Supporting information

Assembly of Organic-inorganic Hybrid Supramolecular Materials Based on $\{P_2W_{18}O_{62}\}^{6-}$ Anion and Cu(II)/Mn(II) Complex

Kai Yu[†,‡], Yang Yu[†,‡], Bodong Jiang[§], Bai-Bin Zhou*[†,‡]

1. Structural figures

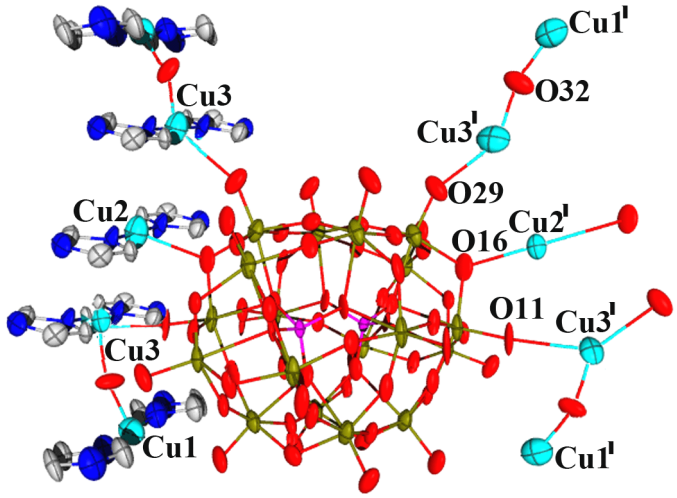

Figure S1. ORTEP view of the basic units in compound **1** with 50% thermal ellipsoids.

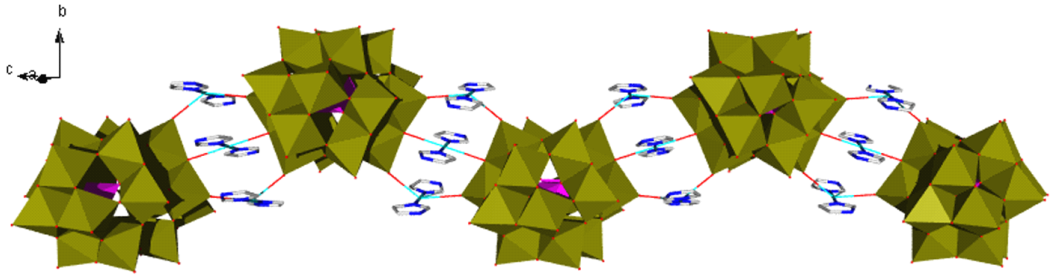

Figure S2. 1-D chain of the hybrids based on $\{P_2W_{18}\}$ units and $\{Cu(imi)_2\}$ linkers in **1**

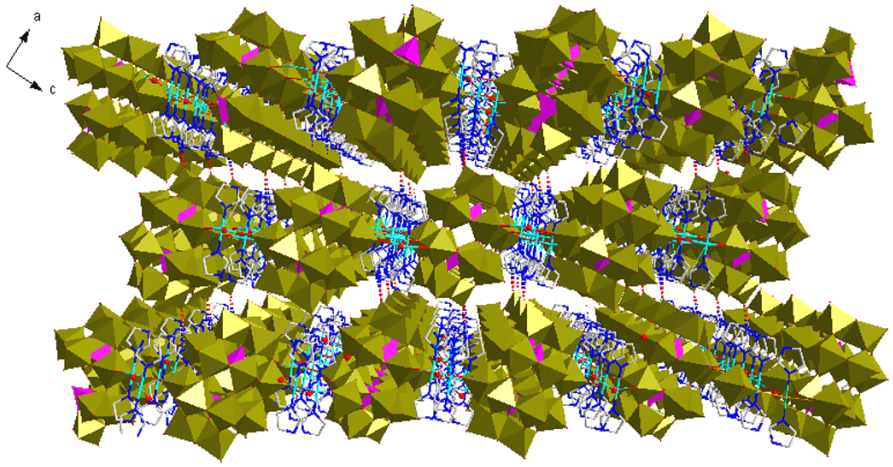

Figure S3 The 3D supramolecular framework along the b axis of **1**. The broken lines represent the hydrogen bonding interactions. The isolated water molecules are omitted for clarity.

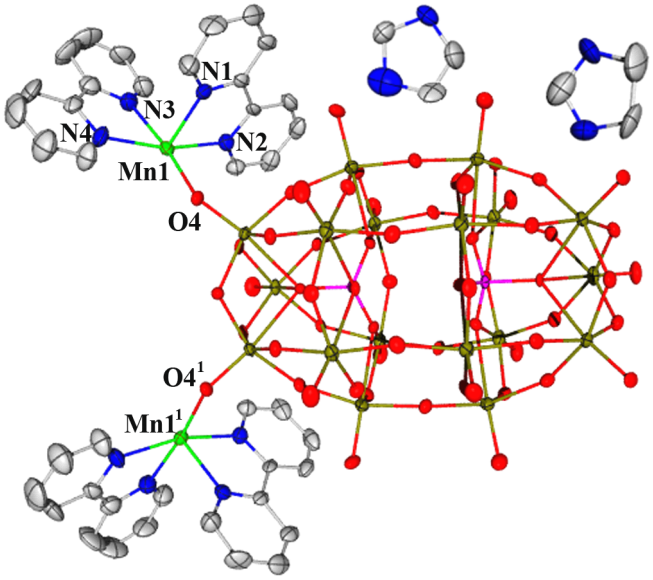

Figure S4. ORTEP view of the basic units in compound **2** with 50% thermal ellipsoids.

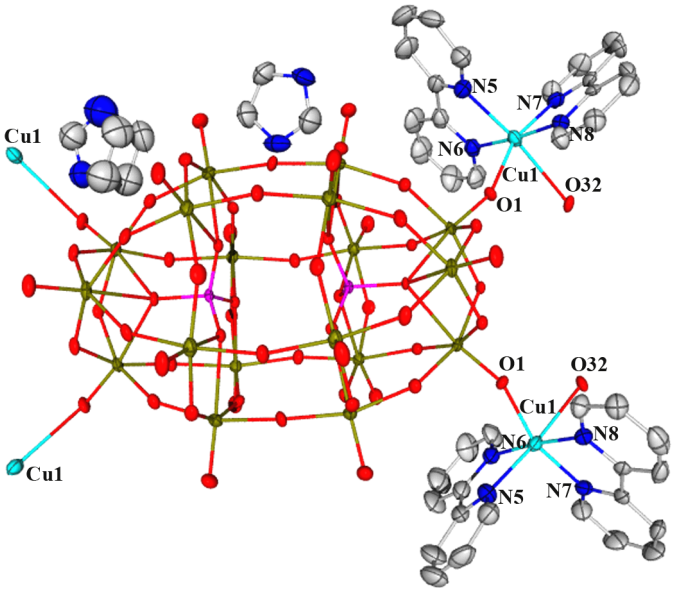

Figure S5. ORTEP view of the basic units in compound **3** with 50% thermal ellipsoids.

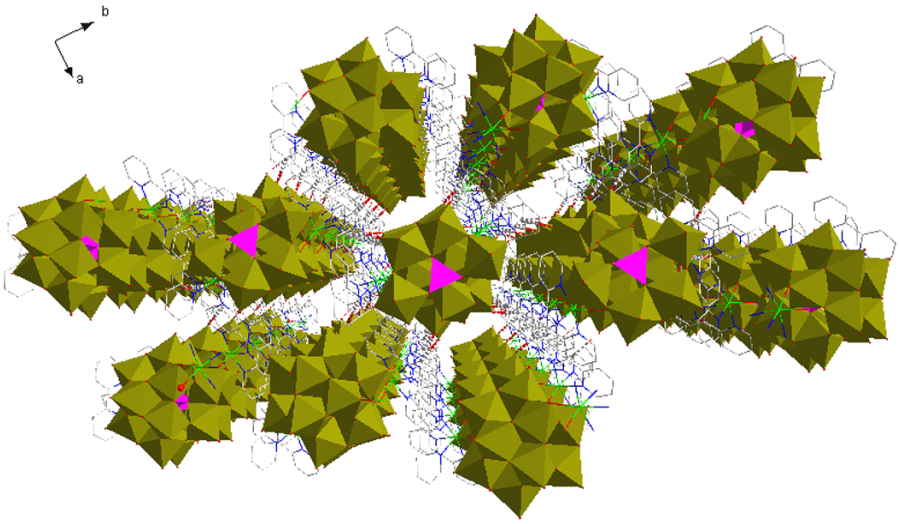

Figure S6. The 3D supramolecular framework along the b axis of **2**. The broken lines represent the hydrogen bonding interactions. The isolated water molecules are omitted for clarity.

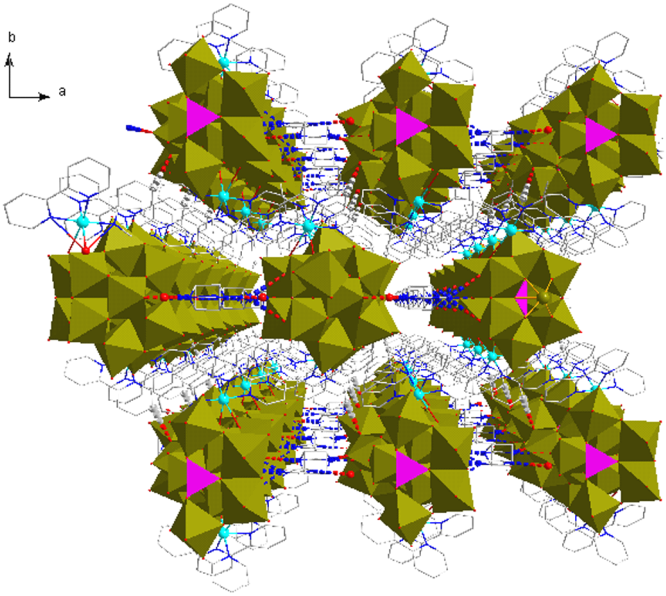

Figure S7. The 3D supramolecular framework along the c axis of **3**. The broken lines represent the hydrogen bonding interactions. The isolated water molecules are omitted for clarity.

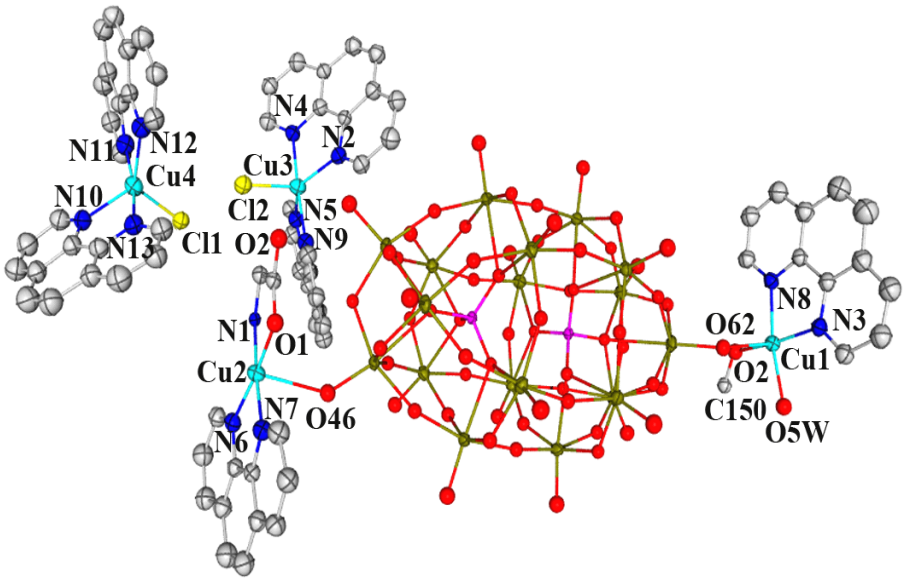

Figure S8. ORTEP view of the basic units in compound **4** with 50% thermal ellipsoids.

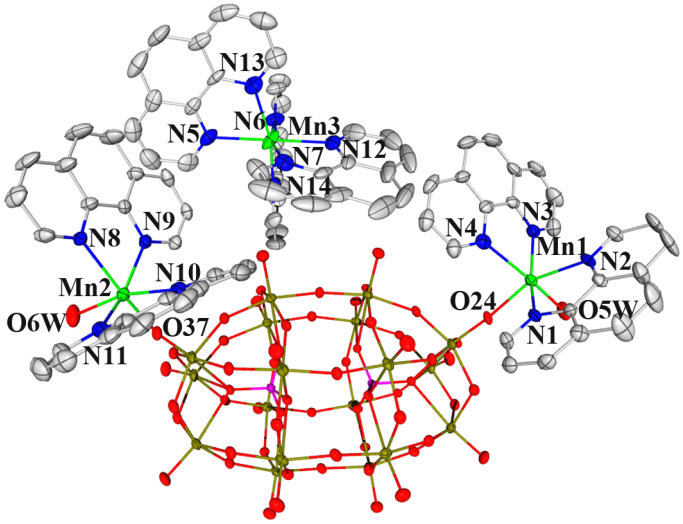

Figure S9. ORTEP view of the basic units in compound **5** with 50% thermal ellipsoids.

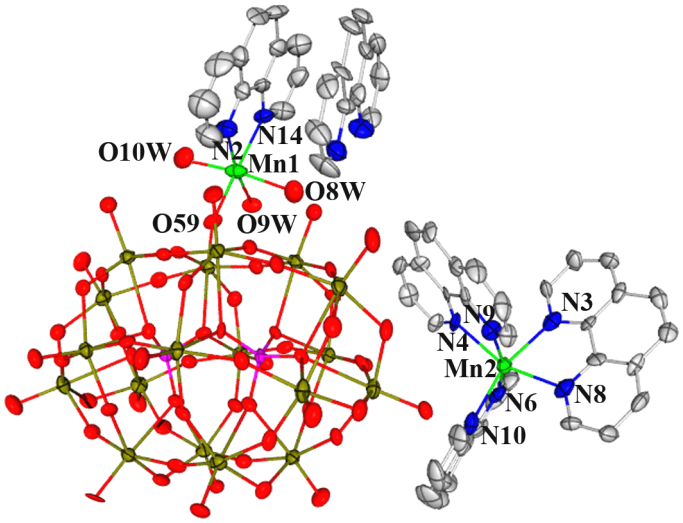

Figure S10. ORTEP view of the basic units in compound **6** with 50% thermal ellipsoids.

2. Structural data

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

W(1)-O(25)	1.723(12)	W(2)-O(20)	1.697(12)	W(3)-O(23)	1.696(12)
W(1)-O(9)	1.874(13)	W(2)-O(21)	1.878(15)	W(3)-O(5)	1.881(11)
W(1)-O(24)	1.890(12)	W(2)-O(19)	1.886(15)	W(3)-O(2)	1.883(13)
W(1)-O(12)	1.904(12)	W(2)-O(13)#1	1.904(11)	W(3)-O(24)	1.921(12)
W(1)-O(14)	1.937(13)	W(2)-O(12)	1.915(11)	W(3)-O(15)	1.926(12)
W(1)-O(1)	2.365(11)	W(2)-O(8)	2.332(12)	W(3)-O(1)	2.380(10)
W(4)-O(28)	1.687(14)	W(5)-O(11)	1.686(12)	W(6)-O(26)	1.695(13)
W(4)-O(18)	1.875(14)	W(5)-O(13)	1.875(11)	W(6)-O(14)	1.891(12)
W(4)-O(3)	1.886(13)	W(5)-O(3)	1.890(14)	W(6)-O(7)	1.894(12)
W(4)-O(15)	1.889(11)	W(5)-O(16)	1.895(15)	W(6)-O(4)	1.904(12)
W(4)-O(17)#1	1.935(11)	W(5)-O(5)	1.930(11)	W(6)-O(2)	1.916(12)
W(4)-O(30)	2.349(13)	W(5)-O(6)	2.333(11)	W(6)-O(1)	2.378(12)
W(7)-O(29)	1.689(15)	W(8)-O(31)	1.693(14)	W(9)-O(27)	1.704(13)
W(7)-O(10)	1.895(11)	W(8)-O(22)	1.867(13)	W(9)-O(17)	1.863(11)
W(7)-O(16)	1.905(13)	W(8)-O(10)#1	1.886(11)	W(9)-O(21)	1.890(14)
W(7)-O(22)	1.908(13)	W(8)-O(19)	1.923(13)	W(9)-O(18)	1.925(13)
W(7)-O(4)	1.911(11)	W(8)-O(7)	1.934(11)	W(9)-O(9)	1.962(11)
W(7)-O(6)	2.341(13)	W(8)-O(8)	2.364(13)	W(9)-O(30)	2.327(13)
Cu(1)-N(1)	1.85(2)	Cu(1)-N(1)#2	1.85(2)	Cu(1)-O(32)	1.939(10)
Cu(1)-O(32)#2	1.939(10)	Cu(2)-N(2)#3	1.933(15)	Cu(2)-N(2)	1.933(15)
Cu(3)-N(4)	1.97(3)	Cu(3)-N(3)	1.92(3)	Cu(3)-O(32)	1.930(10)
P(1)-O(8)	1.542(12)	P(1)-O(30)	1.544(15)	P(1)-O(6)	1.547(12)
P(1)-O(1)	1.568(10)				
O(25)-W(1)-O(9)	101.1(6)	O(20)-W(2)-O(21)	101.9(7)	O(23)-W(3)-O(5)	101.2(6)
O(25)-W(1)-O(24)	101.0(5)	O(20)-W(2)-O(19)	100.1(7)	O(23)-W(3)-O(2)	100.7(6)
O(25)-W(1)-O(12)	101.7(5)	O(20)-W(2)-O(13)#1	99.1(5)	O(23)-W(3)-O(24)	102.8(6)
O(25)-W(1)-O(14)	101.9(6)	O(20)-W(2)-O(12)	97.0(5)	O(23)-W(3)-O(15)	102.9(6)
O(25)-W(1)-O(1)	172.2(5)	O(20)-W(2)-O(8)	173.8(7)	O(23)-W(3)-O(1)	172.5(5)
O(28)-W(4)-O(18)	100.5(7)	O(11)-W(5)-O(13)	99.7(5)	O(26)-W(6)-O(14)	101.2(6)
O(28)-W(4)-O(3)	102.7(7)	O(11)-W(5)-O(3)	102.0(7)	O(26)-W(6)-O(7)	101.6(6)
O(28)-W(4)-O(15)	98.2(6)	O(11)-W(5)-O(16)	100.3(7)	O(26)-W(6)-O(4)	103.2(6)
O(28)-W(4)-O(17)#1	98.0(6)	O(11)-W(5)-O(5)	96.1(5)	O(26)-W(6)-O(2)	101.6(5)
O(28)-W(4)-O(30)	172.8(7)	O(11)-W(5)-O(6)	172.4(6)	O(26)-W(6)-O(1)	172.0(5)
O(29)-W(7)-O(10)	98.4(6)	O(31)-W(8)-O(22)	102.8(7)	O(27)-W(9)-O(17)	100.1(6)
O(29)-W(7)-O(16)	100.0(7)	O(31)-W(8)-O(10)#1	99.5(6)	O(27)-W(9)-O(21)	102.0(7)
O(29)-W(7)-O(22)	102.9(7)	O(31)-W(8)-O(19)	99.7(7)	O(27)-W(9)-O(18)	100.3(7)
O(29)-W(7)-O(4)	97.8(6)	O(31)-W(8)-O(7)	96.7(6)	O(27)-W(9)-O(9)	95.0(6)
O(29)-W(7)-O(6)	172.1(6)	O(31)-W(8)-O(8)	171.8(6)	O(27)-W(9)-O(30)	171.4(6)
N(1)-Cu(1)-N(1)#2	179.998(3)	N(1)-Cu(1)-O(32)	66.3(15)	N(1)-Cu(1)-O(32)#2	113.7(15)
N(2)-Cu(2)-N(2)#3	179.996(3)	N(3)-Cu(3)-O(32)	95.7(16)	N(3)-Cu(3)-N(4)	179.7(19)
N(3)-Cu(3)-O(32)	95.7(16)	N(3)-Cu(3)-N(4)	179.3(17)	Cu(3)-O(32)-Cu(1)	152(2)
O(8)-P(1)-O(30)	111.7(7)	O(8)-P(1)-O(6)	112.2(7)	O(8)-P(1)-O(1)	106.2(6)

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 (°) of compound **2**

W(1)-O(32)	1.699(6)	W(2)-O(35)	1.698(6)	W(3)-O(15)	1.910(5)
W(1)-O(13)	1.877(5)	W(2)-O(3)	1.896(5)	W(3)-O(2)	1.911(5)
W(1)-O(3)	1.890(5)	W(2)-O(30)	1.901(6)	W(3)-O(30)	1.916(6)
W(1)-O(23)	1.907(6)	W(2)-O(22)	1.907(5)	W(3)-O(20)	1.923(2)
W(1)-O(12)	1.947(5)	W(2)-O(26)	1.932(5)	W(3)-O(25)	2.363(5)
W(1)-O(28)	2.364(5)	W(2)-O(25)	2.391(5)	W(3)- O(37)	1.694(6)
W(4)-O(33)	1.698(6)	W(5)-O(31)	1.693(6)	W(6)-O(36)	1.709(8)
W(4)-O(2)	1.899(5)	W(5)-O(6)	1.882(5)	W(6)-O(16)#1	1.885(5)
W(4)-O(19)	1.8999(19)	W(5)-O(22)	1.883(5)	W(6)-O(16)	1.885(5)
W(4)-O(23)	1.905(6)	W(5)-O(17)	1.925(4)	W(6)-O(8)#1	1.933(5)
W(4)-O(16)	1.930(5)	W(5)-O(24)	1.939(5)	W(6)-O(8)	1.933(5)
W(4)-O(28)	2.364(6)	W(5)-O(27)	2.369(6)	W(6)-O(1)	2.400(8)
W(7)-O(34)	1.700(6)	W(8)-O(29)	1.699(8)	W(9)-O(18)	1.726(5)
W(7)-O(13)	1.899(5)	W(8)-O(15)	1.904(6)	W(9)-O(26)	1.877(6)
W(7)-O(6)	1.918(5)	W(8)-O(15)#1	1.904(6)	W(9)-O(24)	1.891(5)
W(7)-O(21)	1.920(3)	W(8)-O(14)#1	1.928(6)	W(9)-O(5)	1.909(4)
W(7)-O(7)	1.961(5)	W(8)-O(14)	1.928(6)	W(9)-O(14)	1.914(5)
W(7)-O(9)	2.378(5)	W(8)-O(11)	2.411(7)	W(9)-O(11)	2.345(5)
W(10)-O(4)	1.731(5)	W(10)-O(12)	1.873(5)	W(10)-O(7)	1.895(6)
W(10)-O(8)	1.900(6)	W(10)-O(10)	1.939(3)	W(10)-O(1)	2.368(5)
P(2)-O(9)	1.519(8)	P(2)-O(28)	1.530(5)	P(2)-O(28)#1	1.531(5)
P(2)-O(1)	1.588(7)	P(1)-O(27)	1.526(8)	P(1)-O(25)#1	1.524(6)
P(1)-O(25)	1.524(5)	P(1)-O(11)	1.585(7)		
Mn(1)-O(18)	2.099(6)	Mn(1)-N(1)	2.178(8)	Mn(1)-N(4)	2.200(8)
Mn(1)-N(2)	2.207(7)	Mn(1)-N(3)	2.262(9)	Mn(1)-O(4)#2	2.304(6)
O(32)-W(1)-O(13)	102.3(3)	O(35)-W(2)-O(3)	99.9(3)	O(37)-W(3)-O(15)	97.2(3)
O(32)-W(1)-O(3)	98.3(2)	O(35)-W(2)-O(30)	101.0(3)	O(37)-W(3)-O(2)	98.8(3)
O(32)-W(1)-O(23)	100.2(3)	O(35)-W(2)-O(22)	101.9(3)	O(37)-W(3)-O(30)	100.9(3)
O(32)-W(1)-O(12)	98.4(2)	O(35)-W(2)-O(26)	98.3(3)	O(37)-W(3)-O(20)	100.9(3)
O(32)-W(1)-O(28)	173.1(3)	O(35)-W(2)-O(25)	174.2(2)	O(37)-W(3)-O(25)	174.4(3)
O(33)-W(4)-O(2)	99.2(3)	O(31)-W(5)-O(6)	99.5(3)	O(36)-W(6)-O(16)#1	102.2(3)
O(33)-W(4)-O(19)	101.5(3)	O(31)-W(5)-O(22)	103.7(3)	O(36)-W(6)-O(16)	102.2(3)
O(33)-W(4)-O(23)	101.1(3)	O(31)-W(5)-O(17)	98.6(3)	O(36)-W(6)-O(8)#1	102.0(3)
O(33)-W(4)-O(16)	96.6(3)	O(31)-W(5)-O(24)	96.7(3)	O(36)-W(6)-O(8)	102.0(3)
O(33)-W(4)-O(28)	173.5(2)	O(31)-W(5)-O(27)	171.0(3)	O(36)-W(6)-O(1)	172.4(3)
O(34)-W(7)-O(13)	103.5(3)	O(29)-W(8)-O(15)	103.1(3)	O(18)-W(9)-O(26)	102.7(2)
O(34)-W(7)-O(6)	98.3(3)	O(29)-W(8)-O(15)#1	103.1(3)	O(18)-W(9)-O(24)	102.1(3)
O(34)-W(7)-O(21)	99.5(3)	O(29)-W(8)-O(14)#1	100.9(3)	O(18)-W(9)-O(5)	100.1(3)
O(34)-W(7)-O(7)	98.0(3)	O(29)-W(8)-O(14)	100.9(3)	O(18)-W(9)-O(14)	100.2(2)
O(34)-W(7)-O(9)	172.4(2)	O(29)-W(8)-O(11)	170.9(4)	O(18)-W(9)-O(11)	171.0(2)
O(4)-W(10)-O(12)	102.5(2)	O(4)-W(10)-O(7)	103.6(3)	O(4)-W(10)-O(8)	98.7(2)
O(4)-W(10)-O(10)	101.1(3)	O(4)-W(10)-O(1)	170.2(2)		
O(9)-P(2)-O(28)	112.1(3)	O(9)-P(2)-O(28)#1	112.1(3)	O(9)-P(2)-O(1)	106.9(4)
O(27)-P(1)-O(25)#1	112.1(3)	O(27)-P(1)-O(25)	112.1(3)	O(27)-P(1)-O(11)	106.2(4)
O(18)-Mn(1)-N(1)	165.1(3)	O(18)-Mn(1)-N(4)	96.5(3)	O(18)-Mn(1)-N(2)	91.2(3)
O(18)-Mn(1)-N(3)	94.5(3)	O(18)-Mn(1)-O(4)#2	86.1(2)		

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

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

W(1)-O(35)	1.696(7)	W(2)-O(32)	1.711(4)	W(3)-O(20)	1.710(5)
W(1)-O(29)	1.902(4)	W(2)-O(28)	1.896(5)	W(3)-O(18)	1.900(4)
W(1)-O(29)#1	1.902(4)	W(2)-O(34)	1.903(4)	W(3)-O(21)	1.9017(16)
W(1)-O(34)#1	1.919(5)	W(2)-O(27)	1.910(4)	W(3)-O(22)	1.912(5)
W(1)-O(34)	1.919(4)	W(2)-O(33)	1.934(3)	W(3)-O(29)	1.918(4)
W(1)-O(30)	2.388(6)	W(2)-O(30)	2.374(4)	W(3)-O(36)	2.353(4)
W(4)-O(23)	1.691(5)	W(5)-O(25)	1.700(5)	W(6)-O(8)	1.704(5)
W(4)-O(16)	1.896(4)	W(5)-O(24)	1.888(5)	W(6)-O(15)	1.885(4)
W(4)-O(24)	1.898(5)	W(5)-O(19)	1.909(4)	W(6)-O(19)	1.887(4)
W(4)-O(22)	1.905(5)	W(5)-O(26)	1.920(3)	W(6)-O(17)	1.920(3)
W(4)-O(28)	1.926(4)	W(5)-O(27)	1.939(4)	W(6)-O(7)	1.938(4)
W(4)-O(36)	2.382(4)	W(5)-O(31)	2.372(4)	W(6)-O(14)	2.354(4)
W(7)-O(9)	1.691(5)	W(8)-O(11)	1.698(5)	W(9)-O(3)	1.709(6)
W(7)-O(16)	1.891(4)	W(8)-O(18)	1.906(4)	W(9)-O(4)#1	1.893(5)
W(7)-O(10)	1.902(5)	W(8)-O(10)	1.916(5)	W(9)-O(4)	1.893(5)
W(7)-O(15)	1.906(5)	W(8)-O(12)	1.9184(16)	W(9)-O(2)#1	1.920(4)
W(7)-O(6)	1.950(4)	W(8)-O(4)	1.923(4)	W(9)-O(2)	1.920(4)
W(7)-O(13)	2.390(4)	W(8)-O(13)	2.366(4)	W(9)-O(5)	2.398(6)
W(10)-O(1)	1.722(4)	W(10)-O(6)	1.870(4)	W(10)-O(7)	1.890(4)
W(10)-O(2)	1.921(4)	W(10)-O(37)	1.921(3)	W(10)-O(5)	2.347(4)
P(2)-O(13)	1.526(4)	P(2)-O(13)#1	1.526(4)	P(2)-O(14)	1.538(6)
P(2)-O(5)	1.588(6)	P(1)-O(36)#1	1.530(4)	P(1)-O(36)	1.530(4)
P(1)-O(31)	1.532(6)	P(1)-O(30)	1.577(6)		
Cu(1)-N(8)	1.981(6)	Cu(1)-N(6)	1.986(6)	Cu(1)-N(7)	2.001(6)
Cu(1)-O(1)	2.006(4)	Cu(1)-N(5)	2.175(6)		
O(35)-W(1)-O(29)	102.2(2)	O(32)-W(2)-O(28)	102.8(2)	O(20)-W(3)-O(18)	99.2(2)
O(35)-W(1)-O(29)#1	102.2(2)	O(32)-W(2)-O(34)	100.9(2)	O(20)-W(3)-O(21)	101.1(3)
O(35)-W(1)-O(34)#1	102.0(2)	O(32)-W(2)-O(27)	102.0(2)	O(20)-W(3)-O(22)	100.7(2)
O(35)-W(1)-O(34)	102.0(2)	O(32)-W(2)-O(33)	99.9(2)	O(20)-W(3)-O(29)	96.5(2)
O(35)-W(1)-O(30)	172.7(3)	O(32)-W(2)-O(30)	170.78(19)	O(20)-W(3)-O(36)	173.7(2)
O(23)-W(4)-O(16)	97.9(2)	O(25)-W(5)-O(24)	103.0(2)	O(8)-W(6)-O(15)	103.0(2)
O(23)-W(4)-O(24)	102.1(2)	O(25)-W(5)-O(19)	98.4(2)	O(8)-W(6)-O(19)	99.7(2)
O(23)-W(4)-O(22)	100.4(2)	O(25)-W(5)-O(26)	99.3(2)	O(8)-W(6)-O(17)	99.1(2)
O(23)-W(4)-O(28)	98.6(2)	O(25)-W(5)-O(27)	97.7(2)	O(8)-W(6)-O(7)	96.9(2)
O(23)-W(4)-O(36)	173.36(19)	O(25)-W(5)-O(31)	172.1(2)	O(8)-W(6)-O(14)	171.1(2)
O(9)-W(7)-O(16)	99.5(2)	O(11)-W(8)-O(18)	98.8(2)	O(3)-W(9)-O(4)#1	102.7(2)
O(9)-W(7)-O(10)	100.9(2)	O(11)-W(8)-O(10)	100.7(2)	O(3)-W(9)-O(4)	102.7(2)
O(9)-W(7)-O(15)	101.4(2)	O(11)-W(8)-O(12)	101.2(3)	O(3)-W(9)-O(2)#1	101.2(2)
O(9)-W(7)-O(6)	98.3(2)	O(11)-W(8)-O(4)	97.3(2)	O(3)-W(9)-O(2)	101.2(2)
O(9)-W(7)-O(13)	174.1(2)	O(11)-W(8)-O(13)	174.3(2)	O(3)-W(9)-O(5)	171.0(3)
O(1)-W(10)-O(6)	102.0(2)	O(1)-W(10)-O(7)	102.7(2)	O(1)-W(10)-O(2)	100.0(2)
O(1)-W(10)-O(37)	100.4(2)	O(1)-W(10)-O(5)	170.70(19)		
O(36)#1-P(1)-O(36)	111.4(3)	O(36)#1-P(1)-O(31)	111.7(2)	O(36)#1-P(1)-O(30)	107.5(2)
O(13)-P(2)-O(13)#1	111.3(4)	O(13)-P(2)-O(14)	112.6(2)	O(13)-P(2)-O(5)	106.9(2)
N(8)-Cu(1)-N(6)	175.2(3)	N(8)-Cu(1)-N(7)	81.7(3)		
N(8)-Cu(1)-N(5)	97.8(3)	N(8)-Cu(1)-O(1)	93.3(2)		

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

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

W(1)-O(45)	1.699(7)	W(2)-O(64)	1.694(7)	W(3)-O(42)	1.699(7)
W(1)-O(9)	1.903(7)	W(2)-O(9)	1.887(7)	W(3)-O(57)	1.896(7)
W(1)-O(24)	1.911(6)	W(2)-O(34)	1.904(6)	W(3)-O(30)	1.906(7)
W(1)-O(54)	1.917(6)	W(2)-O(31)	1.927(6)	W(3)-O(5)	1.925(7)
W(1)-O(14)	1.936(6)	W(2)-O(16)	1.930(7)	W(3)-O(19)	1.928(7)
W(1)-O(17)	2.389(6)	W(2)-O(12)	2.380(6)	W(3)-O(37)	2.355(6)
W(4)-O(59)	1.705(7)	W(5)-O(49)	1.878(7)	W(6)-O(66)	1.719(7)
W(4)-O(8)	1.870(7)	W(5)-O(5)	1.889(7)	W(6)-O(51)	1.900(7)
W(4)-O(34)	1.902(6)	W(5)-O(21)	1.906(6)	W(6)-O(11)	1.908(7)
W(4)-O(57)	1.920(7)	W(5)-O(15)	1.958(7)	W(6)-O(27)	1.910(7)
W(4)-O(7)	1.963(7)	W(5)-O(29)	2.365(6)	W(6)-O(18)	1.911(6)
W(4)-O(37)	2.379(6)	W(5)- O(3)	1.706(7)	W(6)-O(32)	2.367(6)
W(7)-O(40)	1.703(7)	W(8)-O(58)	1.704(7)	W(9)-O(46)	1.732(7)
W(7)-O(6)	1.883(7)	W(8)-O(48)	1.876(7)	W(9)-O(39)	1.867(7)
W(7)-O(18)	1.886(6)	W(8)-O(56)	1.919(7)	W(9)-O(19)	1.906(7)
W(7)-O(31)	1.913(6)	W(8)-O(27)	1.930(7)	W(9)-O(28)	1.908(6)
W(7)-O(48)	1.937(7)	W(8)-O(28)	1.938(6)	W(9)-O(10)	1.936(7)
W(7)-O(12)	2.367(6)	W(8)-O(25)	2.395(6)	W(9)-O(25)	2.376(6)
W(10)-O(61)	1.694(8)	W(11)-O(41)	1.728(7)	W(12)-O(55)	1.705(7)
W(10)-O(11)	1.892(7)	W(11)-O(7)	1.868(7)	W(12)-O(24)	1.891(6)
W(10)-O(22)	1.905(7)	W(11)-O(16)	1.891(7)	W(12)-O(21)	1.901(6)
W(10)-O(52)	1.913(7)	W(11)-O(10)	1.925(7)	W(12)-O(26)	1.917(7)
W(10)-O(23)	1.939(7)	W(11)-O(56)	1.941(7)	W(12)-O(8)	1.921(7)
W(10)-O(36)	2.363(6)	W(11)-O(25)	2.358(6)	W(12)-O(29)	2.385(6)
W(13)-O(67)	1.720(8)	W(14)-O(62)	1.729(7)	W(15)-O(43)	1.719(7)
W(13)-O(23)	1.892(7)	W(14)-O(14)	1.877(6)	W(15)-O(22)	1.895(7)
W(13)-O(20)	1.912(6)	W(14)-O(35)	1.903(7)	W(15)-O(54)	1.905(6)
W(13)-O(38)	1.916(7)	W(14)-O(26)	1.915(7)	W(15)-O(6)	1.906(7)
W(13)-O(35)	1.939(7)	W(14)-O(33)	1.921(7)	W(15)-O(20)	1.911(6)
W(13)-O(13)	2.389(6)	W(14)-O(13)	2.385(6)	W(15)-O(17)	2.361(6)
W(16)-O(63)	1.710(7)	W(17)-O(44)	1.708(7)	W(18)-O(65)	1.690(7)
W(16)-O(15)	1.867(7)	W(17)-O(30)	1.878(7)	W(18)-O(52)	1.901(7)
W(16)-O(50)	1.900(7)	W(17)-O(4)	1.890(7)	W(18)-O(49)	1.911(7)
W(16)-O(38)	1.934(7)	W(17)-O(51)	1.916(7)	W(18)-O(4)	1.918(7)
W(16)-O(33)	1.936(7)	W(17)-O(39)	1.964(7)	W(18)-O(50)	1.929(7)
W(16)-O(13)	2.385(6)	W(17)-O(32)	2.369(6)	W(18)-O(36)	2.391(6)
P(1)-O(12)	1.524(7)	P(1)-O(37)	1.531(6)	P(1)-O(32)	1.532(7)
P(1)-O(25)	1.584(7)	P(2)-O(29)	1.524(7)	P(2)-O(36)	1.530(6)
P(2)-O(17)	1.531(6)	P(2)-O(13)	1.567(7)		
Cu(1)-O(5W)	1.957(8)	Cu(1)-O(2)	1.960(8)	Cu(1)-N(8)	1.968(9)
Cu(1)-N(3)	1.998(9)	Cu(1)-O(62)	2.333(7)	Cu(2)-O(1)	1.965(7)
Cu(2)-N(1)	1.968(7)	Cu(2)-N(7)	1.992(9)	Cu(2)-N(6)	1.998(9)
Cu(2)-O(46)	2.438(7)	Cu(3)-N(9)	1.968(10)	Cu(3)-N(4)	1.974(9)
Cu(3)-N(5)	2.064(10)	Cu(3)-N(2)	2.071(9)	Cu(3)-Cl(2)	2.157(14)
Cu(4)-N(12)	1.961(11)	Cu(4)-N(13)	1.985(11)	Cu(4)-N(11)	2.105(11)
Cu(4)-N(10)	2.138(11)	Cu(4)-Cl(1)	2.355(7)		
O(45)-W(1)-O(9)	98.9(3)	O(64)-W(2)-O(9)	98.3(3)	O(42)-W(3)-O(57)	99.5(3)
O(45)-W(1)-O(24)	102.3(3)	O(64)-W(2)-O(34)	101.8(3)	O(42)-W(3)-O(30)	103.5(3)
O(45)-W(1)-O(54)	100.5(3)	O(64)-W(2)-O(31)	100.6(3)	O(42)-W(3)-O(5)	98.0(3)
O(45)-W(1)-O(14)	97.1(3)	O(64)-W(2)-O(16)	97.4(3)	O(42)-W(3)-O(19)	97.7(3)
O(45)-W(1)-O(17)	172.9(3)	O(64)-W(2)-O(12)	173.4(3)	O(42)-W(3)-O(37)	172.6(3)
O(59)-W(4)-O(8)	99.4(3)	O(3)-W(5)-O(49)	102.5(3)	O(66)-W(6)-O(51)	99.7(3)
O(59)-W(4)-O(34)	102.5(3)	O(3)-W(5)-O(5)	99.3(3)	O(66)-W(6)-O(11)	97.7(3)
O(59)-W(4)-O(57)	99.9(3)	O(3)-W(5)-O(21)	99.9(3)	O(66)-W(6)-O(27)	98.2(3)
O(59)-W(4)-O(7)	97.6(3)	O(3)-W(5)-O(15)	96.0(3)	O(66)-W(6)-O(18)	103.5(3)

O(59)-W(4)-O(37)	171.9(3)	O(3)-W(5)-O(29)	172.0(3)	O(66)-W(6)-O(32)	172.9(3)
O(40)-W(7)-O(6)	99.1(3)	O(58)-W(8)-O(48)	103.3(3)	O(46)-W(9)-O(39)	102.8(3)
O(40)-W(7)-O(18)	101.6(3)	O(58)-W(8)-O(56)	101.5(3)	O(46)-W(9)-O(19)	104.0(3)
O(40)-W(7)-O(31)	100.6(3)	O(58)-W(8)-O(27)	101.9(3)	O(46)-W(9)-O(28)	98.0(3)
O(40)-W(7)-O(48)	97.2(3)	O(58)-W(8)-O(28)	100.5(3)	O(46)-W(9)-O(10)	100.4(3)
O(40)-W(7)-O(12)	173.8(3)	O(58)-W(8)-O(25)	171.1(3)	O(46)-W(9)-O(25)	169.2(3)
O(61)-W(10)-O(11)	99.4(3)	O(41)-W(11)-O(7)	102.2(3)	O(55)-W(12)-O(24)	102.8(3)
O(61)-W(10)-O(22)	102.7(3)	O(41)-W(11)-O(16)	103.1(3)	O(55)-W(12)-O(21)	100.7(3)
O(61)-W(10)-O(52)	100.1(3)	O(41)-W(11)-O(10)	99.0(3)	O(55)-W(12)-O(26)	98.8(3)
O(61)-W(10)-O(23)	97.3(3)	O(41)-W(11)-O(56)	99.5(3)	O(55)-W(12)-O(8)	97.3(3)
O(61)-W(10)-O(36)	173.0(3)	O(41)-W(11)-O(25)	169.4(3)	O(55)-W(12)-O(29)	172.8(3)
O(67)-W(13)-O(23)	102.8(3)	O(62)-W(14)-O(14)	102.9(3)	O(43)-W(15)-O(22)	102.4(3)
O(67)-W(13)-O(20)	103.2(3)	O(62)-W(14)-O(35)	99.6(3)	O(43)-W(15)-O(54)	100.0(3)
O(67)-W(13)-O(38)	100.1(3)	O(62)-W(14)-O(26)	102.9(3)	O(43)-W(15)-O(6)	98.0(3)
O(67)-W(13)-O(35)	100.1(3)	O(62)-W(14)-O(33)	100.5(3)	O(43)-W(15)-O(20)	98.1(3)
O(67)-W(13)-O(13)	169.9(3)	O(62)-W(14)-O(13)	170.5(3)	O(43)-W(15)-O(17)	173.5(3)
O(63)-W(16)-O(15)	102.7(3)	O(44)-W(17)-O(30)	102.2(3)	O(65)-W(18)-O(52)	101.2(3)
O(63)-W(16)-O(50)	103.8(3)	O(44)-W(17)-O(4)	99.2(3)	O(65)-W(18)-O(49)	102.2(3)
O(63)-W(16)-O(38)	101.0(3)	O(44)-W(17)-O(51)	100.3(3)	O(65)-W(18)-O(4)	98.5(3)
O(63)-W(16)-O(33)	98.5(3)	O(44)-W(17)-O(39)	96.7(3)	O(65)-W(18)-O(50)	97.0(3)
O(63)-W(16)-O(13)	169.2(3)	O(44)-W(17)-O(32)	172.6(3)	O(65)-W(18)-O(36)	173.9(3)
O(5W)-Cu(1)-O(2)	92.2(3)	O(5W)-Cu(1)-N(8)	168.8(4)	O(5W)-Cu(1)-N(3)	93.3(3)
O(5W)-Cu(1)-O(62)	90.8(3)	O(1)-Cu(2)-N(1)	83.0(3)	O(1)-Cu(2)-N(7)	94.3(3)
O(1)-Cu(2)-N(6)	174.0(4)	O(1)-Cu(2)-O(46)	92.3(3)	N(9)-Cu(3)-N(4)	176.2(4)
N(9)-Cu(3)-N(5)	82.1(4)	N(9)-Cu(3)-N(2)	97.4(4)	N(9)-Cu(3)-Cl(2)	89.6(5)
N(12)-Cu(4)-N(13)	168.3(5)	N(12)-Cu(4)-N(11)	79.8(4)	N(12)-Cu(4)-N(10)	94.4(4)
N(12)-Cu(4)-Cl(1)	93.8(4)	O(6W)-Sr(2)-O(9W)	140.40(9)		
O(12)-P(1)-O(37)	112.9(4)	O(12)-P(1)-O(32)	112.1(4)	O(12)-P(1)-O(25)	106.4(4)
O(29)-P(2)-O(36)	111.9(4)	O(29)-P(2)-O(17)	111.9(4)	O(29)-P(2)-O(13)	107.5(4)

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

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

W(1)-O(51)	1.707(4)	W(2)-O(54)	1.697(4)	W(3)-O(56)	1.704(4)
W(1)-O(16)	1.873(3)	W(2)-O(18)	1.891(3)	W(3)-O(9)	1.879(3)
W(1)-O(55)	1.908(4)	W(2)-O(7)	1.895(3)	W(3)-O(40)	1.892(4)
W(1)-O(11)	1.914(4)	W(2)-O(50)	1.909(4)	W(3)-O(45)	1.925(4)
W(1)-O(29)	1.950(3)	W(2)-O(44)	1.933(3)	W(3)-O(17)	1.941(3)
W(1)-O(39)	2.342(3)	W(2)--O(1)	2.366(3)	W(3)-O(10)	2.388(3)
W(4)-O(61)	1.705(4)	W(5)-O(32)	1.707(4)	W(6)-O(59)	1.706(4)
W(4)-O(30)	1.892(3)	W(5)-O(8)	1.877(3)	W(6)-O(12)	1.901(4)
W(4)-O(60)	1.897(3)	W(5)-O(21)	1.896(3)	W(6)-O(27)	1.909(3)
W(4)-O(55)	1.910(4)	W(5)-O(6)	1.898(3)	W(6)-O(23)	1.910(4)
W(4)-O(3)	1.926(3)	W(5)-O(5)	1.952(3)	W(6)-O(43)	1.921(3)
W(4)-O(39)	2.381(3)	W(5)-O(20)	2.368(3)	W(6)-O(31)	2.370(3)
W(7)-O(47)	1.710(4)	W(8)-O(62)	1.716(4)	W(9)-O(25)	1.694(4)
W(7)-O(22)	1.882(4)	W(8)-O(29)	1.871(4)	W(9)-O(3)	1.857(3)
W(7)-O(17)	1.884(3)	W(8)-O(34)	1.913(4)	W(9)-O(13)	1.906(3)
W(7)-O(21)	1.922(3)	W(8)-O(14)	1.921(4)	W(9)-O(18)	1.909(3)
W(7)-O(2)	1.945(3)	W(8)-O(53)	1.920(4)	W(9)-O(48)	1.985(3)
W(7)-O(20)	2.370(3)	W(8)-O(26)	2.407(3)	W(9)-O(42)	2.371(3)
W(10)-O(52)	1.696(4)	W(11)-O(49)	1.706(4)	W(12)-O(38)	1.705(4)
W(10)-O(7)	1.887(3)	W(11)-O(4)	1.870(3)	W(12)-O(6)	1.904(4)
W(10)-O(23)	1.903(4)	W(11)-O(27)	1.905(3)	W(12)-O(15)	1.907(3)
W(10)-O(30)	1.904(3)	W(11)-O(53)	1.911(4)	W(12)-O(13)	1.907(4)
W(10)-O(57)	1.949(3)	W(11)-O(41)	1.976(4)	W(12)-O(16)	1.926(3)

W(10)-O(31)	2.362(3)	W(11)-O(26)	2.400(3)	W(12)-O(42)	2.365(3)
W(13)-O(58)	1.707(4)	W(14)-O(24)	1.736(3)	W(15)-O(37)	1.735(3)
W(13)-O(43)	1.882(3)	W(14)-O(48)	1.847(3)	W(15)-O(41)	1.875(4)
W(13)-O(50)	1.901(4)	W(14)-O(44)	1.887(3)	W(15)-O(57)	1.886(3)
W(13)-O(22)	1.908(4)	W(14)-O(33)	1.910(3)	W(15)-O(34)	1.928(4)
W(13)-O(9)	1.946(3)	W(14)-O(40)	1.950(3)	W(15)-O(60)	1.932(3)
W(13)-O(1)	2.363(3)	W(14)-O(10)	2.335(3)	W(15)-O(26)	2.354(3)
W(16)-O(35)	1.709(4)	W(17)-O(36)	1.712(4)	W(18)-O(46)	1.702(4)
W(16)-O(11)	1.875(4)	W(17)-O(2)	1.866(3)	W(18)-O(5)	1.887(3)
W(16)-O(14)	1.907(3)	W(17)-O(19)	1.890(3)	W(18)-O(45)	1.904(4)
W(16)-O(19)	1.923(3)	W(17)-O(12)	1.906(4)	W(18)-O(15)	1.909(3)
W(16)-O(8)	1.926(3)	W(17)-O(4)	1.972(3)	W(18)-O(33)	1.960(3)
W(16)-O(28)	2.359(3)	W(17)-O(28)	2.374(3)	W(18)-O(10)	2.419(3)
P(1)-O(39)	1.523(4)	P(1)-O(31)	1.531(3)	P(1)-O(28)	1.534(4)
P(1)-O(26)	1.568(3)	P(2)-O(20)	1.525(4)	P(2)-O(42)	1.533(3)
P(2)-O(10)	1.574(3)	P(2)- O(1)	1.524(3)		
Mn(1)-O(5W)	2.133(4)	Mn(2)-O(37)	2.183(4)	Mn(3)-N(13)	2.215(5)
Mn(1)-O(24)	2.196(4)	Mn(2)-O(6W)	2.185(4)	Mn(3)-N(7)	2.220(5)
Mn(1)-N(1)	2.263(5)	Mn(2)-N(9)	2.269(5)	Mn(3)-N(14)	2.227(5)
Mn(1)-N(4)	2.274(5)	Mn(2)-N(11)	2.270(5)	Mn(3)-N(12)	2.293(5)
Mn(1)-N(3)	2.274(5)	Mn(2)-N(10)	2.283(5)	Mn(3)-N(6)	2.239(5)
Mn(1)-N(2)	2.275(4)	Mn(2)-N(8)	2.297(4)	Mn(3)-N(5)	2.303(6)
O(51)-W(1)-O(16)	98.53(17)	O(54)-W(2)-O(18)	101.75(17)	O(1)-Mo(3)-O(9)	98.70(10)
O(51)-W(1)-O(55)	99.16(17)	O(54)-W(2)-O(7)	99.66(16)	O(12)-Mo(3)-O(9)	154.55(8)
O(51)-W(1)-O(29)	96.83(16)	O(54)-W(2)-O(50)	100.56(17)	O(11)-Mo(3)-O(9)	86.06(8)
O(51)-W(1)-O(11)	102.29(17)	O(54)-W(2)-O(44)	96.88(16)	O(22)-Mo(3)-O(9)	84.90(9)
O(51)-W(1)-O(39)	173.02(16)	O(54)-W(2)-O(1)	173.44(15)	O(9)-Mo(3)-O(8)	72.18(8)
O(61)-W(4)-O(30)	102.09(17)	O(32)-W(5)-O(8)	98.57(17)	O(59)-W(6)-O(12)	101.37(17)
O(61)-W(4)-O(60)	98.64(16)	O(32)-W(5)-O(21)	100.57(16)	O(59)-W(6)-O(27)	97.95(16)
O(61)-W(4)-O(55)	100.79(17)	O(32)-W(5)-O(6)	102.07(16)	O(59)-W(6)-O(23)	101.29(17)
O(61)-W(4)-O(3)	98.81(16)	O(32)-W(5)-O(5)	96.85(16)	O(59)-W(6)-O(43)	98.49(16)
O(61)-W(4)-O(39)	173.93(16)	O(32)-W(5)-O(20)	173.65(15)	O(59)-W(6)-O(31)	174.32(16)
O(47)-W(7)-O(22)	102.89(17)	O(62)-W(8)-O(29)	103.41(17)	O(25)-W(9)-O(3)	99.30(16)
O(47)-W(7)-O(17)	99.50(16)	O(62)-W(8)-O(34)	104.08(17)	O(25)-W(9)-O(13)	100.14(17)
O(47)-W(7)-O(21)	99.61(17)	O(62)-W(8)-O(14)	99.86(17)	O(25)-W(9)-O(18)	102.48(17)
O(47)-W(7)-O(2)	97.72(16)	O(62)-W(8)-O(53)	101.07(17)	O(25)-W(9)-O(48)	96.67(16)
O(47)-W(7)-O(20)	172.17(15)	O(62)-W(8)-O(26)	172.19(15)	O(25)-W(9)-O(42)	172.55(15)
O(52)-W(10)-O(7)	98.83(16)	O(49)-W(11)-O(4)	101.92(17)	O(38)-W(12)-O(6)	100.45(16)
O(52)-W(10)-O(23)	99.51(17)	O(49)-W(11)-O(27)	103.68(17)	O(38)-W(12)-O(15)	98.45(16)
O(52)-W(10)-O(30)	102.65(17)	O(49)-W(11)-O(53)	100.40(17)	O(38)-W(12)-O(13)	102.01(17)
O(52)-W(10)-O(57)	96.96(16)	O(49)-W(11)-O(26)	169.93(15)	O(38)-W(12)-O(16)	97.93(16)
O(52)-W(10)-O(31)	172.65(15)	O(49)-W(11)-O(41)	100.40(17)	O(38)-W(12)-O(42)	175.18(15)
O(58)-W(13)-O(43)	99.27(17)	O(24)-W(14)-O(48)	101.38(16)	O(37)-W(15)-O(41)	102.39(16)
O(58)-W(13)-O(50)	99.54(17)	O(24)-W(14)-O(44)	101.92(16)	O(37)-W(15)-O(57)	101.36(16)
O(58)-W(13)-O(22)	102.42(17)	O(24)-W(14)-O(33)	100.47(15)	O(37)-W(15)-O(34)	101.63(16)
O(58)-W(13)-O(9)	97.58(17)	O(24)-W(14)-O(40)	100.47(16)	O(37)-W(15)-O(60)	100.41(16)
O(58)-W(13)-O(1)	172.66(16)	O(24)-W(14)-O(10)	171.82(14)	O(37)-W(15)-O(26)	174.06(14)
O(11)-W(16)-O(14)	87.11(15)	O(36)-W(17)-O(2)	99.53(16)	O(46)-W(18)-O(5)	102.59(17)
O(11)-W(16)-O(19)	157.30(15)	O(36)-W(17)-O(19)	100.39(16)	O(46)-W(18)-O(45)	101.50(17)
O(11)-W(16)-O(8)	88.67(15)	O(36)-W(17)-O(12)	102.35(17)	O(46)-W(18)-O(15)	103.72(17)
O(11)-W(16)-O(28)	84.27(13)	O(36)-W(17)-O(4)	96.15(16)	O(46)-W(18)-O(33)	100.59(17)
O(35)-W(16)-O(11)	102.73(17)	O(36)-W(17)-O(28)	172.95(15)	O(46)-W(18)-O(10)	170.02(15)
O(5W)-Mn(1)-O(24)	82.39(15)	O(37)-Mn(2)-O(6W)	82.12(15)	N(13)-Mn(3)-N(7)	89.6(2)
O(5W)-Mn(1)-N(1)	102.66(19)	O(37)-Mn(2)-N(9)	91.82(15)	N(13)-Mn(3)-N(14)	162.6(2)
O(5W)-Mn(1)-N(4)	158.42(19)	O(37)-Mn(2)-N(11)	110.71(16)	N(13)-Mn(3)-N(6)	94.00(19)
O(5W)-Mn(1)-N(3)	92.76(19)	O(37)-Mn(2)-N(10)	93.05(15)	N(13)-Mn(3)-N(12)	106.4(2)
O(5W)-Mn(1)-N(2)	89.11(17)	O(37)-Mn(2)-N(8)	159.67(16)	N(13)-Mn(3)-N(5)	73.8(2)

O(39)-P(1)-O(31)	111.8(2)	O(39)-P(1)-O(28)	111.7(2)	O(39)-P(1)-O(26)	106.61(19)
O(1)-P(2)-O(20)	111.63(19)	O(1)-P(2)-O(42)	111.75(19)	O(1)-P(2)-O(10)	107.07(18)

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

Table S6 Selected bond lengths (Å) and bond angles (°) of compound **6**

W(1)-O(49)	1.701(9)	W(2)-O(24)	1.708(9)	W(3)-O(56)	1.688(9)
W(1)-O(3)	1.888(9)	W(2)-O(20)	1.862(9)	W(3)-O(10)	1.896(9)
W(1)-O(9)	1.893(8)	W(2)-O(15)	1.889(9)	W(3)-O(17)	1.908(9)
W(1)-O(5)	1.908(9)	W(2)-O(54)	1.927(9)	W(3)-O(9)	1.910(8)
W(1)-O(4)	1.935(9)	W(2)-O(30)	1.955(9)	W(3)-O(41)	1.920(9)
W(1)-O(29)	2.378(9)	W(2)-O(22)	2.354(9)	W(3)-O(35)	2.373(9)
W(4)-O(28)	1.703(9)	W(5)-O(25)	1.701(10)	W(6)-O(34)	1.699(9)
W(4)-O(2)	1.891(9)	W(5)-O(13)	1.885(8)	W(6)-O(19)	1.896(9)
W(4)-O(16)	1.907(10)	W(5)-O(15)	1.908(9)	W(6)-O(8)	1.900(9)
W(4)-O(58)	1.923(9)	W(5)-O(17)	1.909(9)	W(6)-O(40)	1.929(9)
W(4)-O(43)	1.923(9)	W(5)-O(12)	1.958(8)	W(6)-O(21)	2.416(8)
W(4)-O(38)	2.387(9)	W(5)-O(35)	2.345(9)	W(6)-O(74)	1.917(9)
W(7)-O(53)	1.721(10)	W(8)-O(31)	1.689(9)	W(9)-O(59)	1.705(10)
W(7)-O(14)	1.887(9)	W(8)-O(3)	1.902(9)	W(9)-O(5)	1.875(9)
W(7)-O(10)	1.897(9)	W(8)-O(13)	1.914(9)	W(9)-O(68)	1.878(9)
W(7)-O(18)	1.916(9)	W(8)-O(23)	1.915(9)	W(9)-O(14)	1.904(9)
W(7)-O(21)	2.333(9)	W(8)-O(6)	1.932(9)	W(9)-O(44)	1.910(9)
W(7)-O(74)	1.889(9)	W(8)-O(29)	2.350(9)	W(9)-O(32)	2.307(9)
W(10)-O(51)	1.698(9)	W(11)-O(45)	1.697(9)	W(12)-O(60)	1.717(10)
W(10)-O(8)	1.893(9)	W(11)-O(43)	1.858(10)	W(12)-O(41)	1.900(9)
W(10)-O(7)	1.905(9)	W(11)-O(19)	1.898(9)	W(12)-O(18)	1.907(10)
W(10)-O(2)	1.909(9)	W(11)-O(44)	1.922(10)	W(12)-O(26)	1.921(10)
W(10)-O(54)	1.913(9)	W(11)-O(36)	1.928(9)	W(12)-O(47)	1.933(9)
W(10)-O(22)	2.391(8)	W(11)-O(32)	2.371(9)	W(12)-O(11)	2.405(8)
W(13)-O(50)	1.678(9)	W(14)-O(57)	1.697(9)	W(15)-O(55)	1.683(9)
W(13)-O(40)	1.885(9)	W(14)-O(33)	1.893(10)	W(15)-O(23)	1.874(9)
W(13)-O(47)	1.911(10)	W(14)-O(58)	1.899(10)	W(15)-O(39)	1.891(9)
W(13)-O(7)	1.926(9)	W(14)-O(36)	1.900(9)	W(15)-O(16)	1.907(9)
W(13)-O(48)	1.947(10)	W(14)-O(42)	1.933(9)	W(15)-O(20)	1.936(9)
W(13)-O(11)	2.390(8)	W(14)-O(1)	2.371(8)	W(15)-O(38)	2.369(9)
W(16)-O(63)	1.727(10)	W(17)-O(52)	1.701(9)	W(18)-O(62)	1.691(10)
W(16)-O(12)	1.875(9)	W(17)-O(4)	1.888(9)	W(18)-O(6)	1.898(9)
W(16)-O(30)	1.882(9)	W(17)-O(46)	1.921(10)	W(18)-O(46)	1.917(9)
W(16)-O(48)	1.901(9)	W(17)-O(42)	1.929(9)	W(18)-O(39)	1.930(9)
W(16)-O(26)	1.944(10)	W(17)-O(68)	1.946(10)	W(18)-O(33)	1.942(9)
W(16)-O(11)	2.332(8)	W(17)-O(1)	2.381(9)	W(18)-O(1)	2.398(9)
Mn(1)-O(9W)	2.109(13)	Mn(1)-O(59)	2.150(10)	Mn(1)-O(10W)	2.169(15)
Mn(1)-N(14)	2.218(13)	Mn(1)-N(2)	2.226(14)	Mn(1)-O(8W)	2.250(11)
Mn(2)-N(10)	2.236(14)	Mn(2)-N(6)	2.240(13)	Mn(2)-N(3)	2.243(14)
Mn(2)-N(8)	2.257(13)	Mn(2)-N(4)	2.257(11)	Mn(2)-N(9)	2.270(12)
P(1)-O(38)	1.521(9)	P(1)-O(32)	1.535(9)	P(1)-O(29)	1.541(9)
P(1)-O(1)	1.579(8)	P(2)-O(22)	1.513(9)	P(2)-O(21)	1.518(9)
P(2)-O(35)	1.532(8)	P(2)-O(11)	1.590(8)		
O(49)-W(1)-O(3)	103.2(4)	O(24)-W(2)-O(20)	99.0(4)	O(56)-W(3)-O(10)	102.8(5)
O(49)-W(1)-O(9)	99.6(4)	O(24)-W(2)-O(15)	100.9(4)	O(56)-W(3)-O(17)	100.8(4)
O(49)-W(1)-O(5)	101.5(4)	O(24)-W(2)-O(54)	100.4(4)	O(56)-W(3)-O(9)	99.2(4)
O(49)-W(1)-O(4)	96.8(4)	O(24)-W(2)-O(30)	97.6(4)	O(56)-W(3)-O(41)	96.8(4)
O(49)-W(1)-O(29)	175.6(4)	O(24)-W(2)-O(22)	174.0(4)	O(56)-W(3)-O(35)	173.6(4)
O(28)-W(4)-O(2)	100.1(4)	O(25)-W(5)-O(13)	98.3(4)	O(34)-W(6)-O(19)	99.6(4)
O(28)-W(4)-O(16)	100.4(4)	O(25)-W(5)-O(15)	103.3(4)	O(34)-W(6)-O(8)	101.2(4)

O(28)-W(4)-O(58)	96.4(4)	O(25)-W(5)-O(17)	98.5(4)	O(34)-W(6)-O(74)	102.4(4)
O(28)-W(4)-O(43)	102.1(4)	O(25)-W(5)-O(12)	98.4(4)	O(34)-W(6)-O(40)	97.1(4)
O(28)-W(4)-O(38)	172.8(4)	O(25)-W(5)-O(35)	172.3(4)	O(34)-W(6)-O(21)	173.7(4)
O(53)-W(7)-O(14)	97.4(4)	O(31)-W(8)-O(3)	100.1(4)	O(59)-W(9)-O(5)	100.8(4)
O(53)-W(7)-O(74)	100.7(4)	O(31)-W(8)-O(13)	98.2(4)	O(59)-W(9)-O(68)	97.2(4)
O(53)-W(7)-O(10)	101.4(4)	O(31)-W(8)-O(23)	103.3(4)	O(59)-W(9)-O(14)	98.5(4)
O(53)-W(7)-O(18)	97.5(4)	O(31)-W(8)-O(6)	96.7(4)	O(59)-W(9)-O(44)	100.5(4)
O(53)-W(7)-O(21)	174.8(4)	O(31)-W(8)-O(29)	173.2(4)	O(59)-W(9)-O(32)	174.5(4)
O(51)-W(10)-O(8)	102.3(4)	O(45)-W(11)-O(43)	103.9(4)	O(60)-W(12)-O(41)	102.0(4)
O(51)-W(10)-O(7)	98.7(4)	O(45)-W(11)-O(19)	98.8(4)	O(60)-W(12)-O(18)	102.6(5)
O(51)-W(10)-O(2)	97.8(4)	O(45)-W(11)-O(44)	98.7(4)	O(60)-W(12)-O(26)	101.1(5)
O(51)-W(10)-O(54)	99.9(5)	O(45)-W(11)-O(36)	98.0(4)	O(60)-W(12)-O(47)	102.1(4)
O(51)-W(10)-O(22)	173.3(4)	O(45)-W(11)-O(32)	171.0(4)	O(60)-W(12)-O(11)	171.3(4)
O(50)-W(13)-O(40)	103.5(4)	O(57)-W(14)-O(33)	100.7(4)	O(55)-W(15)-O(23)	101.2(4)
O(50)-W(13)-O(47)	101.7(4)	O(57)-W(14)-O(58)	103.5(5)	O(55)-W(15)-O(39)	97.2(4)
O(50)-W(13)-O(7)	102.5(4)	O(57)-W(14)-O(36)	102.1(4)	O(55)-W(15)-O(16)	101.7(4)
O(50)-W(13)-O(48)	100.0(4)	O(57)-W(14)-O(42)	100.6(5)	O(55)-W(15)-O(20)	97.3(4)
O(50)-W(13)-O(11)	170.4(4)	O(57)-W(14)-O(1)	171.8(4)	O(55)-W(15)-O(38)	175.7(4)
O(63)-W(16)-O(12)	101.6(4)	O(52)-W(17)-O(4)	101.6(4)	O(62)-W(18)-O(6)	102.1(4)
O(63)-W(16)-O(30)	103.1(4)	O(52)-W(17)-O(46)	102.2(4)	O(62)-W(18)-O(46)	102.3(5)
O(63)-W(16)-O(48)	100.5(4)	O(52)-W(17)-O(42)	101.2(4)	O(62)-W(18)-O(39)	100.6(5)
O(63)-W(16)-O(26)	99.5(4)	O(52)-W(17)-O(68)	100.3(4)	O(62)-W(18)-O(33)	102.7(4)
O(63)-W(16)-O(11)	171.1(4)	O(52)-W(17)-O(1)	173.6(4)	O(62)-W(18)-O(1)	173.5(4)
N(10)-Mn(2)-N(6)	74.6(5)	N(10)-Mn(2)-N(3)	162.9(4)	N(10)-Mn(2)-N(8)	93.4(5)
N(10)-Mn(2)-N(4)	103.9(4)	N(10)-Mn(2)-N(9)	99.8(5)	O(9W)-Mn(1)-O(59)	93.3(5)
O(9W)-Mn(1)-O(10W)	91.4(7)	O(9W)-Mn(1)-N(14)	98.0(5)		
O(9W)-Mn(1)-O(8W)	84.4(6)	O(9W)-Mn(1)-N(2)	171.6(6)		
O(38)-P(1)-O(32)	112.0(5)	O(38)-P(1)-O(29)	111.1(5)	O(38)-P(1)-O(1)	107.0(5)
O(22)-P(2)-O(21)	112.6(5)	O(22)-P(2)-O(35)	112.7(5)	O(22)-P(2)-O(11)	106.2(5)

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

3. Physical characterization

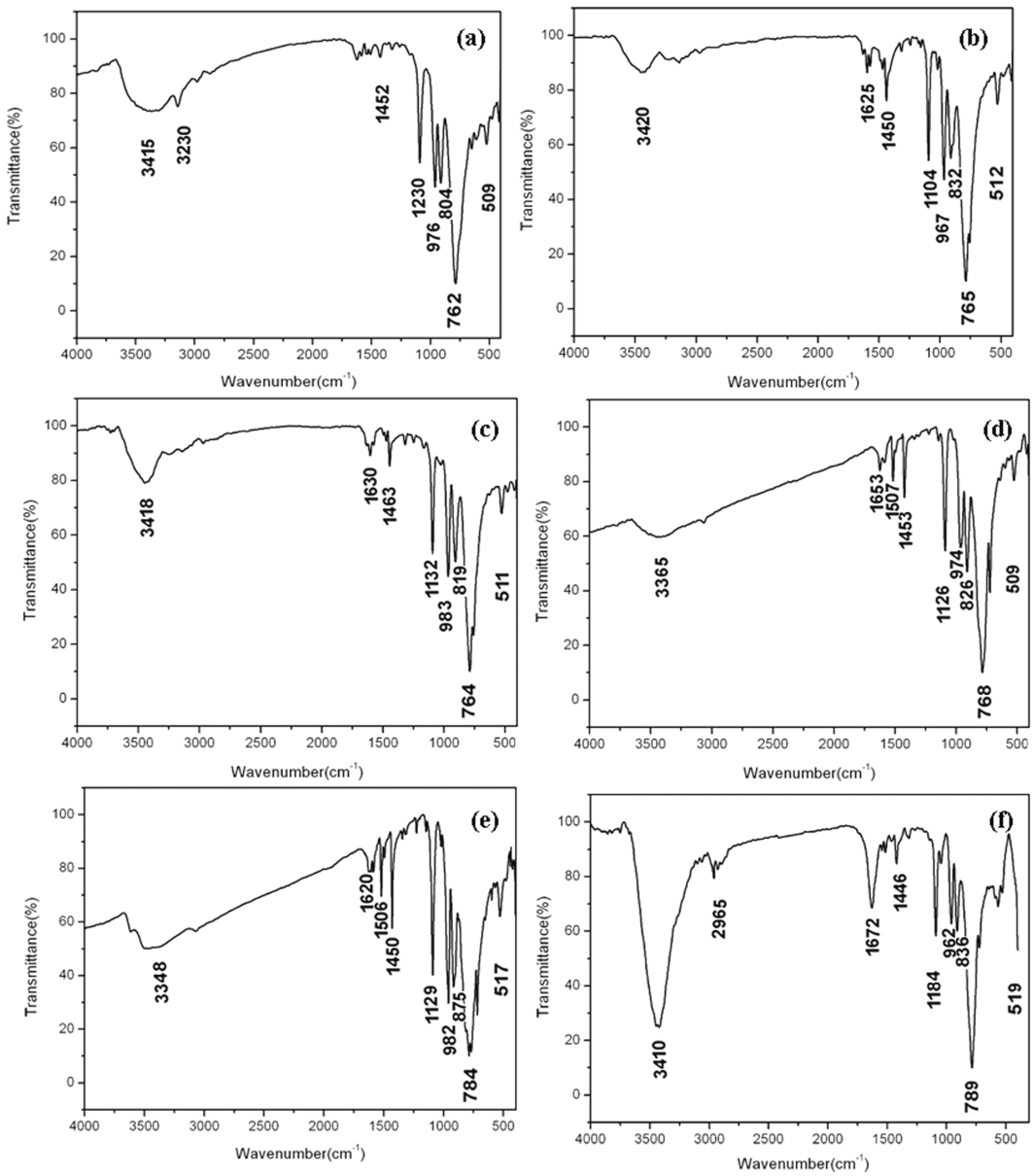

Fig. S11 IR spectra of **(a)** compound **1**, **(b)** compound **2**, **(c)** compound **3, (d)** compound **4, (e)** compound **5,** and **(f)** compound **6.**

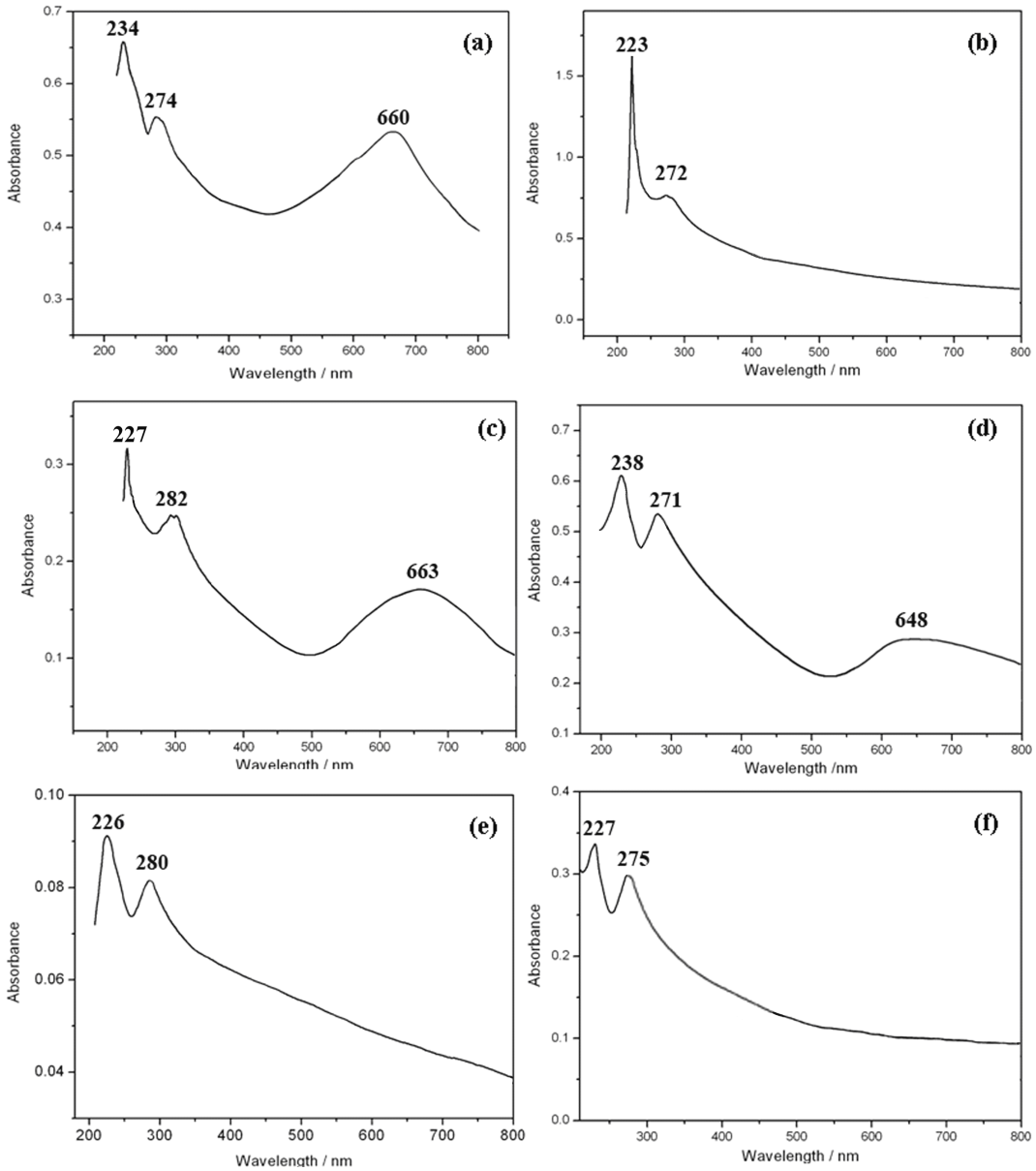

Fig. S12 UV spectra of **(a)** compound **1**, **(b)** compound **2**, **(c)** compound **3, (d)** compound **4, (e)** compound **5,** and **(f)** compound **6.**

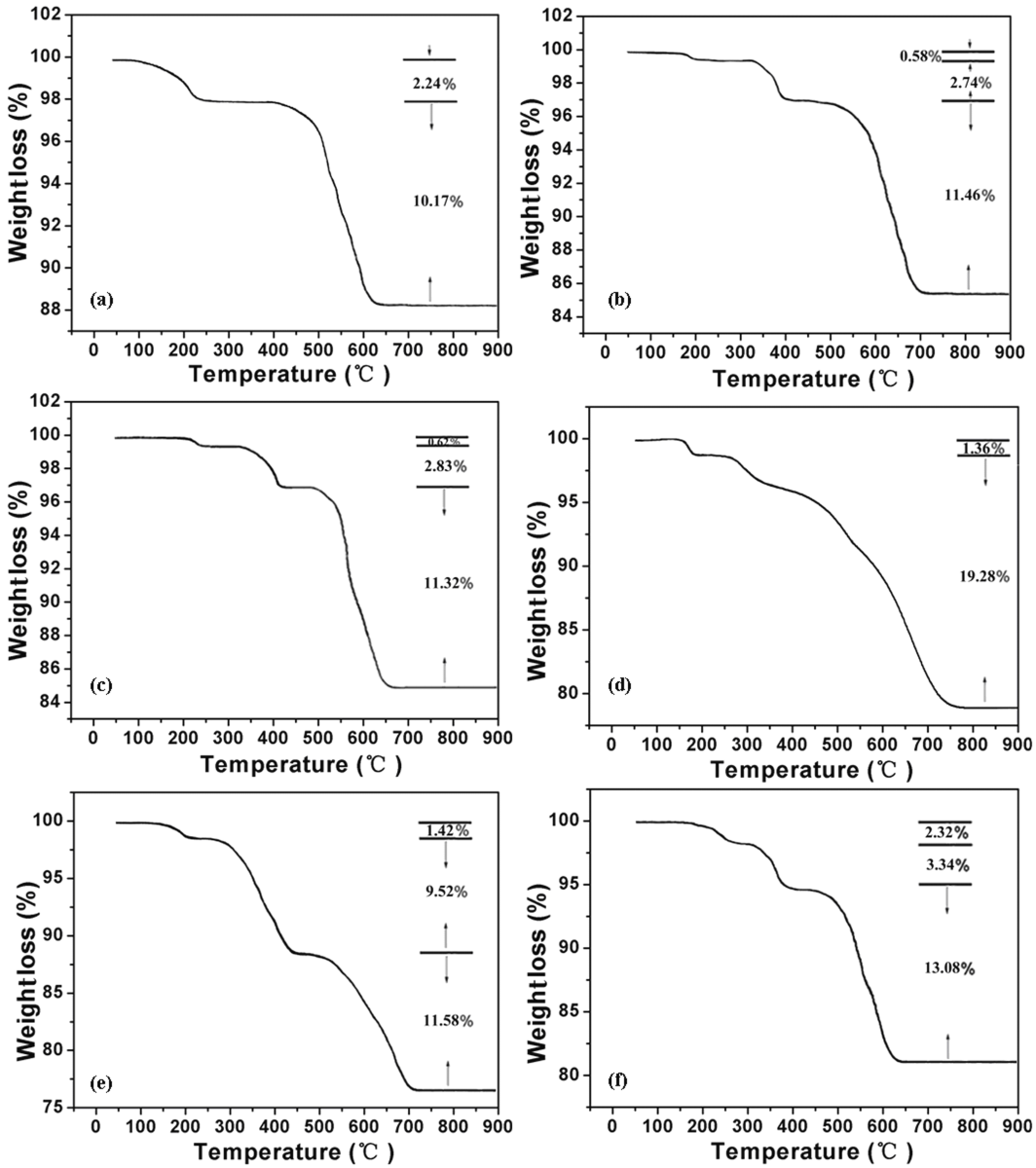

Fig. S13 TG of **(a)** compound **1**, **(b)** compound **2**, **(c)** compound **3**, **(d)** compound **4**, **(e)** compound **5**, and **(f)** compound **6.**

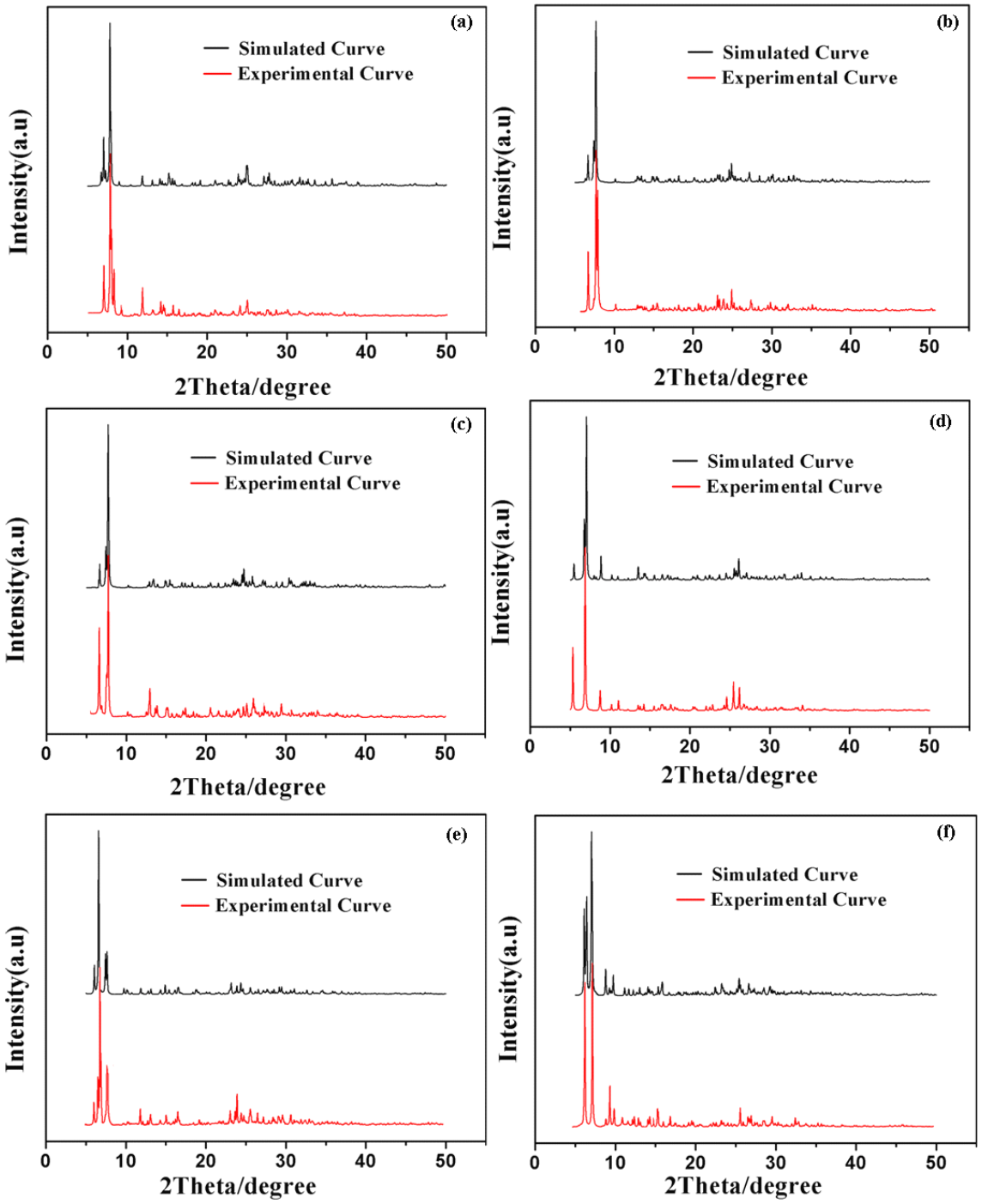

Figure S14. The XPRD contrast curves of compound **1 (a)**, compound **2 (b)**, compound **3 (c),** compound **4 (d),** compound **5 (e),** and compound **6 (f).**

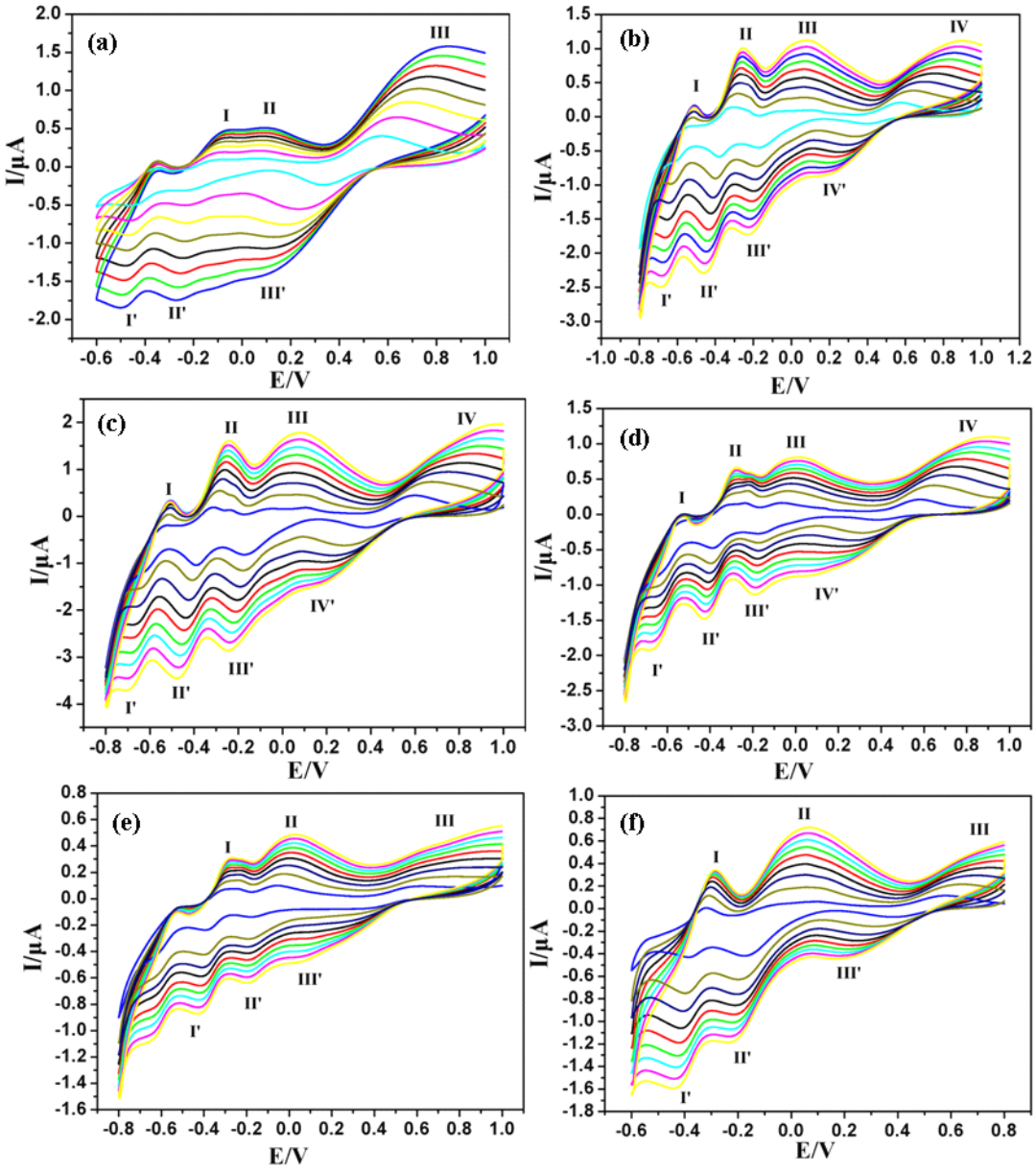

Fig. S15 Cyclic voltammograms of **(a) 1-CPE, (b) 2-CPE, (c) 3-CPE, (d) 4-CPE, (d) 5-CPE,** and **(e) 6-CPE,** rates (from inner to outer: 20, 50, 80, 110, 140, 170, 200, 230, 260 mV s^{-1}).

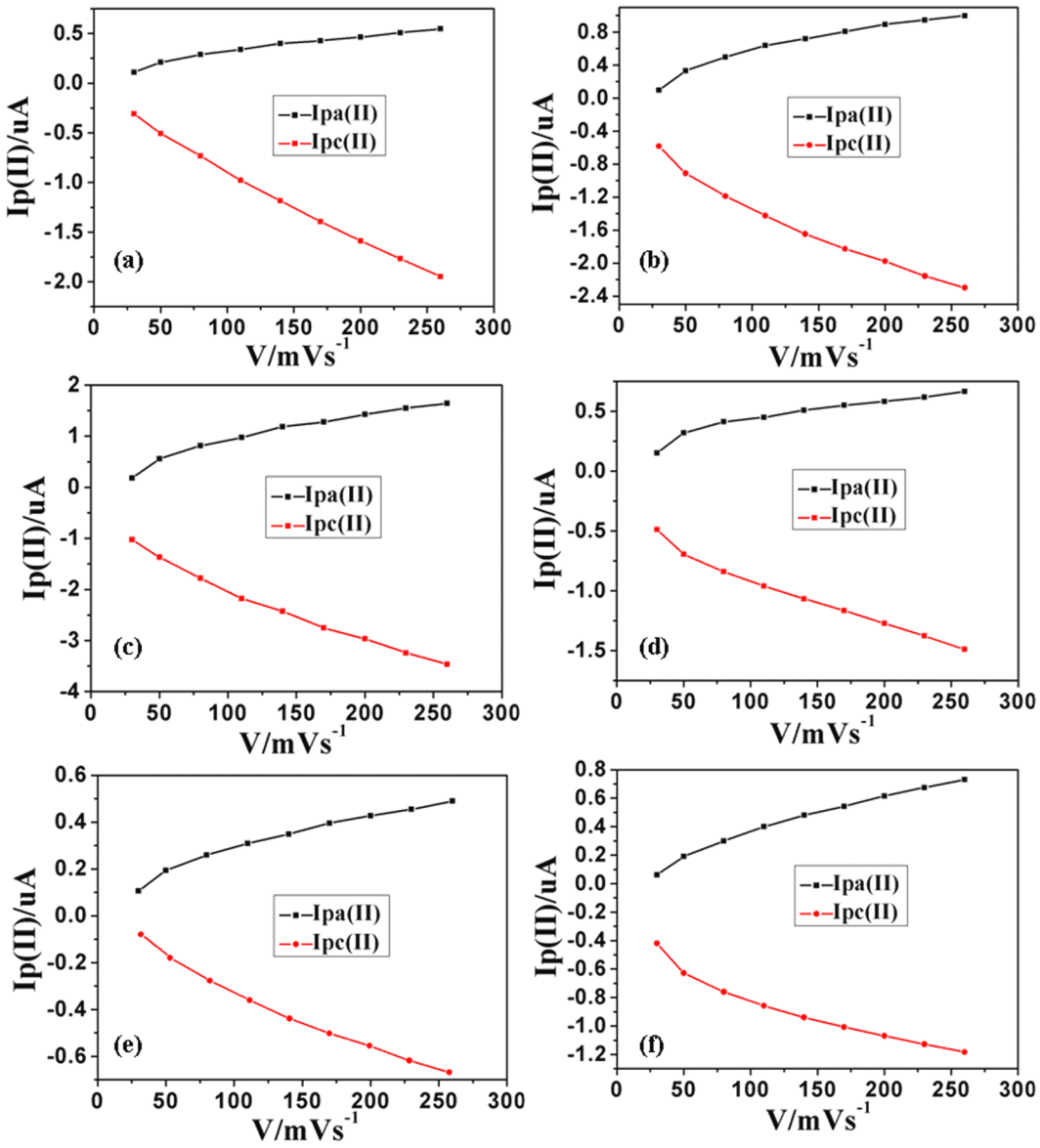

Fig. S16 The dependence of anodic peak II current on scan rates for compound **1 (a)**, compound **2 (b)**, compound **3 (c),** compound **4 (d),** compound **5 (e),** and compound **6 (f).**

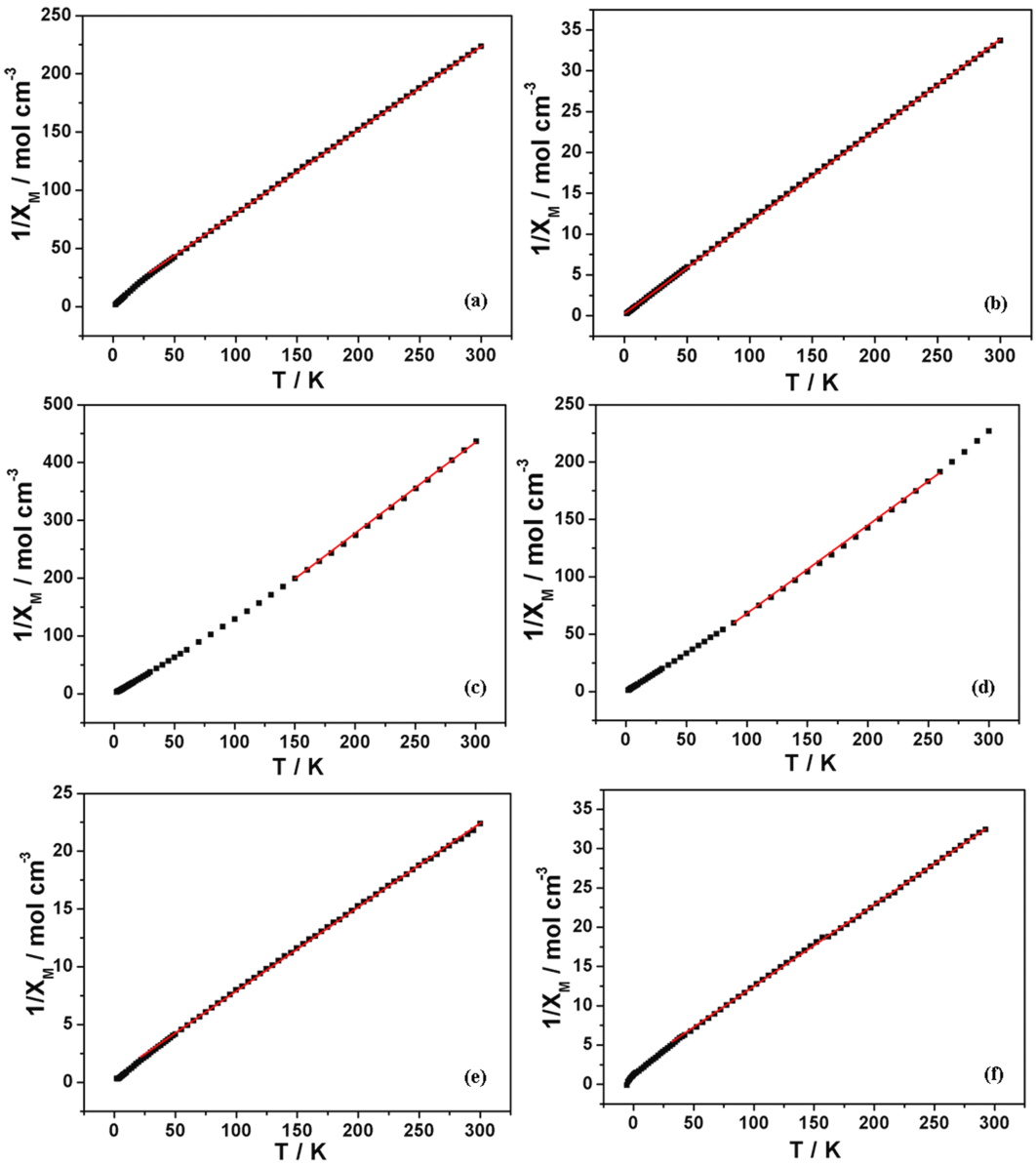

Fig. S17 Temperature dependences of χ_m^{-1} for compound **1 (a)**, compound **2 (b)**, compound **3 (c),** compound **4 (d),** compound **5 (e),** and compound **6 (f).**