

## **Supporting Information**

Fig. S1 The PXRD patterns for complexes 1-6. Red line-simulated and black line-experimental.



Fig. S2 The TG curves of complexes 1-6.

Table S1 Selected bond	lengths	(Å) and a	ingles (°)	for complex 1
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Co(1)-O(7)	1.9937(15)	Co(2)-O(10)	2.1251(14)
Co(1)-O(3)#1	2.0652(14)	Co(2)-O(8)#4	2.0238(15)
Co(1)-O(5)#2	2.0569(14)	Co(2)-O(2)#5	2.1204(15)
Co(1)-O(6)#1	2.0098(14)	Co(2)-O(6)	2.1900(15)
Co(1)-O(10)#1	2.1436(13)	Co(2)-O(6)#3	2.0169(14)
Co(2)-O(9)	2.1423(16)	O(6)#3-Co(2)-O(2)#5	110.73(6)
O(6)#1-Co(1)-O(5)#2	99.57(6)	O(7)-Co(1)-O(6)#1	102.62(6)
O(7)-Co(1)-O(3)#1	106.01(6)	O(6)#1-Co(1)-O(3)#1	149.69(6)
O(7)-Co(1)-O(10)#1	91.91(6)	O(6)#1-Co(1)-O(10)#1	81.51(6)
O(3)#1-Co(1)-O(10)#1	87.77(6)	O(6)#3-Co(2)-O(8)#4	95.98(6)
O(8)#4-Co(2)-O(2)#5	93.29(6)	O(6)#3-Co(2)-O(10)	89.65(6)
O(2)#5-Co(2)-O(10)	87.15(6)	O(6)#3-Co(2)-O(9)	161.36(6)
O(2)#5-Co(2)-O(9)	86.07(6)	O(10)-Co(2)-O(9)	82.96(6)
O(8)#4-Co(2)-O(6)	99.94(6)	O(2)#5-Co(2)-O(6)	158.57(6)
O(9)-Co(2)-O(6)	77.00(6)	O(8)#4-Co(2)-O(9)	90.89(6)
O(7)-Co(1)-O(5)#2	102.03(6)	O(6)#3-Co(2)-O(6)	84.73(6)
O(5)#2-Co(1)-O(3)#1	84.10(6)	O(10)-Co(2)-O(6)	77.90(5)
O(5)#2-Co(1)-O(10)#1	165.36(6)	O(8)#4-Co(2)-O(10)	173.79(6)

Symmetry codes: #1: -0.5+*x*, *y*, 0.5-*z*; #2: 1-*x*, 0.5+*y*, 0.5-*z*; #3: 2-*x*, -*y*, 1-*z*; #4: 1.5-*x*, -*y*, 0.5+*z*; #5: 1-*x*, -*y*, 1-*z* 

Mn(1)-O(8)	2.086(2)	Mn(2)-O(5)#3	2.074(2)
Mn(1)-O(4)#1	2.087(2)	Mn(2)-O(8)#4	2.103(2)
Mn(1)-O(6)#2	2.101(2)	Mn(2)-O(3)#5	2.186(2)
Mn(1)-O(1)	2.166(2)	Mn(2)-O(7)	2.232(2)
Mn(1)-O(7)	2.208(2)	Mn(2)-O(9)	2.260(2)
O(8)-Mn(1)-O(4)#1	103.54(9)	Mn(2)-O(8)	2.268(2)
O(8)-Mn(1)-O(6)#2	101.83(9)	O(5)#3-Mn(2)-O(8)#4	95.47(9)
O(4)#1-Mn(1)-O(6)#2	99.67(9)	O(5)#3-Mn(2)-O(3)#5	94.11(9)
O(8)-Mn(1)-O(1)	148.34(9)	O(8)#4-Mn(2)-O(3)#5	113.34(9)
O(4)#1-Mn(1)-O(1)	105.73(9)	O(5)#3-Mn(2)-O(7)	172.95(9)
O(6)#2-Mn(1)-O(1)	84.97(8)	O(8)#4-Mn(2)-O(7)	90.35(8)
O(8)-Mn(1)-O(7)	81.67(8)	O(3)#5-Mn(2)-O(7)	87.20(8)
O(4)#1-Mn(1)-O(7)	92.10(9)	O(5)#3-Mn(2)-O(9)	93.63(10)
O(6)#2-Mn(1)-O(7)	166.46(9)	O(8)#4-Mn(2)-O(9)	158.06(9)
O(1)-Mn(1)-O(7)	85.42(8)	O(3)#5-Mn(2)-O(9)	85.79(9)
O(3)#5-Mn(2)-O(8)	157.29(8)	O(7)-Mn(2)-O(9)	79.55(9)
O(7)-Mn(2)-O(8)	77.25(8)	O(5)#3-Mn(2)-O(8)	99.41(9)
O(9)-Mn(2)-O(8)	75.27(8)	O(8)#4-Mn(2)-O(8)	83.56(9)

Table S2 Selected bond lengths (Å) and angles (°) for complex 2

Symmetry codes: #1: *x*-0.5, *y*, -*z*+1.5; #2: -*x*+1.5, *y*+1, *z*; #3: -*x*+1.5, -*y*, *z*+1.5; #4: -*x*+1, -*y*, -*z*+2; #5: -*x*+2, -*y*, -*z*+2.

Zn(1)-O(2)#4	2.044(2)	Zn(2) -O(8)	1.998(2)
Zn(1) -O(5)	2.0850(19)	Zn(2) -O(9)	2.125(2)
Zn(1)-O(8)#2	1.979(2)	Zn(2)-O(3)#5	2.0082(19)
Zn(2)-O(6)#1	2.1297(19)	Zn(2)-O(8)#2	2.228(2)
Zn(1) -O(1)	2.1583(19)	Zn(2) -O(1)	2.1525(18)
Zn(1)-O(4)#3	1.9748(18)		
O(4)#3-Zn(1)-O(8)#2	105.97(8)	O(4)#3-Zn(1)-O(5)	106.12(8)
O(4)#3-Zn(1)-O(2)#4	103.26(8)	O(8)#2-Zn(1)-O(5)	146.30(8)
O(8)#2-Zn(1)-O(2)#3	99.76(8)	O(2)#3-Zn(1)-O(5)	82.63(8)
O(5)-Zn(1)-O(1)	86.31(8)	O(1)-Zn(1)-Zn(2)	43.48(5)
O(4)#3-Zn(1)-Zn(2)	122.43(6)	O(8)-Zn(2)-O(3)#5	96.56(8)
O(8)#2-Zn(1)-Zn(2)	45.21(6)	O(8)-Zn(2)-O(9)	160.64(8)
O(2)#4-Zn(1)-Zn(2)	126.57(5)	O(3)#5-Zn(2)-O(9)	90.49(8)
O(5)-Zn(1)-Zn(2)	106.96(6)	O(8)-Zn(2)-O(6)#1	111.89(8)
O(6)#1-Zn(2)-O(1)	86.66(7)	O(3)#5-Zn(2)-O(8)#2	102.08(8)
O(8)-Zn(2)-O(8)#2	84.02(9)	O(9)-Zn(2)-O(8)#2	76.87(8)
O(4)#3-Zn(1)-O(1)	94.34(8)	O(8)-Zn(2)-O(1)	89.62(7)
O(8)#2-Zn(1)-O(1)	81.28(8)	O(3)#5-Zn(2)-O(1)	173.34(8)
O(2)#3-Zn(1)-O(1)	161.24(7)	O(9)-Zn(2)-O(1)	82.86(8)
O(3)#5-Zn(2)-O(6)#1	93.32(8)	O(6)#1-Zn(2)-O(8)#2	156.58(7)
O(9)-Zn(2)-O(6)#1	85.56(8)	O(1)-Zn(2)-O(8)#2	76.01(7)

Table S3 Selected bond lengths (Å) and angles (°) for complex  ${\bf 3}$ 

Symmetry codes: #1: 1-x, -y, 2-z; #2: 2-x, -y, 2-z; #3: 0.5+x, y, 1.5-z; #4: 1.5-x, 0.5+y, z; #5: 1.5-x, -y, 0.5+z.

Zn(1)-O(1)	2.064(3)	Zn(2)-O(2)	1.941(3)
Zn(1)-O(9)	2.108(3)	Zn(2)-O(3)#3	1.951(3)
Zn(1)-O(4)#2	2.066(3)	Zn(2)-O(9)	1.960(3)
Zn(1)-O(9)#1	2.077(3)	Zn(2)-O(8)	2.020(3)
Zn(1)-O(10)	2.072(3)	Zn(1)-O(6)#2	2.168(3)
O(1)-Zn(1)-O(4)#2	89.30(13)	O(1)-Zn(1)-O(10)	84.99(12)
O(1)-Zn(1)-O(9)#1	176.08(12)	O(4)#2-Zn(1)-O(9)	168.97(12)
O(4)#2-Zn(1)-O(9)#1	93.19(12)	O(10)-Zn(1)-O(9)	100.89(12)
O(10)-Zn(1)-O(9)#1	98.03(12)	O(9)#1-Zn(1)-O(9)	84.14(12)
O(1)-Zn(1)-O(9)	92.86(12)	O(1)-Zn(1)-O(6)#2	90.85(12)
O(1)-Zn(1)-Zn(1)#1	134.49(9)	O(9)-Zn(1)-Zn(1)#1	41.69(8)
O(4)#2-Zn(1)-Zn(1)#1	134.68(9)	O(6)#2-Zn(1)-Zn(1)#1	78.37(8)
O(10)-Zn(1)-Zn(1)#1	102.80(9)	O(1)-Zn(1)-Zn(2)	67.52(9)
O(9)#1-Zn(1)-Zn(1)#1	42.45(8)	O(4)#2-Zn(1)-Zn(2)	135.17(9)
Zn(1)#1-Zn(1)-Zn(2)	71.14(2)	O(2)-Zn(2)-O(3)#3	124.80(13)
O(3)#3-Zn(2)-O(9)	107.47(13)	O(9)-Zn(2)-O(8)	100.79(13)
O(2)-Zn(2)-O(8)	101.74(14)	O(2)-Zn(2)-Zn(1)	83.92(9)
O(3)#3-Zn(2)-O(8)	98.63(13)	O(3)#3-Zn(2)-Zn(1)	116.14(9)
O(4)#2-Zn(1)-O(10)	90.07(12)	O(10)-Zn(1)-Zn(2)	123.32(9)
O(4)#2-Zn(1)-O(6)#2	92.39(12)	O(9)#1-Zn(1)-Zn(2)	108.64(8)
O(10)-Zn(1)-O(6)#2	175.14(12)	O(9)-Zn(1)-Zn(2)	37.69(8)
O(9)#1-Zn(1)-O(6)#2	86.03(11)	O(6)#2-Zn(1)-Zn(2)	52.41(8)
O(9)-Zn(1)-O(6)#2	76.78(11)	O(2)-Zn(2)-O(9)	117.99(13)
O(8)-Zn(2)-Zn(1)	133.21(9)	O(9)-Zn(2)-Zn(1)	41.11(8)

Table S4 Selected bond lengths (Å) and angles (°) for complex 4

Symmetry codes: #1: -*x*, -*y*, 1-*z*; #2: -0.5+*x*, *y*, 0.5-*z*; #3: -*x*, -0.5+*y*, 0.5-*z*.

Zn(1)-N(1)	2.002(2)	Zn(3)-O(12)#2	1.957(2)
Zn(1)-O(8)	1.9136(18)	Zn(3)-O(14)	1.956(2)
Zn(1)-O(16)	1.941(2)	Zn(3)-O(10)	1.943(2)
Zn(1)-O(2)#1	1.934(2)	Zn(3)-N(3)#3	2.038(2)
Zn(2)-O(10)	2.2000(19)	Zn(4)-O(8)	2.1764(19)
Zn(2)-O(17)	2.1145(19)	Zn(4)-O(6)	2.016(2)
Zn(2)-N(4)	2.129(2)	Zn(4)-O(10)	2.073(2)
Zn(2)-O(9)	2.1250(19)	Zn(4)-N(2)#3	2.111(2)
Zn(2)-O(11)#2	2.062(2)	Zn(4)-O(1)#2	2.021(2)
Zn(2)-O(8)	2.064(2)	N(4)-Zn(2)-O(10)	176.38(9)
O(8)-Zn(1)-O(2)#1	108.90(9)	O(8)-Zn(1)-O(16)	110.70(9)
O(11)#2-Zn(2)-O(17)	84.66(8)	O(2)#2-Zn(1)-O(16)	103.58(10)
O(8)-Zn(2)-O(17)	90.00(8)	O(8)-Zn(1)-N(1)	118.89(9)
O(11)#2-Zn(2)-O(9)	87.79(8)	O(8)-Zn(2)-N(4)	98.21(9)
O(8)-Zn(2)-O(9)	96.92(8)	O(17)-Zn(2)-N(4)	91.52(9)
O(17)-Zn(2)-O(9)	171.92(9)	O(9)-Zn(2)-N(4)	91.61(9)
O(11)#2-Zn(2)-N(4)	91.97(9)	O(11)#2-Zn(2)-O(10)	91.35(8)
O(10)-Zn(3)-O(14)	116.66(9)	O(14)-Zn(3)-N(3)#3	101.81(9)
O(10)-Zn(3)-O(12)#2	104.26(9)	O(12)#2-Zn(3)-N(3)#3	99.20(10)
O(14)-Zn(3)-O(12)#2	115.36(10)	O(6)-Zn(4)-O(1)#1	101.59(9)
O(10)-Zn(3)-N(3)#3	118.71(10)	O(6)-Zn(4)-O(10)	111.25(8)
O(6)-Zn(4)-O(8)	87.78(8)	O(1)#1-Zn(4)-O(8)	96.18(8)
N(2)#3-Zn(4)-O(8)	171.89(9)	O(2)#1-Zn(1)-N(1)	108.82(9)
O(1)#1-Zn(4)-O(10)	146.47(9)	O(16)-Zn(1)-N(1)	104.84(10)
O(6)-Zn(4)-N(2)#3	94.73(9)	O(11)#2-Zn(2)-O(8)	168.63(8)
O(1)#4-Zn(4)-N(2)#3	90.88(9)	O(8)-Zn(2)-O(10)	78.61(7)
O(10)-Zn(4)-N(2)#3	92.93(9)	O(17)-Zn(2)-O(10)	90.22(8)
O(10)-Zn(4)-O(8)	78.97(7)	O(9)-Zn(2)-O(10)	87.08(8)

Table S5 Selected bond lengths (Å) and angles (°) for complex  ${\bf 5}$ 

Symmetry codes: #1: *x*, 0.5–*y*, 0.5+*z*; #2 :*x*, 1.5–*y*, –0.5+*z*; #3: 1+*x*, *y*, *z*.

Cd(1)-O(8)	2.219(2)	Cd(2)-O(7)#1	2.276(2)
Cd(1)-O(1)	2.379(2)	Cd(2)-O(8)#2	2.254(2)
Cd(1)-O(6)#1	2.289(2)	Cd(2)-O(5)#2	2.379(2)
Cd(1)-N(3)	2.317(3)	Cd(2)-O(8)	2.318(2)
Cd(1)-O(3)	2.328(2	Cd(2)-O(1)	2.319(2)
Cd(1)-N(1)	2.331(3)	Cd(2)-N(2)#3	2.310(3)
O(8)-Cd(1)-N(1)	160.17(10)	O(8)-Cd(1)-O(1)	76.75(8)
O(6)#1-Cd(1)-N(1)	89.85(10)	O(6)#1-Cd(1)-O(1)	96.37(9)
N(3)-Cd(1)-N(1)	95.85(12)	N(3)-Cd(1)-O(1)	173.41(10)
O(3)-Cd(1)-N(1)	88.38(9)	O(3)-Cd(1)-O(1)	87.29(8)
O(3)-Cd(1)-Cd(2)	108.00(6)	O(8)#2-Cd(2)-O(7)#1	169.84(9)
N(1)-Cd(1)-Cd(2)	120.02(8)	O(8)#2-Cd(2)-N(2)#3	99.35(10)
O(1)-Cd(1)-Cd(2)	42.48(5)	O(7)#1-Cd(2)-N(2)#3	85.18(10)
O(8)#2-Cd(2)-O(1)	96.43(8)	N(2)#3-Cd(2)-O(1)	106.34(10)
O(7)#1-Cd(2)-O(1)	90.94(9)	O(8)-Cd(2)-O(1)	76.06(8)
N(2)#3-Cd(2)-O(5)#2	92.95(10)	O(8)-Cd(2)-O(5)#2	84.24(9)
O(8)-Cd(1)-N(3)	103.86(11)	O(8)#2-Cd(2)-O(8)	82.89(9)
O(6)#1-Cd(1)-N(3)	90.18(10)	O(7)#1-Cd(2)-O(8)	92.17(8)
O(8)-Cd(1)-O(6)#1	92.21(9)	N(2)#3-Cd(2)-O(8)	176.42(9)
N(3)-Cd(1)-O(3)	86.14(10)	O(8)#2-Cd(2)-O(5)#2	90.21(8)
O(8)-Cd(1)-O(3)	90.77(8)	O(7)#1-Cd(2)-O(5)#2	80.44(9)
O(6)#1-Cd(1)-O(3)	175.73(9)	O(1)-Cd(2)-O(5)#2	158.20(9)
N(1)-Cd(1)-O(1)	83.42(10)	O(6)#1-Cd(1)-Cd(2)	76.24(6)
O(8)-Cd(1)-Cd(2)	42.03(6)	N(3)-Cd(1)-Cd(2)	141.03(9)

## Table S6 Selected bond lengths $({\rm \AA})$ and angles (°) for complex 6

Symmetry codes:#1:0.5+*x*, 0.5-*y*, 0.5+*z*; #2: 1-*x*, -*y*, 1-*z*; #3: 1.5-*x*, -0.5+*y*, 0.5-*z*.