Electronic Supplementary Material (ESI) for CrystEngComm.

Support Information

Crystal Structure, Magnetism, and Dielectric Properties Based on Axial chirality Ligand 2, 2′-Dinitro-4, 4′-Biphenyldicarboxylic Acid

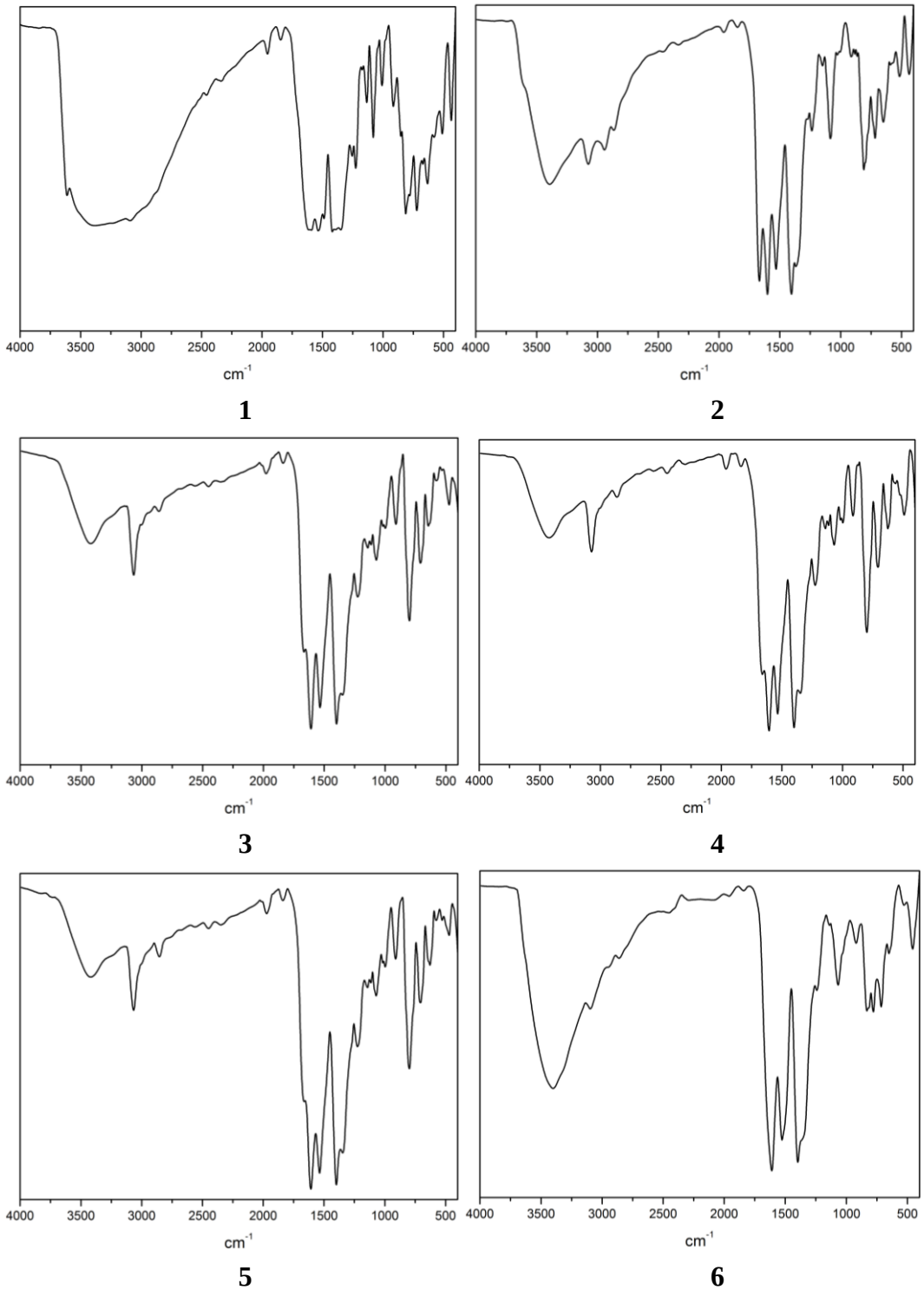


Figure S1: The measurement of IR of complexes **1-6**.

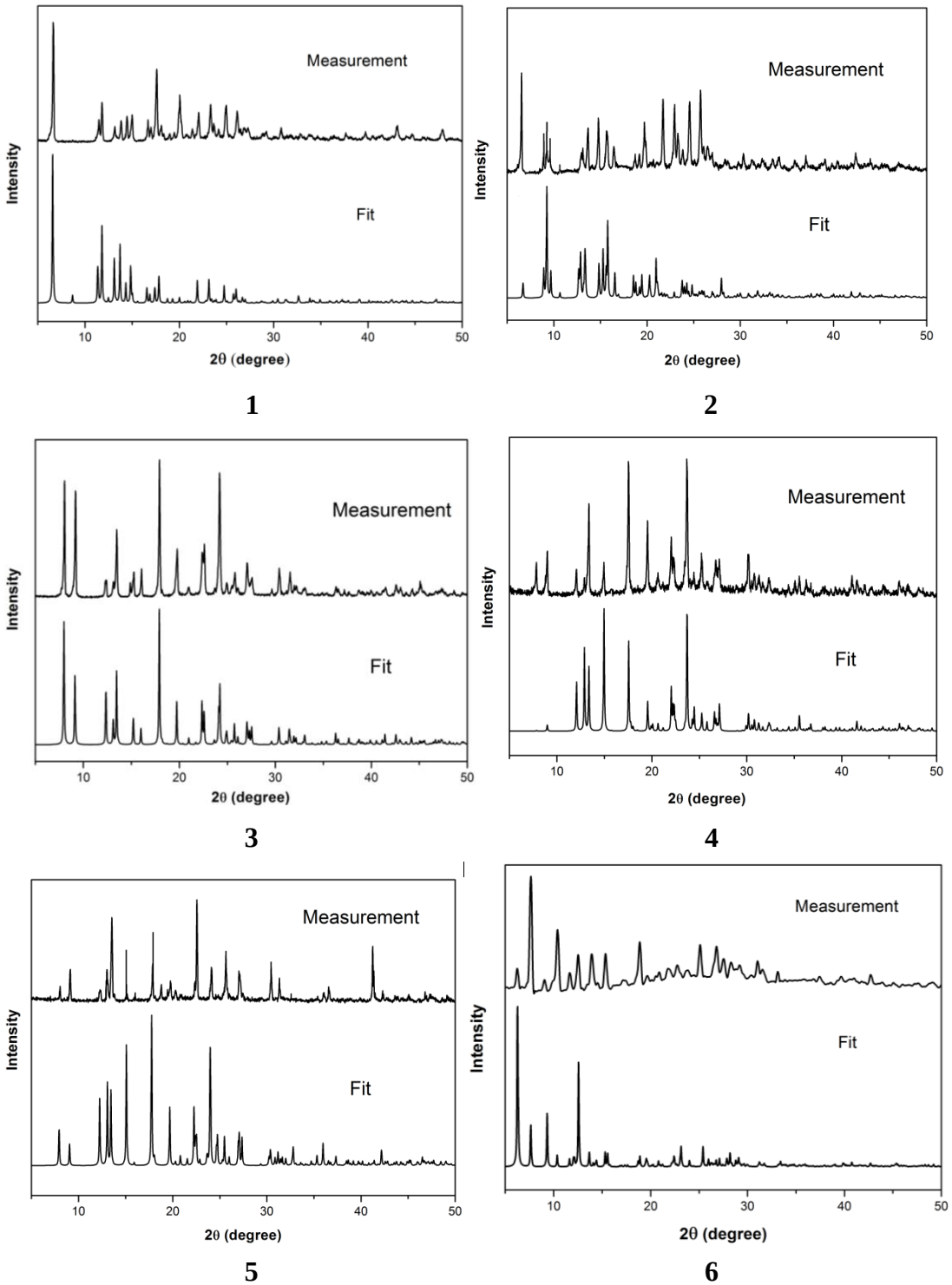


Figure S2: XRPD pattern of compounds **1**-**6**, where the lower line is the simulated pattern.

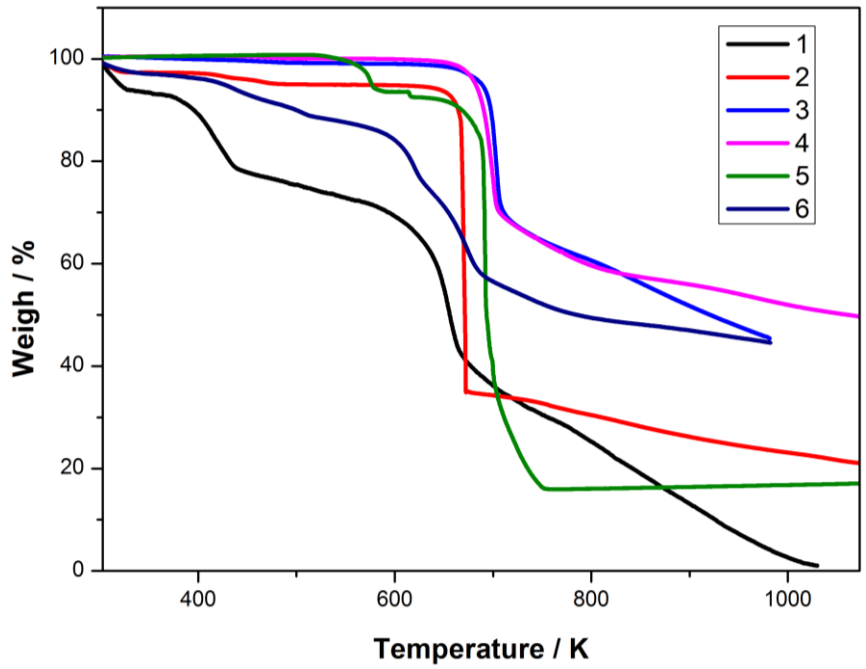


Figure S3: The thermal gravimetric (TG) stability of complexes of **1**–**6**.

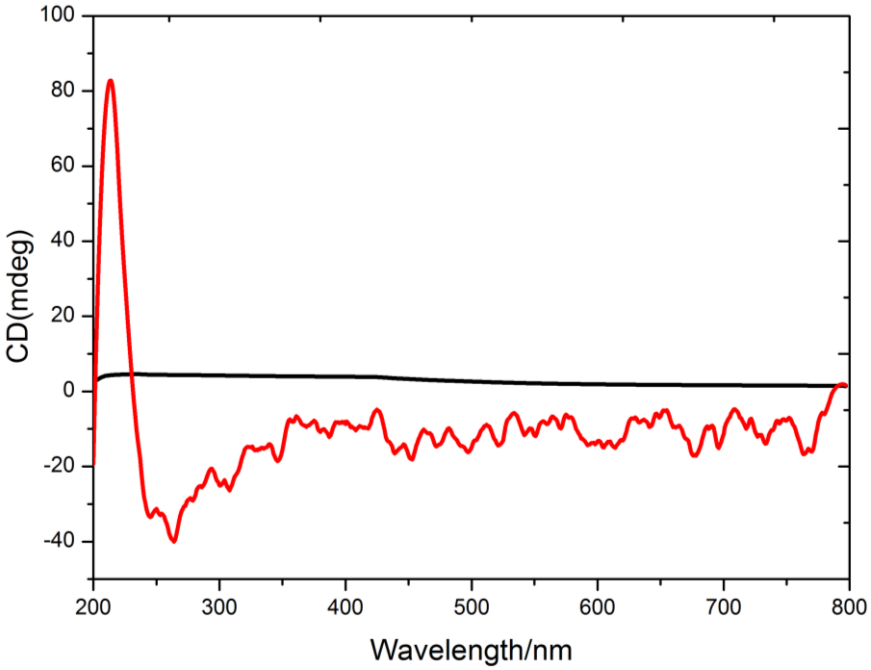


Figure S4: Circular Dichroism (CD) of ligand by using KBr pellets at room temperature

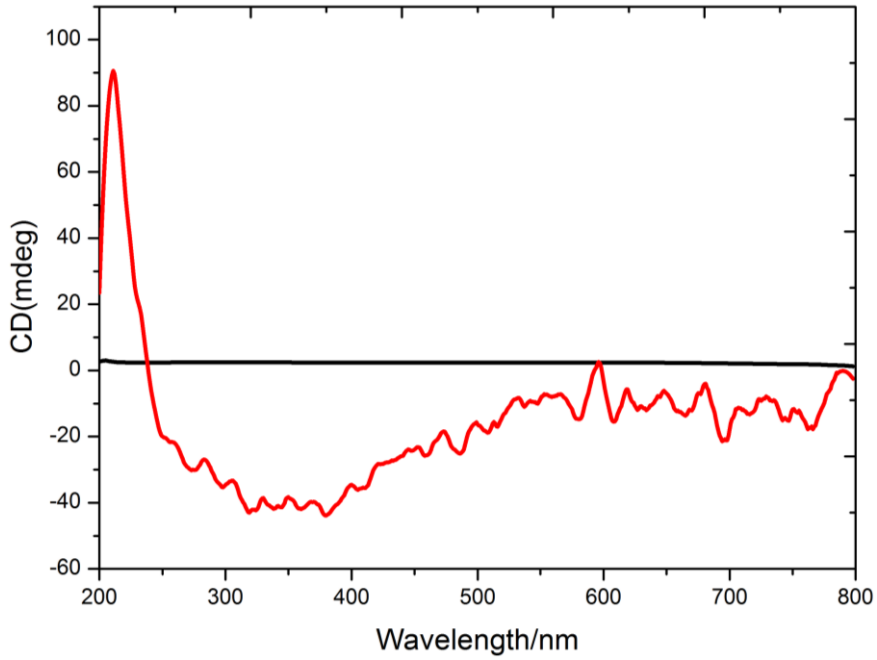
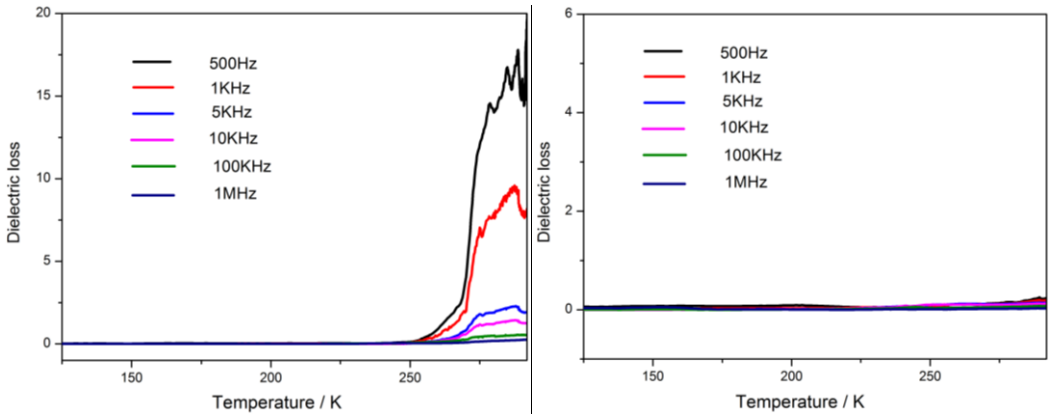
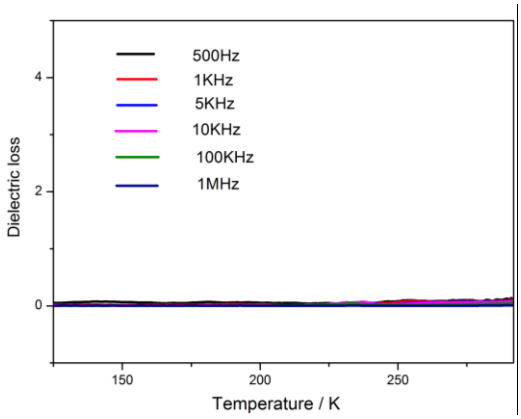


Figure S5: Circular Dichroism (CD) of complex **1** by using KBr pellets at room temperature

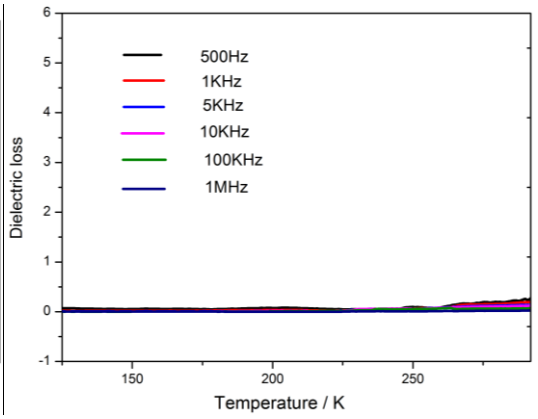


(a)

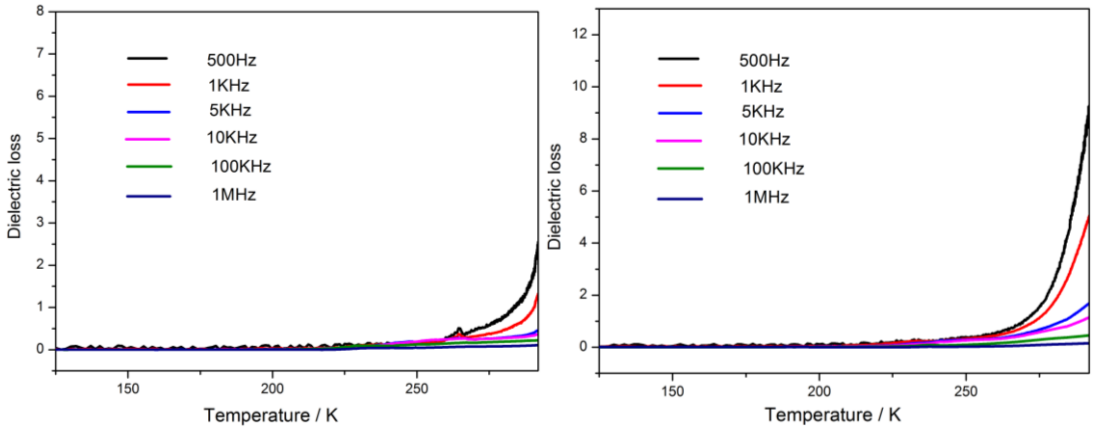
(b)



(c)



(d)



(e) (f)

Figure S6: Dielectric loss of complexes **1-6** as a function of temperature at several frequencies, measured based on pellets from their powdered samples from 125 K to 292 K.

Table S1: Selected Bond Lengths (Å) and Bond Angles (°) of **1**

Ni(1)−O(1)	2.116(3)	Ni(1)− N(1)	2.055(5)	Ni(1)− O (3)	2.021(3)
Ni(1)−N(2)	2.075(5)	Ni (1)−O(2)	2.142(4)	Ni(1)−O(9)	2.116(4)
O(3)−Ni(1)− N(1)	96.68(17)	O(3)−Ni(1)−N(2)	88.09(16)	N(2)−Ni(1)−N(1)	92.64(18)
O(3)−Ni(1)−O(1)	163.32(16)	N(1)−Ni(1)−O(1)	99.89(17)	O(1)−Ni(1)−N(2)	89.18(17)
O(3)−Ni(1)−O(9)	90.38(14)	N(1)−Ni(1)−O(9)	89.31(18)	N(2)−Ni(1)−O(9)	177.64(18)
O(3)−Ni(1)−O(2)	101.08(15)	O(9)−Ni(1)−O(2)	89.28(16)	N(1)−Ni(1)−O(2)	162.20(16)
N(2)−Ni(1)−O(2)	89.26(17)	O(1)−Ni(1)−O(9)	91.78(15)	O(1)−Ni(1)−O(2)	62.42(15)

Table S2: Selected Bond Lengths (Å) and Bond Angles (°) of **2**

Ni(1)−O(1)	2.033(5)	Ni(2)−O(8)	2.022(6)	Ni(2)−N(5)	2.085(8)
Ni(1)−O(13)	2.071(5)	Ni (2)−O(9)	2.140(5)	Ni(2)−O(7)$^{\#1}$	2.004(5)
Ni(1)−N(1)	2.113(6)	Ni (2)−O(10)	2.142(5)	Ni(2)−N(6)$^{\#2}$	2.072(8)
O(1)−Ni(1)−O(13)	91.54(18)	O(1)−Ni(1)−N(1)	91.0(2)	O(13)−Ni(1)−N(1)	92.1(2)
O(8)−Ni(2)−O(9)	93.7(2)	O(8)−Ni(2)−O(10)	155.5(2)	O(8)−Ni(2)−N(5)	86.0(3)
O(10)−Ni(2)−N(5)	91.5(2)	O(9)−Ni(2)−O(10)	61.9(2)	O(9)−Ni(2)−N(5)	88.9(3)
O(7)−Ni(2)−N(6)$^{\#2}$	94.6(3)	O(8)−Ni(2)−O(7)$^{\#1}$	108.4(2)	O(8)−Ni(2)−N(6)$^{\#2}$	92.2(3)
O(9)−Ni(2)−O(7)$^{\#1}$	157.7(2)	O(9)−Ni(2)−N(6)$^{\#2}$	87.7(3)	O(10)−Ni(2)−O(7)$^{\#1}$	96.0(2)
O(10)−Ni(2)−N(5)	91.5(2)	O(7)−Ni(2)−N(5)$^{\#1}$	89.2(3)	N(5)−Ni(2)−N(6)$^{\#2}$	176.1(3)

Symmetry transformation: #1 2-x,2-y,2-z； #2 x,2-y,1/2+z

Table S3: Selected Bond Lengths (Å) and Bond Angles (°) of **3-5**

Ni(1)−O(0AA)	2.061(4)	Ni(1)−O(1AA)	2.070(4)	Ni(1)−N(2)	2.091(4)
Mn(1)−O(1)	2.127(2)	Mn(1)−O(2)$^{\#1}$	2.158(2)	Mn(1)−N(2)	2.282(3)
Co(1)−O(1)	2.090(3)	Co(1)−O(2)	2.077(2)	Co(1)−N(3)	2.154(3)
O(0AA)−Ni(1)−O(1AA)	88.62(16)	O(0AA)−Ni(1)−N(2)	84.99(16)	O(0AA)−Ni(1)− O(0AA)$^{\#1}$	174.27(16)
O(0AA)−Ni(1)−O(1AA)$^{\#1}$	95.60(16)	O(0AA)−Ni(1)−N(2)$^{\#1}$	91.06(16)	O(1AA)−Ni(1)−N(2)	90.93(16)
O(1AA)−Ni(1)−O(1AA)$^{\#1}$	85.24(16)	O(1AA)−Ni(1)−N(2)$^{\#1}$	176.11(16)	N(2)−Ni(1)−N(2)$^{\#1}$	92.91(16)

O(1)−Mn(1)−O(2)	99.93(9)	O(1)−Mn(1)−N(2)	90.19(10)	O(1)−Mn(1)−O(1)$^{\#1}$	89.15(14)
O(1)−Mn(1)−O(2)$^{\#1}$	89.48(9)	O(1)−Mn(1)−N(2)$^{\#1}$	176.68(10)	O(2)−Mn(1)−N(2)$^{\#1}$	83.31(9)
O(2)−Mn(1)−O(2)$^{\#1}$	166.83(13)	O(2)−Mn(1)−N(2)	87.43(9)	N(2)−Mn(1)−N(2)$^{\#1}$	90.64(10)
O(1)−Co(1)−O(2)	96.32(10)	O(1)−Co(1)−N(3)	90.88(10)	O(1)−Co(1)−O(1)$^{\#2}$	86.11(10)
O(1)−Co(1)−O(2)$^{\#2}$	89.23(10)	O(1)−Co(1)−N(3)$^{\#2}$	176.78(11)	O(2)−Co(1)−N(3)	89.97(10)
O(2)−Co(1)−O(2)$^{\#2}$	172.41(11)	O(2)−Co(1)−N(3)$^{\#2}$	84.76(10)	N(3)−Co(1)−N(3)$^{\#2}$	92.15(11)

Symmetry transformation: #1 1-x, y, 1/2-z ;#2 -x, y, 5/2-z

Table S4: Selected Bond Lengths (Å) and Bond Angles (°) of **6**

Zn(1)−O(13)	1.935(5)	Zn(1)−N(2)	2.117(17)	Zn(2)−N(1)	2.09(3)
Zn(1)−O(12)	1.943(5)	Zn(2)−O(13)$^{\#1}$	2.053(5)	Zn(2)−O(1)	2.162(6)
Zn(1)−O(2)	1.976(5)	Zn(2)−O(5)	2.058(5)	Zn(2)−O(11)	2.132(5)
O(2)−Zn(1)−O(12)	120.0(3)	O(2)−Zn(1)−O(13)	101.4(2)	O(2)−Zn(1)−N(2)	103.2(11)
O(12)−Zn(1)−O(13)	115.3(2)	O(12)−Zn(1)−N(2)	105.9(10)	O(13)−Zn(1)−N(2)	110.3(12)
O(1)−Zn(2)−O(5)	87.6(2)	O(1)−Zn(2)−O(11)	87.6(2)	O(1)−Zn(2)−O(13)	86.3(3)
O(1)−Zn(2)−N(1)	87.0(6)	O(5)−Zn(2)−O(11)	172.4(2)	O(5)−Zn(2)−O(13)	93.5(2)
O(5)−Zn(2)−N(1)	91.1(8)	O(11)−Zn(2)−O(13)$^{\#1}$	92.1(2)	O(11)−Zn(2)−N(1)$^{\#1}$	82.8(8)

Symmetry transformation: #11/2-x,1/2-y,-z