Synthesis and characterization of two {Mo_6}-based/templated metal-organic frameworks

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Table S1 Selected bond lengths [Å] and angles [deg] for **1**

Ni(1)-O(1)#1	2.087(13)	Mo(1)-O(4)	1.974(10)
Ni(1)-O(1)	2.087(13)	Mo(1)-O(3)	2.338(2)
Ni(1)-N(1)	2.095(10)	Mo(1)-O(2)#4	2.339(17)
Ni(1)-N(1)#2	2.095(10)	Mo(2)-O(5)	1.659(15)
Ni(1)-N(1)#1	2.095(10)	Mo(2)-O(4)	1.946(9)
Ni(1)-N(1)#3	2.095(10)	Mo(2)-O(4)#5	1.946(9)
Mo(1)-O(1)	1.733(13)	Mo(2)-O(4)#6	1.946(9)
Mo(1)-O(2)	1.768(14)	Mo(2)-O(4)#7	1.946(9)
Mo(1)-O(4)#3	1.974(10)	Mo(2)-O(3)	2.287(2)
O(1)#1-Ni(1)-O(1)	180	O(4)-Mo(2)-O(4)#5	87.87(11)
O(1)#1-Ni(1)-N(1)	90.6(4)	O(5)-Mo(2)-O(4)#6	101.1(3)
O(1)-Ni(1)-N(1)	89.4(4)	O(4)-Mo(2)-O(4)#6	87.87(11)
O(1)#1-Ni(1)-N(1)#2	89.4(4)	O(4)#5-Mo(2)-O(4)#6	157.8(6)
O(1)-Ni(1)-N(1)#2	90.6(4)	O(5)-Mo(2)-O(4)#7	101.1(3)
N(1)-Ni(1)-N(1)#2	87.8(6)	O(4)-Mo(2)-O(4)#7	157.8(6)
O(1)#1-Ni(1)-N(1)#1	89.4(4)	O(4)#5-Mo(2)-O(4)#7	87.87(11)
O(1)-Ni(1)-N(1)#1	90.6(4)	O(4)#6-Mo(2)-O(4)#7	87.87(11)
N(1)-Ni(1)-N(1)#1	180	O(5)-Mo(2)-O(3)	180
N(1)#2-Ni(1)-N(1)#1	92.2(6)	O(4)-Mo(2)-O(3)	78.9(3)
O(1)#1-Ni(1)-N(1)#3	90.6(4)	O(4)#5-Mo(2)-O(3)	78.9(3)
O(1)-Ni(1)-N(1)#3	89.4(4)	O(4)#6-Mo(2)-O(3)	78.9(3)
N(1)-Ni(1)-N(1)#3	92.2(6)	O(4)#7-Mo(2)-O(3)	78.9(3)
N(1)#2-Ni(1)-N(1)#3	180	Mo(1)-O(1)-Ni(1)	171.2(7)
N(1)#1-Ni(1)-N(1)#3	87.8(6)	Mo(1)-O(2)-Mo(1)#5	106.4(7)
O(1)-Mo(1)-O(2)	104.9(7)	Mo(2)#9-O(3)-Mo(2)	180
O(1)-Mo(1)-O(4)#3	101.2(3)	Mo(2)#9-O(3)-Mo(1)#9	90
O(2)-Mo(1)-O(4)#3	95.8(3)	Mo(2)-O(3)-Mo(1)#9	90
O(1)-Mo(1)-O(4)	101.2(3)	Mo(2)#9-O(3)-Mo(1)#4	90

O(2)-Mo(1)-O(4)	95.8(3)	Mo(2)-O(3)-Mo(1)#4	90
O(4)#3-Mo(1)-O(4)	151.2(5)	Mo(1)#9-O(3)-Mo(1)#4	90
O(1)-Mo(1)-O(3)	167.3(4)	Mo(2)#9-O(3)-Mo(1)	90
O(2)-Mo(1)-O(3)	87.7(5)	Mo(2)-O(3)-Mo(1)	90
O(4)#3-Mo(1)-O(3)	77.1(3)	Mo(1)#9-O(3)-Mo(1)	180
O(4)-Mo(1)-O(3)	77.1(3)	Mo(1)#4-O(3)-Mo(1)	90
O(1)-Mo(1)-O(2)#4	91.5(5)	Mo(2)#9-O(3)-Mo(1)#5	90
O(2)-Mo(1)-O(2)#4	163.6(7)	Mo(2)-O(3)-Mo(1)#5	90
O(4)#3-Mo(1)-O(2)#4	80.7(3)	Mo(1)#9-O(3)-Mo(1)#5	90
O(4)-Mo(1)-O(2)#4	80.7(3)	Mo(1)#4-O(3)-Mo(1)#5	180
O(3)-Mo(1)-O(2)#4	75.9(3)	Mo(1)-O(3)-Mo(1)#5	90
O(5)-Mo(2)-O(4)	101.1(3)	Mo(2)-O(4)-Mo(1)	113.1(4)
O(5)-Mo(2)-O(4)#5	101.1(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y,-z ; #2 -x+1,-y,z ; #3 x,y,-z ; #4 -y,x,z ; #5 -x,-y,z ; #6 y,-x,z ; #7 y,-x,-z
#8 -x+3/2,-y+1/2,-z+1/2 ; #9 -x,-y,-z

Table S2 Selected bond lengths [Å] and angles [deg] for **2.**

Zn(1)-O(12)#1	1.897(12)	Zn(2)-O(11)	1.928(12)
Zn(1)-O(13)	1.929(13)	Zn(2)-O(14)#3	1.941(13)
Zn(1)-N(1)	1.986(17)	Zn(2)-N(8)	2.007(17)
Zn(1)-N(5)#2	2.022(14)	Zn(2)-N(4)#4	2.021(17)
Mo(1)-O(2')	1.19(3)	Mo(2)-O(7)	1.93(2)
Mo(1)-O(2)	1.68(3)	Mo(2)-O(1)	2.259(2)
Mo(1)-O(9)	1.69(3)	Mo(2)-Mo(3)#5	3.195(4)
Mo(1)-O(7)#5	1.889(19)	Mo(3)-O(10)	1.66(3)
Mo(1)-O(5)	1.95(2)	Mo(3)-O(4)	1.74(3)
Mo(1)-O(10)#5	2.09(3)	Mo(3)-O(8)#5	1.86(2)
Mo(1)-O(1)	2.334(3)	Mo(3)-O(6)	1.91(2)
Mo(2)-O(3)	1.66(2)	Mo(3)-O(9)	2.09(2)
Mo(2)-O(5)	1.889(18)	Mo(3)-O(1)	2.305(3)
Mo(2)-O(6)	1.89(2)	Mo(3)-Mo(2)#5	3.195(4)
Mo(2)-O(8)	1.91(2)		

O(12)#1-Zn(1)-O(13)	116.7(5)	O(6)-Mo(2)-O(8)	153.7(9)
O(12)#1-Zn(1)-N(1)	111.3(6)	O(3)-Mo(2)-O(7)	99.8(9)
O(13)-Zn(1)-N(1)	105.6(6)	O(5)-Mo(2)-O(7)	155.8(8)
O(12)#1-Zn(1)-N(5)#2	103.3(6)	O(6)-Mo(2)-O(7)	87.5(11)
O(13)-Zn(1)-N(5)#2	106.8(6)	O(8)-Mo(2)-O(7)	86.2(11)
N(1)-Zn(1)-N(5)#2	113.2(7)	O(3)-Mo(2)-O(1)	175.8(9)
O(11)-Zn(2)-O(14)#3	106.2(5)	O(5)-Mo(2)-O(1)	78.4(6)
O(11)-Zn(2)-N(8)	122.9(6)	O(6)-Mo(2)-O(1)	76.0(7)
O(14)#3-Zn(2)-N(8)	107.3(6)	O(8)-Mo(2)-O(1)	77.7(6)
O(11)-Zn(2)-N(4)#4	97.8(6)	O(7)-Mo(2)-O(1)	77.4(6)

O(14)#3-Zn(2)-N(4)#4	113.5(6)	O(3)-Mo(2)-Mo(3)#5	130.6(8)
N(8)-Zn(2)-N(4)#4	109.2(7)	O(5)-Mo(2)-Mo(3)#5	83.0(7)
O(2')-Mo(1)-O(2)	44.1(16)	O(6)-Mo(2)-Mo(3)#5	122.1(7)
O(2')-Mo(1)-O(9)	129.9(16)	O(8)-Mo(2)-Mo(3)#5	31.6(6)
O(2)-Mo(1)-O(9)	101.7(12)	O(7)-Mo(2)-Mo(3)#5	80.3(7)
O(2')-Mo(1)-O(7)#5	128.3(16)	O(1)-Mo(2)-Mo(3)#5	46.15(7)
O(2)-Mo(1)-O(7)#5	103.6(12)	O(10)-Mo(3)-O(4)	104.8(12)
O(9)-Mo(1)-O(7)#5	88.6(10)	O(10)-Mo(3)-O(8)#5	89.6(11)
O(2')-Mo(1)-O(5)	76.5(16)	O(4)-Mo(3)-O(8)#5	103.2(12)
O(2)-Mo(1)-O(5)	104.7(12)	O(10)-Mo(3)-O(6)	83.7(11)
O(9)-Mo(1)-O(5)	82.2(10)	O(4)-Mo(3)-O(6)	104.9(13)
O(7)#5-Mo(1)-O(5)	151.5(8)	O(8)#5-Mo(3)-O(6)	152.0(9)
O(2')-Mo(1)-O(10)#5	75.9(16)	O(10)-Mo(3)-O(9)	149.4(11)
O(2)-Mo(1)-O(10)#5	110.3(13)	O(4)-Mo(3)-O(9)	105.1(11)
O(9)-Mo(1)-O(10)#5	147.9(10)	O(8)#5-Mo(3)-O(9)	89.7(9)
O(7)#5-Mo(1)-O(10)#5	86.2(11)	O(6)-Mo(3)-O(9)	82.6(9)
O(5)-Mo(1)-O(10)#5	87.4(9)	O(10)-Mo(3)-O(1)	78.5(9)
O(2')-Mo(1)-O(1)	136.7(14)	O(4)-Mo(3)-O(1)	176.6(9)
O(2)-Mo(1)-O(1)	179.2(11)	O(8)#5-Mo(3)-O(1)	77.4(6)
O(9)-Mo(1)-O(1)	77.6(6)	O(6)-Mo(3)-O(1)	74.5(6)
O(7)#5-Mo(1)-O(1)	76.2(6)	O(9)-Mo(3)-O(1)	71.5(7)
O(5)-Mo(1)-O(1)	75.5(5)	O(10)-Mo(3)-Mo(2)#5	83.7(9)
O(10)#5-Mo(1)-O(1)	70.5(8)	O(4)-Mo(3)-Mo(2)#5	135.5(11)
O(3)-Mo(2)-O(5)	104.4(10)	O(8)#5-Mo(3)-Mo(2)#5	32.4(6)
O(3)-Mo(2)-O(6)	107.2(11)	O(6)-Mo(3)-Mo(2)#5	119.5(6)
O(5)-Mo(2)-O(6)	86.7(10)	O(9)-Mo(3)-Mo(2)#5	79.5(6)
O(3)-Mo(2)-O(8)	99.0(10)	O(1)-Mo(3)-Mo(2)#5	44.99(7)
O(5)-Mo(2)-O(8)	88.6(10)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 ; #2 -x+1,-y,-z ; #3 -x,-y+1,-z+1 ; #4 -x+2,-y+2,-z+1 ; #5 -x+1,-y,-z

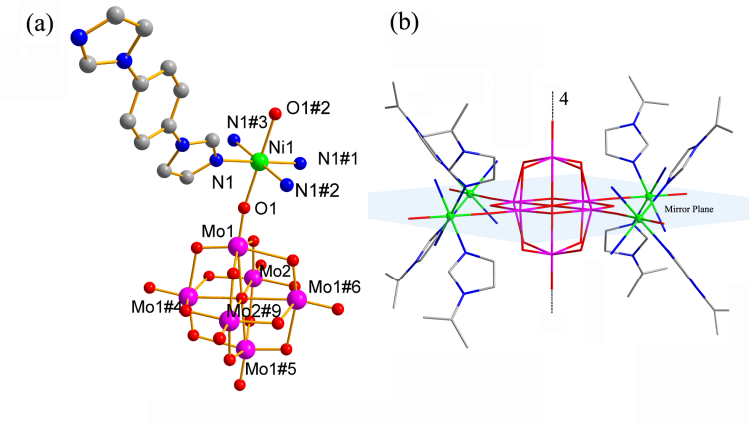

Fig. S1 (a) Coordination mode of Ni ion; (b) The coordination mode of $[Mo_6O_{19}]^{4-}$ anion (Symmetry code: #5 -x, y, z; #6 x, -y, z; #7 -x,-y, z; #8 -x,-y,-z+1)

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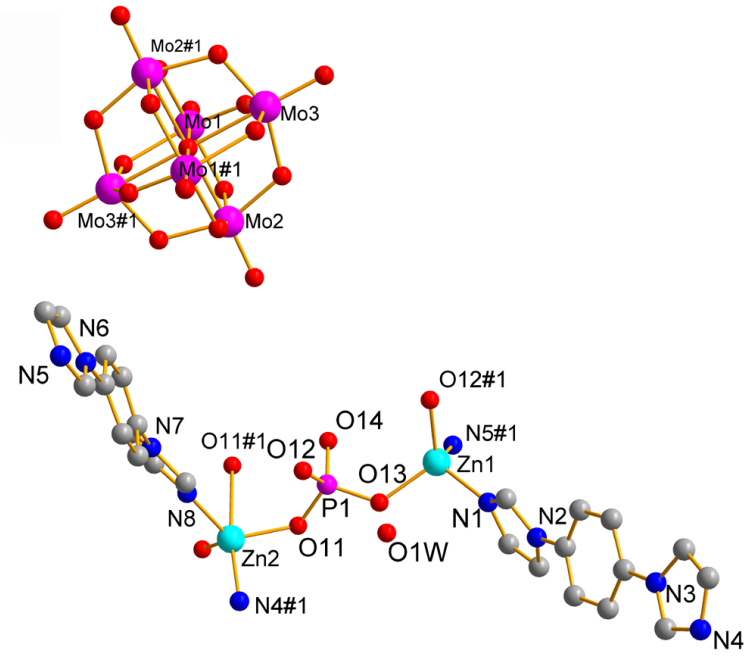

Fig. S2 Coordination mode of Zn^{II} ion (symmetry code: #1 -x+1,-y+1,-z+1).

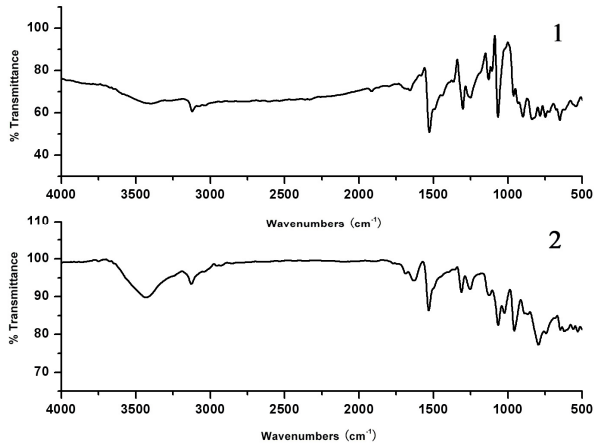

Fig. S3 The IR spectra for compounds **1** and **2**.

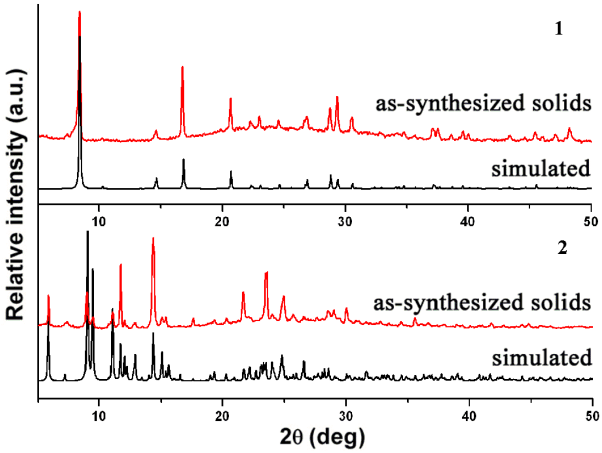

Fig. S4 The PXRD patterns for compounds **1** and **2.**

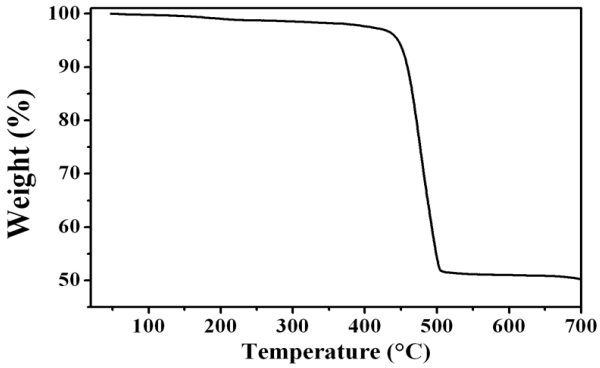

Fig. S5 TG curve of compound **1.**

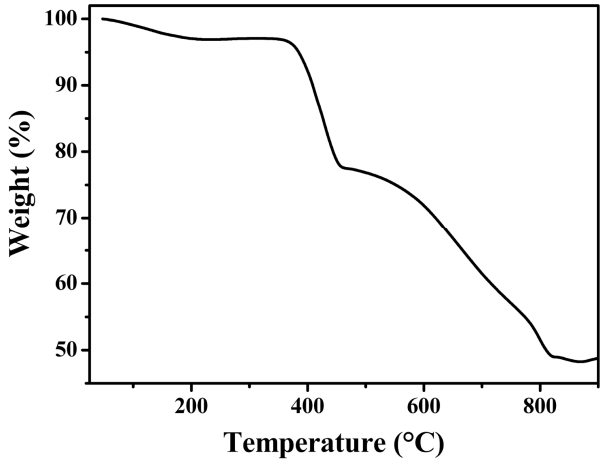

Fig. S6 TG curve of compound **2.**