

Table S1 Selected Bond Distances (Å) and Angles (deg) for Complexes **1-6**

Complex 1			
Ni(1)-O(1)	2.045(4)	Ni(1)-O(5) ^{#1}	2.264(4)
Ni(1)-O(2)	2.038(4)	Ni(1)-N(1)	2.077(5)
Ni(1)-O(4) ^{#1}	2.059(4)	Ni(1)-N(6) ^{#2}	2.080(5)
O(5)-Ni(1) ^{#3}	2.264(4)		
O(1)-Ni(1)-N(6) ^{#2}	94.15(17)	N(1)-Ni(1)-O(5) ^{#1}	86.54(16)
O(1)-Ni(1)-C(00R) ^{#1}	124.50(17)	O(1)-Ni(1)-O(4) ^{#1}	94.26(16)
O(2)-Ni(1)-O(1)	94.93(16)	N(1)-Ni(1)-C(00R) ^{#1}	91.18(18)
O(1)-Ni(1)-N(1)	91.61(17)	N(6) ^{#2} -Ni(1)-O(5) ^{#1}	90.76(16)
O(2)-Ni(1)-O(5) ^{#1}	109.95(15)	N(6) ^{#2} -Ni(1)-C(00R) ^{#1}	90.45(18)
O(2)-Ni(1)-N(1)	85.07(18)	C(7)-N(1)-Ni(1)	132.0(3)
O(2)-Ni(1)-N(6) ^{#2}	88.51(17)	C(1)-O(2)-Ni(1)	123.0(4)
O(2)-Ni(1)-C(00R) ^{#1}	140.51(17)	C(00R)-O(4)-Ni(1) ^{#3}	94.4(4)
O(4) ^{#1} -Ni(1)-O(5) ^{#1}	60.91(15)	C(00R)-O(5)-Ni(1) ^{#3}	84.9(3)
O(4) ^{#1} -Ni(1)-N(1)	95.05(18)	C(6)-N(1)-Ni(1)	121.6(4)
O(4) ^{#1} -Ni(1)-N(6) ^{#2}	90.46(17)		
Complex 2			
Ni(1)-O(2)	1.9934(12)	Ni(1)-O(5) ^{#1}	2.0823(13)
Ni(1)-O(1)	2.0719(12)	Ni(1)-N(1) ^{#2}	2.1053(15)
Ni(1)-O(4) ^{#1}	2.1362(12)	Ni(1)-N(6)	2.0879(15)
O(2)-Ni(1)-O(1)	94.47(5)	O(5)-C(25)-Ni(1) ^{#3}	59.01(9)
O(2)-Ni(1)-O(5) ^{#1}	105.41(5)	O(1)-Ni(1)-N(1) ^{#2}	92.64(6)
O(2)-Ni(1)-N(1) ^{#2}	90.17(6)	O(1)-Ni(1)-N(6)	89.16(5)
O(2)-Ni(1)-N(6)	87.19(6)	O(1)-Ni(1)-C(25) ^{#1}	128.81(6)
O(2)-Ni(1)-C(25) ^{#1}	136.69(5)	C(19)-O(2)-Ni(1)	127.05(12)
O(1)-Ni(1)-O(4) ^{#1}	97.25(5)	O(5) ^{#1} -Ni(1)-O(4) ^{#1}	62.86(5)
O(5) ^{#1} -Ni(1)-N(6)	91.05(6)	O(5) ^{#1} -Ni(1)-N(1) ^{#2}	88.11(6)
N(6)-Ni(1)-C(25) ^{#1}	94.10(6)	C(25)-O(4)-Ni(1) ^{#3}	86.95(10)
N(1) ^{#2} -Ni(1)-O(4) ^{#1}	89.69(5)	C(25)-O(5)-Ni(1) ^{#3}	89.63(10)
N(1) ^{#2} -Ni(1)-C(25) ^{#1}	86.73(6)	C(7)-N(1)-Ni(1) ^{#4}	121.84(13)
N(6)-Ni(1)-O(4) ^{#1}	92.57(5)	C(6)-N(1)-Ni(1) ^{#4}	132.54(12)
C(13)-N(6)-Ni(1)	130.24(12)	C(12)-N(6)-Ni(1)	123.37(12)
Complex 3			
Ni(1)-O(1)	2.026(2)	Ni(1)-O(4) ^{#1}	2.086(3)
Ni(1)-O(5) ^{#1}	2.158(2)	Ni(1)-N(1) ^{#2}	2.084(3)
Ni(1)-O(2)	2.030(3)	Ni(1)-N(6)	2.062(3)
O(1)-Ni(1)-O(2)	94.91(11)	N(1) ^{#2} -Ni(1)-C(26) ^{#1}	94.56(12)
O(1)-Ni(1)-O(4) ^{#1}	100.32(10)	N(6)-Ni(1)-O(5) ^{#1}	86.14(11)
O(1)-Ni(1)-N(1) ^{#2}	89.32(11)	N(6)-Ni(1)-O(4) ^{#1}	87.16(12)
O(1)-Ni(1)-N(6)	95.58(11)	O(4)-C(26)-Ni(1) ^{#3}	58.59(19)
O(1)-Ni(1)-C(26) ^{#1}	131.35(11)	N(6)-Ni(1)-C(26) ^{#1}	84.35(12)
N(1) ^{#2} -Ni(1)-O(4) ^{#1}	94.78(12)	C(26)-O(5)-Ni(1) ^{#3}	86.8(2)
O(2)-Ni(1)-O(5) ^{#1}	102.50(10)	C(19)-O(2)-Ni(1)	123.9(2)
O(2)-Ni(1)-O(4) ^{#1}	164.76(9)	C(26)-O(4)-Ni(1) ^{#3}	90.4(2)
O(2)-Ni(1)-N(1) ^{#2}	85.63(12)	C(7)-N(1)-Ni(1) ^{#4}	120.4(2)
O(2)-Ni(1)-N(6)	91.09(11)	O(5)-N(1)-Ni(1) ^{#3}	61.84(18)

O(2)-Ni(1)-C(26) ^{#1}	133.73(12)	N(1) ^{#2} -Ni(1)-O(5) ^{#1}	90.04(11)
O(4) ^{#1} -Ni(1)-O(5) ^{#1}	62.28(10)		

Complex 4

Mn(1)-O(4)	2.087(3)	Mn(1)-N(1)	2.274(4)
Mn(1)-O(2) ^{#1}	2.249(3)	N(6)-Mn(1) ^{#4}	2.267(4)
Mn(1)-O(1) ^{#1}	2.290(3)	Mn(1)-O(5)	2.113(2)
O(4)-Mn(1)-O(2) ^{#1}	118.16(10)	N(6) ^{#2} -Mn(1)-O(1) ^{#1}	98.00(12)
O(4)-Mn(1)-O(5)	96.30(11)	O(5)-Mn(1)-C(1) ^{#1}	115.70(11)
O(4)-Mn(1)-N(6) ^{#2}	86.39(13)	N(6) ^{#2} -Mn(1)-C(1) ^{#1}	102.84(12)
O(4)-Mn(1)-N(1)	93.89(12)	N(1)-Mn(1)-O(1) ^{#1}	82.08(12)
O(4)-Mn(1)-C(1) ^{#1}	146.40(11)	N(1)-Mn(1)-C(1) ^{#1}	79.97(13)
O(2) ^{#1} -Mn(1)-O(1) ^{#1}	58.00(8)	C(6)-O(4)-Mn(1)	132.0(2)
O(2) ^{#1} -Mn(1)-N(6) ^{#2}	97.81(12)	C(1)-O(2)-Mn(1) ^{#3}	90.1(2)
O(2) ^{#1} -Mn(1)-N(1)	86.99(13)	C(1)-O(1)-Mn(1) ^{#3}	88.4(2)
O(5)-Mn(1)-N(1)	84.63(17)	C(25)-N(6)-Mn(1) ^{#4}	136.5(3)
C(7)-N(1)-Mn(1)	118.9(3)	C(18)-N(6)-Mn(1) ^{#4}	115.9(3)
O(5)-Mn(1)-O(2) ^{#1}	145.00(11)	O(1)-C(1)-Mn(1) ^{#3}	62.44(18)
O(5)-Mn(1)-O(1) ^{#1}	87.17(10)	C(13)-N(1)-Mn(1)	134.2(3)
O(5)-Mn(1)-N(6) ^{#2}	89.80(16)		

Complex 5

Mn(1)-O(1)	2.2982(14)	Mn(1)-N(7)	2.2466(18)
Mn(1)-O(1) ^{#1}	2.4382(15)	Mn(1)-N(6)	2.2856(16)
Mn(1)-O(1S)	2.1503(15)	Mn(1)-N(1) ^{#2}	2.3306(17)
Mn(1)-O(4)	2.3921(15)		
O(1)-Mn(1)-O(1) ^{#1}	71.25(6)	N(7)-Mn(1)-N(1) ^{#2}	83.21(6)
O(1)-Mn(1)-O(4)	139.90(5)	N(6)-Mn(1)-O(1)	86.47(5)
O(1)-Mn(1)-N(1) ^{#2}	90.01(5)	N(6)-Mn(1)-O(1) ^{#1}	91.64(5)
O(1S)-Mn(1)-O(1)	147.26(6)	N(6)-Mn(1)-O(4)	90.19(5)
O(1S)-Mn(1)-O(1) ^{#1}	76.22(5)	C(2)-N(1)-Mn(1) ^{#3}	140.13(13)
O(1S)-Mn(1)-O(4)	72.73(5)	N(1) ^{#2} -Mn(1)-O(1) ^{#1}	96.53(5)
O(1S)-Mn(1)-N(7)	141.04(6)	N(1) ^{#2} -Mn(1)-O(4)	86.18(5)
O(1S)-Mn(1)-N(6)	98.23(6)	Mn(1)-O(1)-Mn(1) ^{#1}	108.75(6)
O(1S)-Mn(1)-N(1) ^{#2}	90.04(6)	C(19)-O(1)-Mn(1)	118.00(12)
O(4)-Mn(1)-O(1) ^{#1}	148.84(5)	C(19)-O(1)-Mn(1) ^{#1}	132.97(12)
N(7)-Mn(1)-O(1)	71.34(6)	Mn(1)-O(1S)-H(1SA)	110.2
N(7)-Mn(1)-O(1) ^{#1}	142.59(5)	C(24)-O(4)-Mn(1)	119.35(13)
N(7)-Mn(1)-O(4)	68.57(6)	C(21)-N(7)-Mn(1)	121.99(13)
N(7)-Mn(1)-N(6)	86.36(6)	C(20)-N(7)-Mn(1)	118.64(13)
C(17)-N(6)-Mn(1)	132.28(12)	C(1)-N(1)-Mn(1) ^{#3}	114.87(13)
C(18)-N(6)-Mn(1)	122.66(13)		

Complex 6

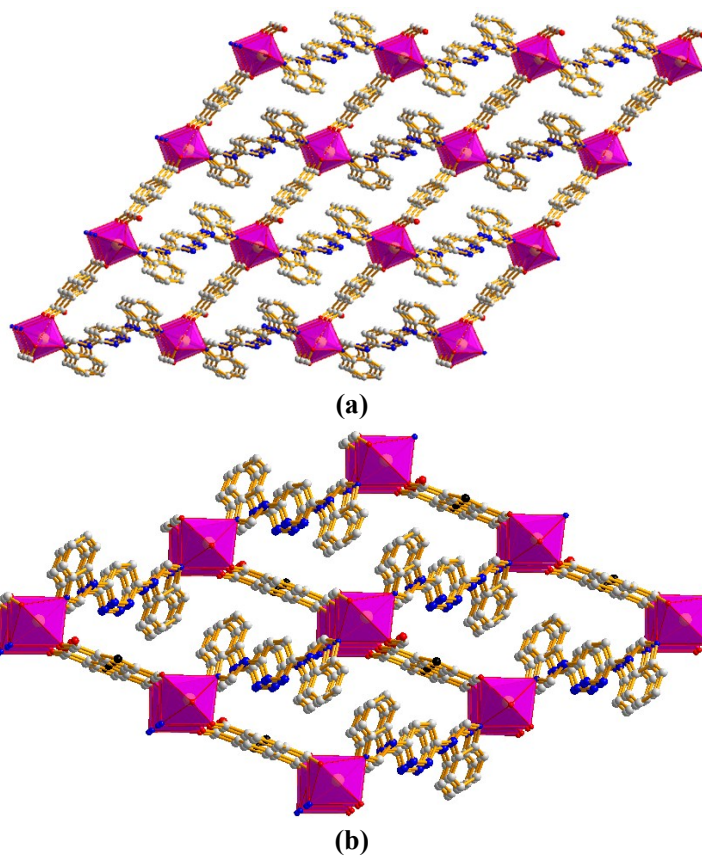
Mn(1)-O(1)	2.152(2)	Mn(1)-O(4)	2.1521(18)
Mn(1)-O(2)	2.1380(19)	Mn(1)-N(1)	2.242(2)
Mn(1)-N(2)	2.263(2)		
O(1)-Mn(1)-O(3) ^{#1}	56.08(7)	N(1)-Mn(1)-O(3) ^{#1}	87.55(8)
O(1)-Mn(1)-N(1)	93.10(8)	C(18) ^{#4} -N(1)-Mn(1)	124.70(17)
O(1)-Mn(1)-N(2)	92.85(8)	N(2)-Mn(1)-O(3) ^{#1}	87.13(8)
O(2)-Mn(1)-O(1)	93.04(7)	C(1)-N(2)-Mn(1)	122.70(19)

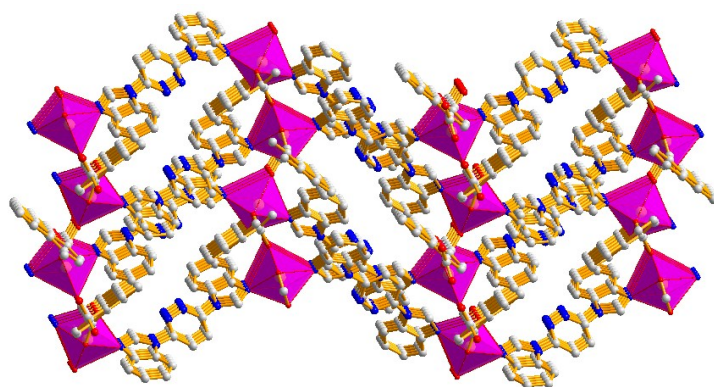
O(2)-Mn(1)-O(3) ^{#1}	148.93(7)	C(19)-O(2)-Mn(1)	145.63(17)
O(2)-Mn(1)-O(4)	97.13(7)	C(30)-O(3)-Mn(1) ^{#2}	83.49(17)
O(2)-Mn(1)-N(1)	91.29(8)	C(19) ^{#3} -O(4)-Mn(1)	132.11(16)
O(2)-Mn(1)-N(2)	98.81(8)	C(12) ^{#4} -N(1)-Mn(1)	128.7(2)
C(7)-N(2)-Mn(1)	130.95(17)	O(4)-Mn(1)-N(1)	88.68(8)
O(4)-Mn(1)-O(3) ^{#1}	113.87(7)	O(4)-Mn(1)-N(2)	83.65(8)

Symmetry codes

for 1, #1 $x+1/2, -y+3/2, z-1/2$ #2 $x-1/2, y+1/2, z-1$ #3 $x-1/2, -y+3/2, z+1/2$
for 2, #1 $1/2+X, 1/2+Y, +Z$ #2 $1-X, 1+Y, 3/2-Z$ #3 $-1/2+X, -1/2+Y, +Z$ #4 $1-X, -1+Y, 3/2-Z$
for 3, #1 $-1/2+X, -Y, 1/2+Z$ #2 $1+X, -1+Y, +Z$ #3 $1/2+X, -Y, -1/2+Z$ #4 $-1+X, 1+Y, +Z$
for 4, #1 $x, -y, z+1/2$ #2 $x-1/2, -y+3/2, z-1/2$ #3 $x, -y, z-1/2$ #4 $x+1/2, -y+3/2, z+1/2$
for 5, #1 $-x+2, -y+1, -z+1$ #2 $x+1, y-1, z$ #3 $x-1, y+1, z$
for 6, #1 $-x+3/2, y-1/2, -z+1/2$ #2 $-x+3/2, y+1/2, -z+1/2$ #3 $-x+1/2, y-1/2, -z+1/2$
#4 $x+1/2, -y+1/2, z+1/2$

Fig. S1.





(c)

Fig. S1. (a) The 3D framework structure of **3**; (b) the 3D framework structure of **4**; (c) the 3D framework structure of **6**.

Fig. S2. PXRD patterns of 1-6.

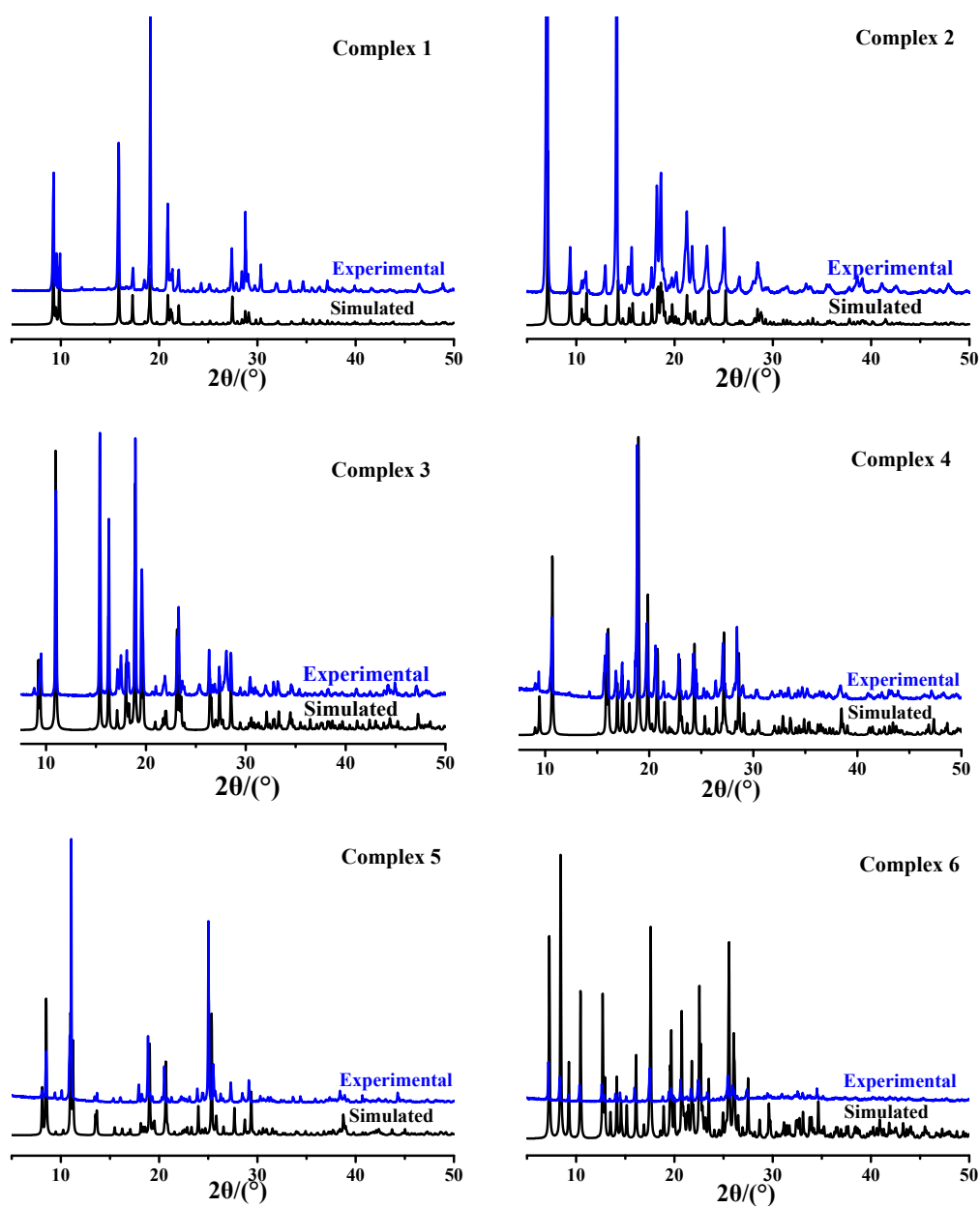


Fig. S3. TG curves for complexes 1-6.

