O(38)	87.4(4)	O(36)-Mo(3)-O(22)	155.1(5)
O(44)-Mo(1)-O(37)	84.7(4)	O(62)-Mo(2)-O(23)	153.1(5)	O(36)-Mo(3)-O(25)	88.1(5)
O(62)-Mo(1)-O(34)	154.2(5)	O(62)-Mo(2)-O(7)	85.5(4)	O(36)-Mo(3)-O(29)	72.7(4)
O(62)-Mo(1)-O(16)	82.4(5)	O(62)-Mo(2)-O(38)	84.7(4)	O(22)-Mo(3)-O(25)	82.8(5)
O(62)-Mo(1)-O(37)	83.6(4)	O(23)-Mo(2)-O(38)	71.1(4)	O(22)-Mo(3)-O(29)	83.1(4)
O(34)-Mo(1)-O(16)	90.4(5)	O(23)-Mo(2)-O(7)	78.4(5)	O(25)-Mo(3)-O(29)	81.5(4)
O(34)-Mo(1)-O(37)	70.9(4)	O(7)-Mo(2)-O(38)	78.7(4)	O(21)-Mo(6)-O(44)	100.9(5)
O(16)-Mo(1)-O(37)	82.7(4)	O(3)-Mo(5)-O(13)	99.9(5)	O(21)-Mo(6)-O(39)	102.8(5)
O(6)-Mo(4)-O(17)	99.7(5)	O(3)-Mo(5)-O(5)	104.4(6)	O(21)-Mo(6)-O(40)	100.1(5)
O(6)-Mo(4)-O(15)	100.4(6)	O(3)-Mo(5)-O(15)	99.9(6)	O(21)-Mo(6)-O(46)	92.1(5)
O(6)-Mo(4)-O(26)	102.9(6)	O(3)-Mo(5)-O(9)	92.8(5)	O(21)-Mo(6)-O(12)	169.3(5)
O(6)-Mo(4)-O(14)	92.1(5)	O(3)-Mo(5)-O(33)	170.0(5)	O(44)-Mo(6)-O(39)	91.2(5)
O(6)-Mo(4)-O(33)	171.0(5)	O(13)-Mo(5)-O(5)	90.5(5)	O(44)-Mo(6)-O(40)	94.8(5)
O(17)-Mo(4)-O(15)	92.4(5)	O(13)-Mo(5)-O(15)	94.5(5)	O(44)-Mo(6)-O(46)	167.0(5)
O(17)-Mo(4)-O(26)	90.6(5)	O(13)-Mo(5)-O(9)	166.6(4)	O(44)-Mo(6)-O(12)	86.2(4)
O(17)-Mo(4)-O(14)	167.8(5)	O(13)-Mo(5)-O(33)	86.1(4)	O(39)-Mo(6)-O(40)	154.8(5)

O(17)-Mo(4)-O(33)	86.0(4)	O(5)-Mo(5)-O(15)	154.0(5)	O(39)-Mo(6)-O(46)	86.4(5)
O(15)-Mo(4)-O(26)	155.6(5)	O(5)-Mo(5)-O(9)	82.2(4)	O(39)-Mo(6)-O(12)	84.9(4)
O(15)-Mo(4)-O(14)	88.5(5)	O(5)-Mo(5)-O(33)	83.3(4)	O(40)-Mo(6)-O(46)	82.3(4)
O(15)-Mo(4)-O(33)	72.2(4)	O(15)-Mo(5)-O(33)	71.6(4)	O(40)-Mo(6)-O(12)	71.2(4)
O(26)-Mo(4)-O(14)	83.7(5)	O(15)-Mo(5)-O(9)	87.5(5)	O(46)-Mo(6)-O(12)	80.8(4)
O(26)-Mo(4)-O(33)	83.9(4)	O(9)-Mo(5)-O(33)	82.0(4)	O(10)-Mo(9)-O(14)	104.1(6)
O(14)-Mo(4)-O(33)	82.7(4)	O(4)-Mo(8)-O(31)	102.4(5)	O(10)-Mo(9)-O(53)	102.4(5)
O(20)-Mo(7)-O(13)	98.7(5)	O(4)-Mo(8)-O(61)	100.9(5)	O(10)-Mo(9)-O(28)	98.9(5)
O(20)-Mo(7)-O(49)	104.2(6)	O(4)-Mo(8)-O(46)	102.1(5)	O(10)-Mo(9)-O(31)	98.8(5)
O(20)-Mo(7)-O(36)	99.5(6)	O(4)-Mo(8)-O(50)	100.6(5)	O(10)-Mo(9)-O(42)	168.2(5)
O(20)-Mo(7)-O(35)	94.9(5)	O(4)-Mo(8)-O(42)	172.9(5)	O(14)-Mo(9)-O(53)	90.8(5)
O(20)-Mo(7)-O(29)	170.9(5)	O(31)-Mo(8)-O(61)	92.1(5)	O(14)-Mo(9)-O(28)	90.5(5)
O(13)-Mo(7)-O(49)	91.5(5)	O(31)-Mo(8)-O(46)	155.0(5)	O(14)-Mo(9)-O(31)	156.9(5)
O(13)-Mo(7)-O(36)	90.6(5)	O(31)-Mo(8)-O(50)	89.9(5)	O(14)-Mo(9)-O(42)	84.8(4)
O(13)-Mo(7)-O(35)	166.3(4)	O(31)-Mo(8)-O(42)	73.7(4)	O(53)-Mo(9)-O(28)	157.7(5)
O(13)-Mo(7)-O(29)	84.2(4)	O(61)-Mo(8)-O(46)	88.0(5)	O(53)-Mo(9)-O(31)	87.4(5)
O(49)-Mo(7)-O(36)	155.5(5)	O(61)-Mo(8)-O(50)	157.5(4)	O(53)-Mo(9)-O(42)	84.9(4)
O(49)-Mo(7)-O(35)	83.7(5)	O(61)-Mo(8)-O(42)	85.3(4)	O(28)-Mo(9)-O(42)	73.0(4)
O(49)-Mo(7)-O(29)	84.2(4)	O(46)-Mo(8)-O(50)	80.9(5)	O(28)-Mo(9)-O(31)	82.8(5)
O(36)-Mo(7)-O(29)	71.8(4)	O(46)-Mo(8)-O(42)	81.4(4)	O(31)-Mo(9)-O(42)	72.1(4)
O(36)-Mo(7)-O(35)	88.6(5)	O(50)-Mo(8)-O(42)	73.7(4)	O(24)-Mo(12)-O(22)	102.0(6)
O(35)-Mo(7)-O(29)	82.5(4)	O(57)-Mo(11)-O(26)	104.5(6)	O(24)-Mo(12)-O(41)	100.5(5)
O(43)-Mo(10)-O(39)	103.7(5)	O(57)-Mo(11)-O(48)	99.9(6)	O(24)-Mo(12)-O(23)	101.5(6)
O(43)-Mo(10)-O(48)	100.9(6)	O(57)-Mo(11)-O(41)	95.7(5)	O(24)-Mo(12)-O(47)	92.4(5)
O(43)-Mo(10)-O(61)	96.8(5)	O(57)-Mo(11)-O(53)	96.3(5)	O(24)-Mo(12)-O(38)	170.2(5)
O(43)-Mo(10)-O(58)	96.3(5)	O(57)-Mo(11)-O(54)	171.3(5)	O(22)-Mo(12)-O(41)	95.9(5)
O(43)-Mo(10)-O(54)	172.2(5)	O(26)-Mo(11)-O(48)	155.6(5)	O(22)-Mo(12)-O(23)	152.7(5)
O(39)-Mo(10)-O(48)	155.4(5)	O(26)-Mo(11)-O(41)	88.8(5)	O(22)-Mo(12)-O(47)	85.5(5)
O(39)-Mo(10)-O(61)	87.1(5)	O(26)-Mo(11)-O(53)	87.9(5)	O(22)-Mo(12)-O(38)	83.9(4)
O(39)-Mo(10)-O(58)	88.2(5)	O(26)-Mo(11)-O(54)	84.1(4)	O(41)-Mo(12)-O(23)	93.4(5)
O(39)-Mo(10)-O(54)	84.1(4)	O(48)-Mo(11)-O(41)	89.6(5)	O(41)-Mo(12)-O(47)	166.4(5)
O(48)-Mo(10)-O(61)	90.7(5)	O(48)-Mo(11)-O(53)	88.6(5)	O(41)-Mo(12)-O(38)	86.5(4)
O(48)-Mo(10)-O(58)	88.4(5)	O(48)-Mo(11)-O(54)	71.5(4)	O(23)-Mo(12)-O(38)	71.0(4)
O(48)-Mo(10)-O(54)	71.3(4)	O(41)-Mo(11)-O(54)	84.0(4)	O(23)-Mo(12)-O(47)	79.8(5)
O(61)-Mo(10)-O(54)	84.4(4)	O(41)-Mo(11)-O(53)	167.9(5)	O(47)-Mo(12)-O(38)	80.2(4)
O(61)-Mo(10)-O(58)	166.8(4)	O(53)-Mo(11)-O(54)	84.1(4)	O(52)-Mo(15)-O(49)	104.7(6)
O(58)-Mo(10)-O(54)	82.9(4)	O(19)-Mo(14)-O(55)	100.4(5)	O(52)-Mo(15)-O(34)	99.6(6)
O(8)-Mo(13)-O(9)	105.4(5)	O(19)-Mo(14)-O(5)	103.1(6)	O(52)-Mo(15)-O(55)	99.2(5)
O(8)-Mo(13)-O(28)	101.1(5)	O(19)-Mo(14)-O(40)	99.0(6)	O(52)-Mo(15)-O(45)	93.7(5)
O(8)-Mo(13)-O(56)	101.6(5)	O(19)-Mo(14)-O(56)	93.1(5)	O(52)-Mo(15)-O(37)	170.3(5)
O(8)-Mo(13)-O(50)	96.4(5)	O(19)-Mo(14)-O(12)	169.3(5)	O(49)-Mo(15)-O(34)	155.4(5)
O(8)-Mo(13)-O(42)	167.3(5)	O(55)-Mo(14)-O(5)	93.7(5)	O(49)-Mo(15)-O(55)	88.5(5)
O(9)-Mo(13)-O(28)	94.5(5)	O(55)-Mo(14)-O(40)	94.8(5)	O(49)-Mo(15)-O(45)	85.5(5)
O(9)-Mo(13)-O(56)	91.2(5)	O(55)-Mo(14)-O(56)	166.5(4)	O(49)-Mo(15)-O(37)	84.5(4)
O(9)-Mo(13)-O(50)	157.6(5)	O(55)-Mo(14)-O(12)	86.1(4)	O(34)-Mo(15)-O(55)	91.9(5)

O(9)-Mo(13)-O(42)	86.7(4)	O(5)-Mo(14)-O(40)	154.5(5)	O(34)-Mo(15)-O(45)	88.8(5)
O(28)-Mo(13)-O(56)	154.1(5)	O(5)-Mo(14)-O(56)	83.0(4)	O(34)-Mo(15)-O(37)	71.0(4)
O(28)-Mo(13)-O(50)	86.1(5)	O(5)-Mo(14)-O(12)	84.8(4)	O(55)-Mo(15)-O(37)	84.0(4)
O(28)-Mo(13)-O(42)	73.8(4)	O(40)-Mo(14)-O(12)	71.8(4)	O(55)-Mo(15)-O(45)	166.8(4)
O(56)-Mo(13)-O(42)	81.4(4)	O(40)-Mo(14)-O(56)	83.1(4)	O(45)-Mo(15)-O(37)	83.8(4)
O(56)-Mo(13)-O(50)	79.3(4)	O(56)-Mo(14)-O(12)	80.6(4)	O(51)-Mo(18)-O(35)	105.7(6)
O(50)-Mo(13)-O(42)	71.9(4)	O(18)-Mo(17)-O(30)	104.4(6)	O(51)-Mo(18)-O(45)	103.7(6)
O(59)-Mo(16)-O(60)	103.9(6)	O(18)-Mo(17)-O(25)	103.3(6)	O(51)-Mo(18)-O(60)	98.4(6)
O(59)-Mo(16)-O(16)	105.1(6)	O(18)-Mo(17)-O(47)	100.2(6)	O(51)-Mo(18)-O(30)	100.5(6)
O(59)-Mo(16)-O(7)	100.6(5)	O(18)-Mo(17)-O(32)	100.0(6)	O(51)-Mo(18)-O(27)	164.6(5)
O(59)-Mo(16)-O(32)	96.9(6)	O(18)-Mo(17)-O(27)	170.6(5)	O(35)-Mo(18)-O(45)	95.8(5)
O(59)-Mo(16)-O(27)	168.3(5)	O(30)-Mo(17)-O(25)	95.2(6)	O(35)-Mo(18)-O(60)	154.6(5)
O(60)-Mo(16)-O(16)	96.1(6)	O(30)-Mo(17)-O(47)	153.4(5)	O(35)-Mo(18)-O(30)	83.9(5)
O(60)-Mo(16)-O(7)	153.1(5)	O(30)-Mo(17)-O(32)	93.0(6)	O(35)-Mo(18)-O(27)	84.9(4)
O(60)-Mo(16)-O(32)	92.4(6)	O(30)-Mo(17)-O(27)	73.7(4)	O(45)-Mo(18)-O(60)	86.0(5)
O(60)-Mo(16)-O(27)	74.1(5)	O(25)-Mo(17)-O(47)	88.9(5)	O(45)-Mo(18)-O(30)	154.9(5)
O(16)-Mo(16)-O(7)	88.0(5)	O(25)-Mo(17)-O(32)	152.4(5)	O(45)-Mo(18)-O(27)	85.9(4)
O(16)-Mo(16)-O(32)	153.7(5)	O(25)-Mo(17)-O(27)	86.1(4)	O(60)-Mo(18)-O(27)	69.9(4)
O(16)-Mo(16)-O(27)	86.6(4)	O(47)-Mo(17)-O(27)	80.3(4)	O(60)-Mo(18)-O(30)	84.0(5)
O(7)-Mo(16)-O(27)	79.7(4)	O(47)-Mo(17)-O(32)	72.6(5)	O(30)-Mo(18)-O(27)	69.1(4)
O(7)-Mo(16)-O(32)	73.7(5)	O(32)-Mo(17)-O(27)	71.1(4)	O(37)-As(3)-O(29)	111.9(5)
O(32)-Mo(16)-O(27)	71.8(4)	O(56)-As(2)-O(46)	101.8(5)	O(37)-As(3)-O(38)	110.8(5)
O(47)-As(1)-O(7)	102.7(5)	O(56)-As(2)-O(50)	83.9(5)	O(37)-As(3)-O(27)	106.5(5)
O(47)-As(1)-O(32)	84.0(5)	O(46)-As(2)-O(50)	81.7(5)	O(29)-As(3)-O(38)	111.0(5)
O(7)-As(1)-O(32)	82.7(5)	N(9)-Cu(1)-N(11)	175.5(9)	O(29)-As(3)-O(27)	107.4(5)
O(33)-As(4)-O(54)	112.0(5)	N(4)-Cu(2)-N(2)	179.0(8)	O(38)-As(3)-O(27)	109.1(5)
O(33)-As(4)-O(12)	111.0(5)	N(5)-Na(1)-N(7)	171.6(12)	O(43)#2-Na(1)-O(48)	146.3(5)
O(33)-As(4)-O(42)	107.5(5)	N(5)-Na(1)-O(43)#2	88.4(8)	N(7)-Na(1)-O(43)#2	85.4(9)
O(54)-As(4)-O(12)	111.3(5)	N(5)-Na(1)-O(48)	86.9(8)	N(7)-Na(1)-O(48)	95.3(9)
O(54)-As(4)-O(42)	106.3(5)	O(12)-As(4)-O(42)	108.5(5)		

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

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

Mo(1)-O(1)	1.688(12)	Mo(2)-O(12)	1.663(12)	Mo(3)-O(8)	1.644(12)
Mo(1)-O(10)#3	1.810(11)	Mo(2)-O(13)	1.840(12)	Mo(3)-O(11)#4	1.80(3)
Mo(1)-O(7)#4	1.924(11)	Mo(2)-O(11)	1.85(3)	Mo(3)-O(9)	1.864(17)
Mo(1)-O(2)	1.928(12)	Mo(2)-O(9)	1.860(17)	Mo(3)-O(7)	1.943(11)
Mo(1)-O(2)#3	2.028(12)	Mo(2)-O(10)	2.083(11)	Mo(3)-O(13)#5	1.961(12)
Mo(1)-O(3)	2.351(9)	Mo(2)-O(6A)	2.6(6)	Mo(3)-O(6A)#4	2.2(7)
Cu(1)-N(5)#1	1.878(18)	Mo(2)-O(6B)#3	2.3(11)	Mo(3)-O(6B)#3	2.7(9)
Cu(1)-N(5)	1.878(18)	As(1)-O(6B)	2.0(14)	As(1)-O(6A)	1.500(8)
Cu(2)-N(2)	1.86(2)	As(1)-O(6B)#3	2.0(14)	As(1)-O(6A)#3	1.500(8)
Cu(2)-O(12)	2.589(2)	Cu(2)-O(12)#3	2.591(2)	As(1)-O(6A)#4	1.500(8)
Cu(2)-N(2)#2	1.86(2)	As(1)-O(6B)#4	2.0(14)	O(9)-Mo(2)-O(10)	85.3(5)
O(1)-Mo(1)-O(10)#3	105.1(6)	O(12)-Mo(2)-O(13)	99.7(6)	O(9)-Mo(2)-O(6A)	99(10)
O(1)-Mo(1)-O(7)#4	103.0(6)	O(12)-Mo(2)-O(11)	104.4(10)	O(9)-Mo(2)-O(6B)#3	65(10)
O(1)-Mo(1)-O(2)	99.2(6)	O(12)-Mo(2)-O(9)	100.0(11)	O(10)-Mo(2)-O(6A)	71(10)
O(1)-Mo(1)-O(2)#3	96.8(5)	O(12)-Mo(2)-O(10)	92.7(5)	O(10)-Mo(2)-O(6B)#3	98(10)
O(1)-Mo(1)-O(3)	166.9(6)	O(12)-Mo(2)-O(6A)	154(10)	O(6A)-Mo(2)-O(6B)#3	46(10)
O(10)#3-Mo(1)-O(7)#4	89.7(5)	O(12)-Mo(2)-O(6B)#3	160(10)	O(8)-Mo(3)-O(11)#4	106.3(10)
O(10)#3-Mo(1)-O(2)	92.6(5)	O(13)-Mo(2)-O(11)	91.0(10)	O(8)-Mo(3)-O(9)	99.5(11)
O(10)#3-Mo(1)-O(2)#3	158.1(5)	O(13)-Mo(2)-O(9)	95.1(7)	O(8)-Mo(3)-O(7)	98.0(6)
O(10)#3-Mo(1)-O(3)	86.4(4)	O(13)-Mo(2)-O(10)	167.3(5)	O(8)-Mo(3)-O(13)#5	96.1(6)
O(7)#4-Mo(1)-O(2)	156.2(5)	O(13)-Mo(2)-O(6A)	96(10)	O(8)-Mo(3)-O(6A)#4	167(10)
O(7)#4-Mo(1)-O(2)#3	84.3(5)	O(13)-Mo(2)-O(6B)#3	71(10)	O(8)-Mo(3)-O(6B)#3	151(10)
O(7)#4-Mo(1)-O(3)	83.0(4)	O(11)-Mo(2)-O(9)	153.4(12)	O(11)#4-Mo(3)-O(9)	154.1(13)
O(2)-Mo(1)-O(3)	73.6(4)	O(11)-Mo(2)-O(10)	83.2(9)	O(11)#4-Mo(3)-O(7)	88.4(9)
O(2)#3-Mo(1)-O(3)	71.9(4)	O(11)-Mo(2)-O(6A)	54(10)	O(11)#4-Mo(3)-O(13)#5	85.2(10)
O(2)-Mo(1)-O(2)#3	84.8(7)	O(11)-Mo(2)-O(6B)#3	93(10)	O(11)#4-Mo(3)-O(6A)#4	64(10)
O(9)-Mo(3)-O(7)	89.8(5)	O(7)-Mo(3)-O(13)#5	165.7(5)	O(11)#4-Mo(3)-O(6B)#3	98(10)
O(9)-Mo(3)-O(13)#5	90.4(7)	O(7)-Mo(3)-O(6A)#4	74(10)	O(13)#5-Mo(3)-O(6B)#3	70(10)
O(9)-Mo(3)-O(6A)#4	91(10)	O(7)-Mo(3)-O(6B)#3	98(10)	O(13)#5-Mo(3)-O(6A)#4	92(10)
O(9)-Mo(3)-O(6B)#3	57(10)	O(6A)#4-Mo(3)-O(6B)#3	42(10)	O(6B)#3-As(1)-O(6B)#4	90(10)
O(6A)#4-As(1)-O(6A)#3	119(10)	O(6A)#3-As(1)-O(6B)#3	138(10)	O(6B)-As(1)-O(6B)#4	90(10)
O(6A)#4-As(1)-O(6A)	119(10)	O(6A)#3-As(1)-O(6B)#4	65(10)	O(6B)-As(1)-O(6B)#3	90(10)
O(6A)#4-As(1)-O(6B)#4	138(10)	O(6A)-As(1)-O(6B)	138(10)	N(5)#1-Cu(1)-N(5)	179.7(12)
O(6A)#4-As(1)-O(6B)	65(10)	O(6A)-As(1)-O(6B)#4	59(10)	N(2)-Cu(2)-N(2)#2	169.5(14)
O(6A)#4-As(1)-O(6B)#3	59(10)	O(6A)#3-As(1)-O(6B)#3	138(10)	O(6A)#4-As(1)-O(6B)#4	138(10)
O(6A)-As(1)-O(6B)	138(10)	O(6A)#3-As(1)-O(6A)	119(10)	O(6A)#3-As(1)-O(6B)	59(10)

Symmetry transformations used to generate equivalent atoms: #1 $x-y+1/3, -y+2/3, -z+13/6$; #2 $x-y+1/3, -y+2/3, -z+1/6$; #3 $-y, x-y, z$;

3. Physical characterization

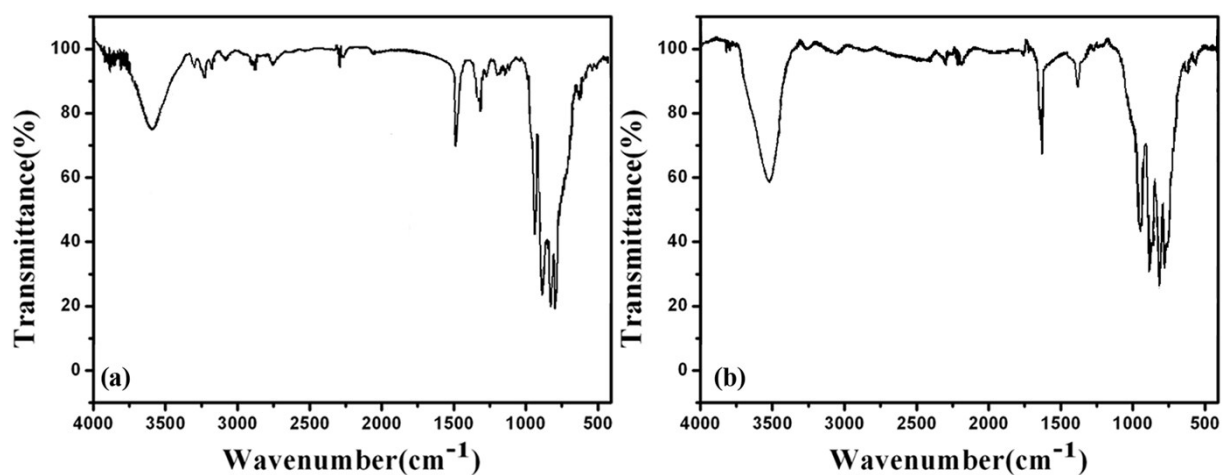


Fig. S6 IR spectra of compounds 1 and 2.

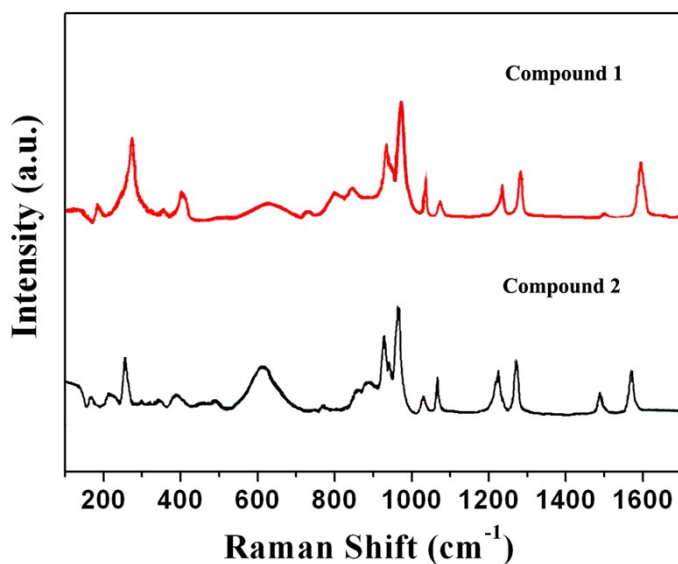


Fig. S7 Raman spectra for compounds 1 and 2.

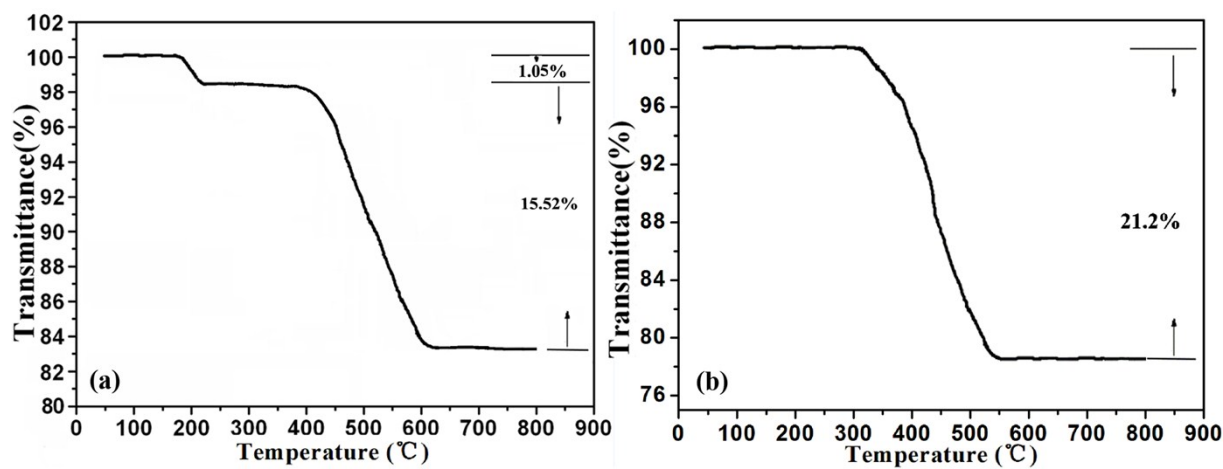


Fig. S8 TG curves of compounds 1 and 2.

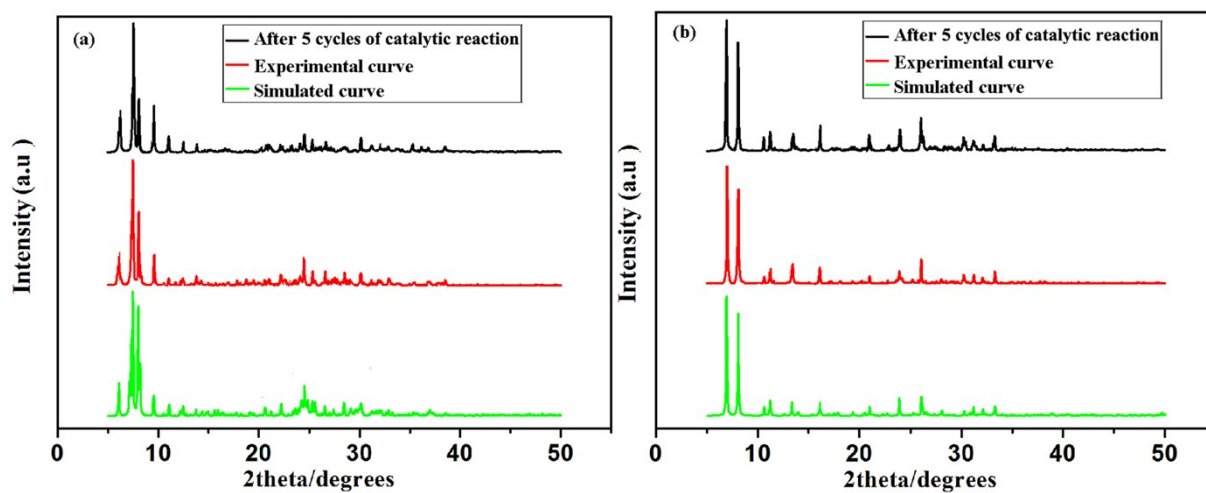


Fig. S9 The PXR D contrast curves of compounds **1** and **2**.

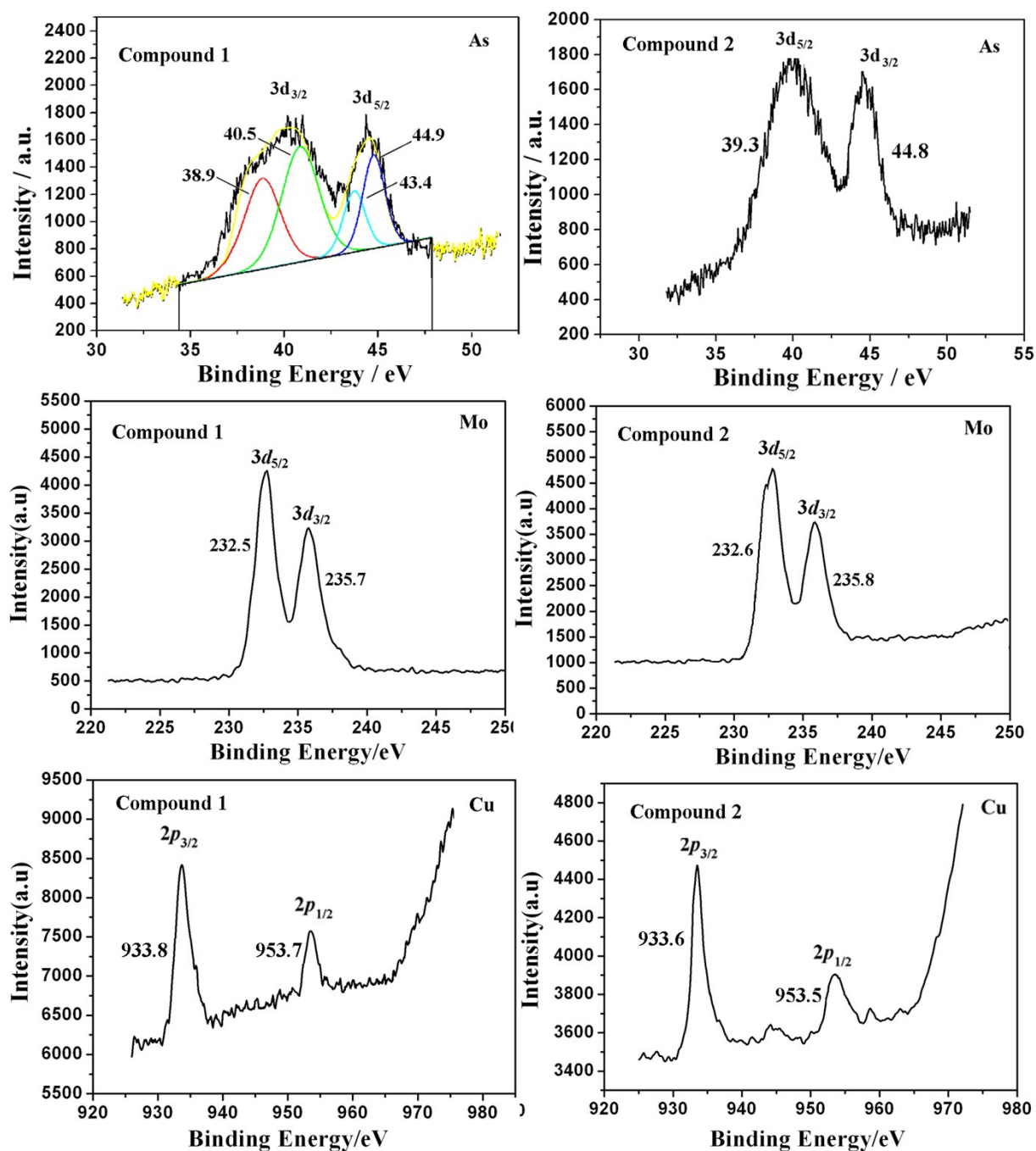


Fig. S10 The X-ray photoelectron spectroscopy (XPS) of compounds 1 and 2.

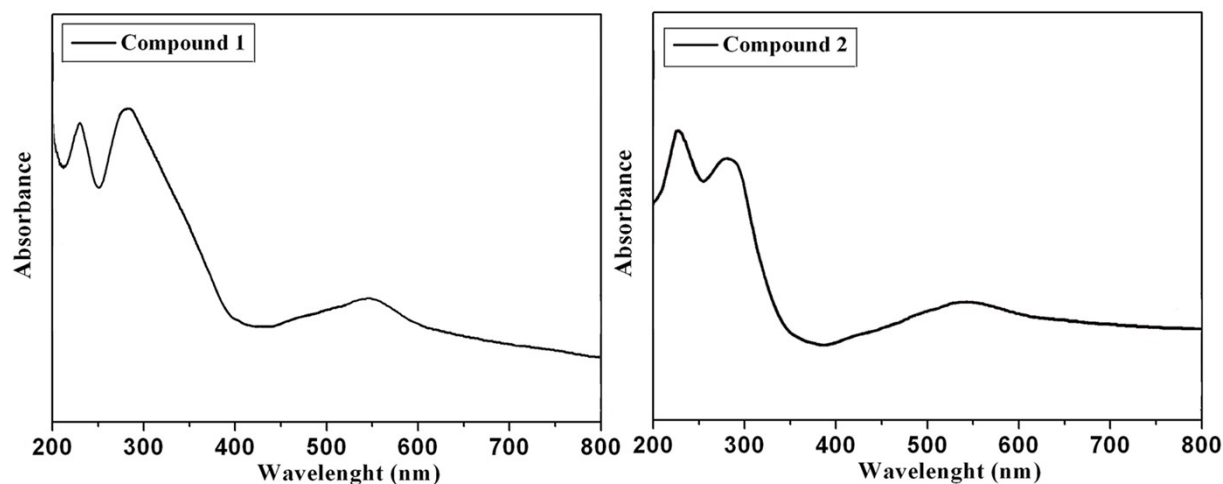


Fig. S11 The UV-vis spectra of compounds 1 and 2 in solid state at room temperature.

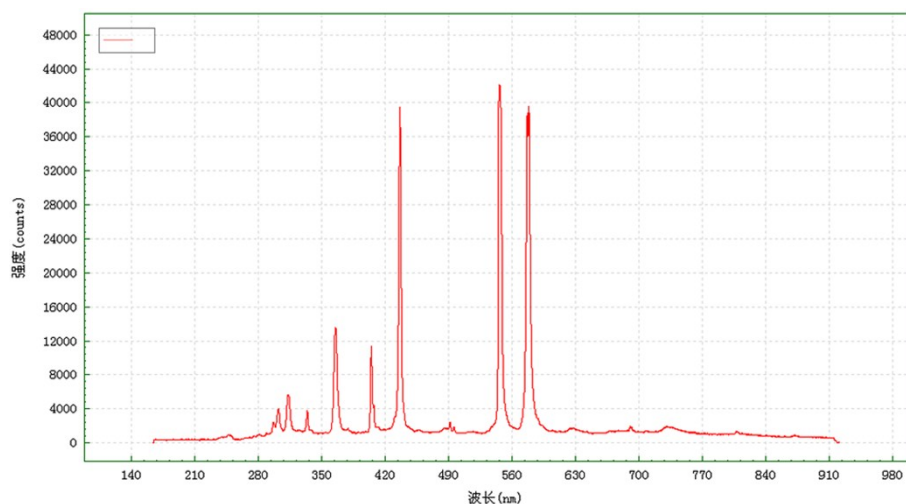


Figure S12 The light spectrum of the photocatalytic reaction

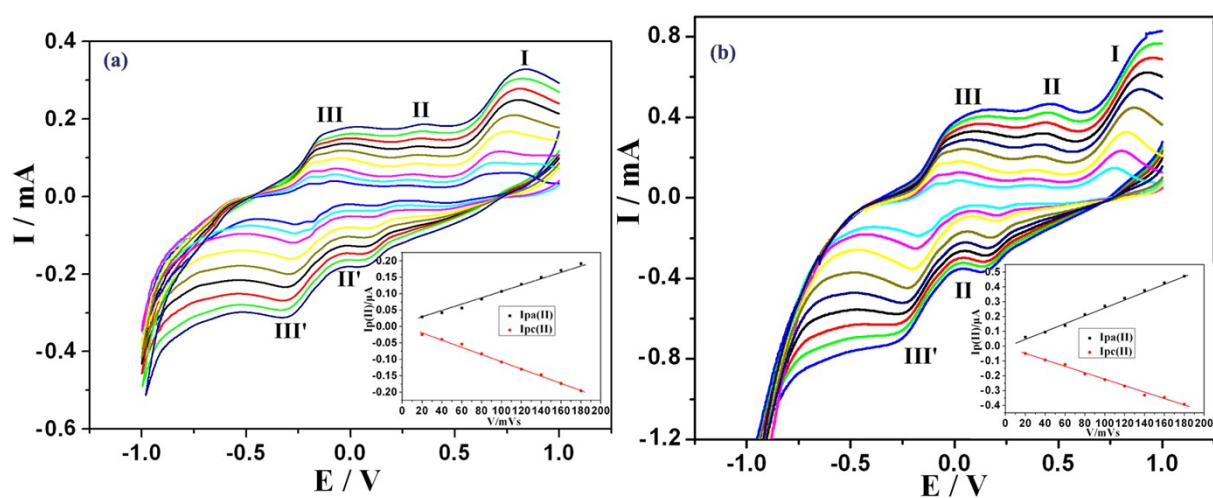


Fig. S13 Cyclic voltammograms of (a) 1-CPE and (b) 2-CPE in the 0.1 M H_2SO_4 solution at different scan rate. rates (from inner to outer: 20, 40, 60, 80, 100, 120, 140, 160, 180 mV s^{-1} ; Insert plots: The dependence of anodic and cathodic peak II current on scan rates.) Potentials vs. SCE.