Supporting information of

Syntheses, crystal structures and properties of three cyano-bridged one-dimensional

coordination polymers based on macrocyclic metallic tectons

Xiang Jiang[&], Bo Tao[&], Xiaoli Yu, Yunhong Wang*, Hua Xia*

Faculty of Material Science and Chemistry, China University of Geosciences, Wuhan, 430074,

China

[&] *Both authors contributed equally to this work.*

Table S1: Selected bond lengths (Å) and angles (°) for the complexes **1-3**.

Complex **1**		Complex **2**		Complex **3**	
Ni1-N1	2.15(3)	Ni1-N2	2.105(3)	Ni2-N4	2.157(4)
Ni1-N3	2.00(4)	Ni1-N4	2.080(3)	Ni2-N8	2.120(4)
Ni1-N4	2.17(3)	Ni1-N5	2.065(4)	Ni2-N9	2.047(3)
Ni1-N6	2.15(2)	Ni1-N6	2.120(4)	Ni3-N2	2.135(3)
Ni1-N7	2.16(3)	Ni1-N7	2.137(4)	Ni3-N5	2.046(4)
Ni1-N9[a]	2.109(12)	Ni1-N10[b]	2.094(3)	Ni3-N6	2.132(4)
Ni2-C13	1.853(9)	Ni2-C1	1.881(4)	Ni2-C1	1.854(5)
Ni2-C14	1.848(9)	Ni2-C2	1.857(3)	Ni2-C2	1.867(5)
Ni2-C15	1.850(7)	Ni2-C3	1.868(4)	Ni2-C3	1.878(5)
Ni2-C16	1.874(15)	Ni2-C4	1.863(3)	Ni2-C4	1.862(5)
N1-Ni1-N3	95.3(15)	N2-Ni1-N4	89.34(12)	N4-Ni2-N8	90.95(14)
N1-Ni1-N4	170.4(11)	N2-Ni1-N5	88.94(12)	N4-Ni2-N9	91.89(13)
N1-Ni1-N6	85.0(10)	N2-Ni1-N6	90.53(12)	N4-Ni2-N8[c]	89.05(14)
N1-Ni1-N7	105.3(10)	N2-Ni1-N7	91.08(11)	N4-Ni2-N9[c]	88.11(13)
N1-Ni1-N9[a]	92.1(8)	N2-Ni1-N10[b]	177.19(11)	N8-Ni2-N9	85.61(14)
N3-Ni1-N4	91.1(15)	N4-Ni1-N5	85.97(14)	N4[c]-Ni2-N8	89.05(14)
N3-Ni1-N6	176.7(13)	N4-Ni1-N6	178.58(15)	N8-Ni2-N9[c]	94.39(14)
N3-Ni1-N7	89.9(13)	N4-Ni1-N7	93.28(15)	N4[c]-Ni2-N9	88.11(13)
N3-Ni1-N9[a]	95.2(11)	N4-Ni1-N10[b]	88.90(12)	N8[c]-Ni2-N9	94.39(14)
N4-Ni1-N6	89.0(9)	N5-Ni1-N6	92.62(14)	N4[c]-Ni2-N8[c]	90.95(14)
N4-Ni1-N7	81.8(10)	N5-Ni1-N7	179.24(14)	N4[c]-Ni2-N9[c]	91.89(13)
N4-Ni1-N9[a]	80.2(7)	N5-Ni1-N10[b]	88.76(12)	N8[c]-Ni2-N9[c]	85.61(14)
N6-Ni1-N7	86.9(10)	N6-Ni1-N7	88.14(15)	N2-Ni3-N5	87.65(14)
N6-Ni1-N9[a]	88.1(7)	N6-Ni1-N10[b]	91.18(12)	N2-Ni3-N6	89.77(13)
N7-Ni1-N9[a]	161.4(10)	N7-Ni1-N10[b]	91.20(11)	N2-Ni3-N5[d]	92.35(14)
C13-Ni2-C14	89.8(4)	C1-Ni2-C2	89.98(15)	N2-Ni3-N6[d]	90.23(13)
C13-Ni2-C15	168.2(4)	C1-Ni2-C3	177.41(16)	N5-Ni3-N6	86.41(14)
C13-Ni2-C16	91.2(5)	C1-Ni2-C4	91.91(15)	N2[d]-Ni3-N5	92.35(14)
C14-Ni2-C15	90.4(4)	C2-Ni2-C3	88.38(15)	N5-Ni3-N6[d]	93.59(14)
C14-Ni2-C16	178.4(5)	C2-Ni2-C4	177.71(16)	N2[d]-Ni3-N6	90.23(13)
C15-Ni2-C16	88.9(5)	C3-Ni2-C4	89.78(15)	N5[d]-Ni3-N6	93.59(14)
				N2[d]-Ni3-N5[d]	87.65(14)
				N2[d]-Ni3-N6[d]	89.77(13)
				N5[d]-Ni3-N6[d]	86.41(14)
				C1-Ni2-C2	86.9(2)
				C1-Ni2-C3	174.7(2)
				C1-Ni2-C4	87.6(2)
				C2-Ni2-C3	93.4(2)
				C2-Ni2-C4	174.3(2)
				C3-Ni2-C4	92.3(2)

Symmetry code a: 2/3-x+y,1/3+y,-1/6+z; b: 1/2+x,3/2-y,1/2+z; c: 1-x,2-y,1-z; d: -1-x,1-y,-z
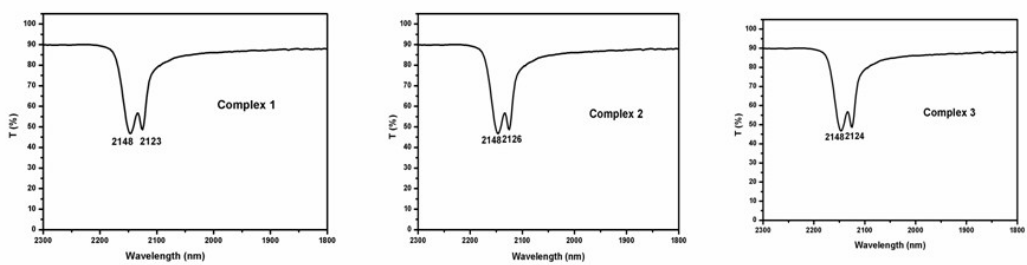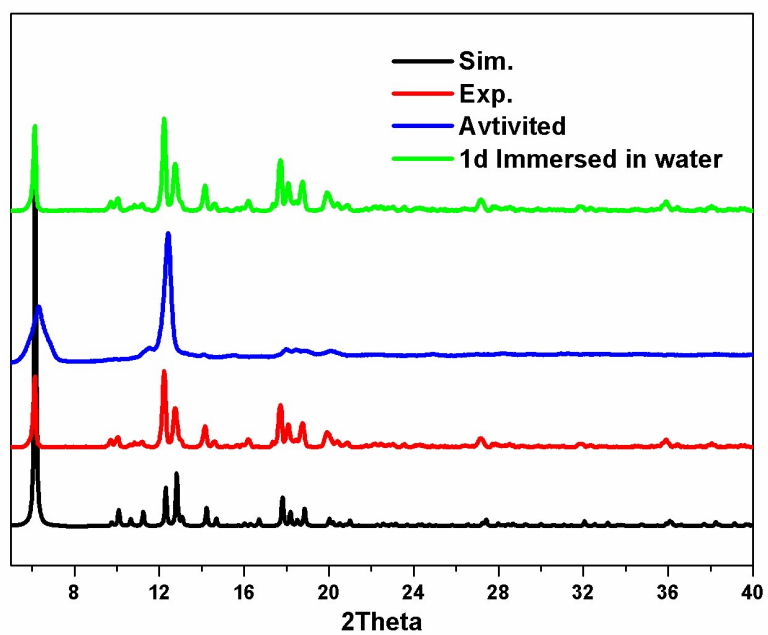
Figure S1: The split IR of -CN in complexes **1-3**;

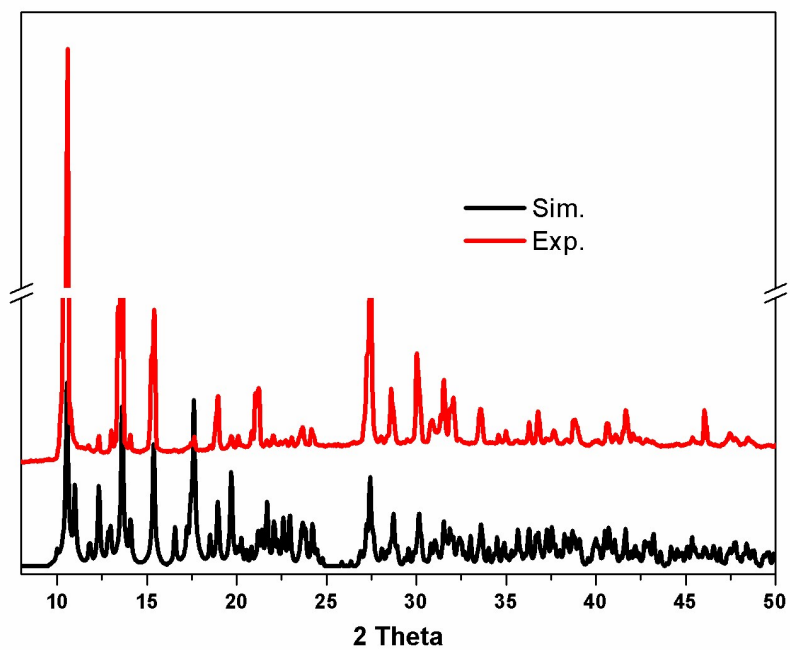Figure S2: XRD of complex **1** (simulated, experimental, desolvated and restoration)

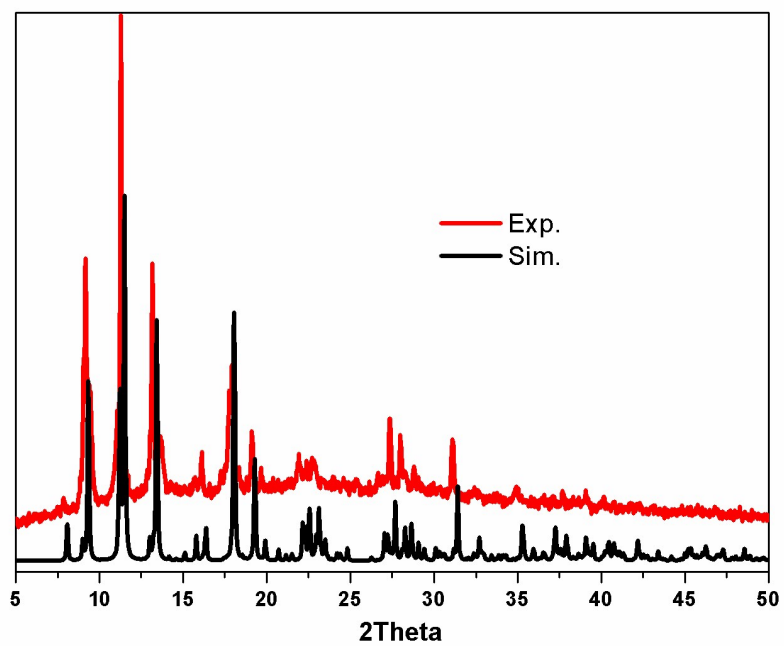Figure S3: XRD of complex **2** (simulated, experimental)

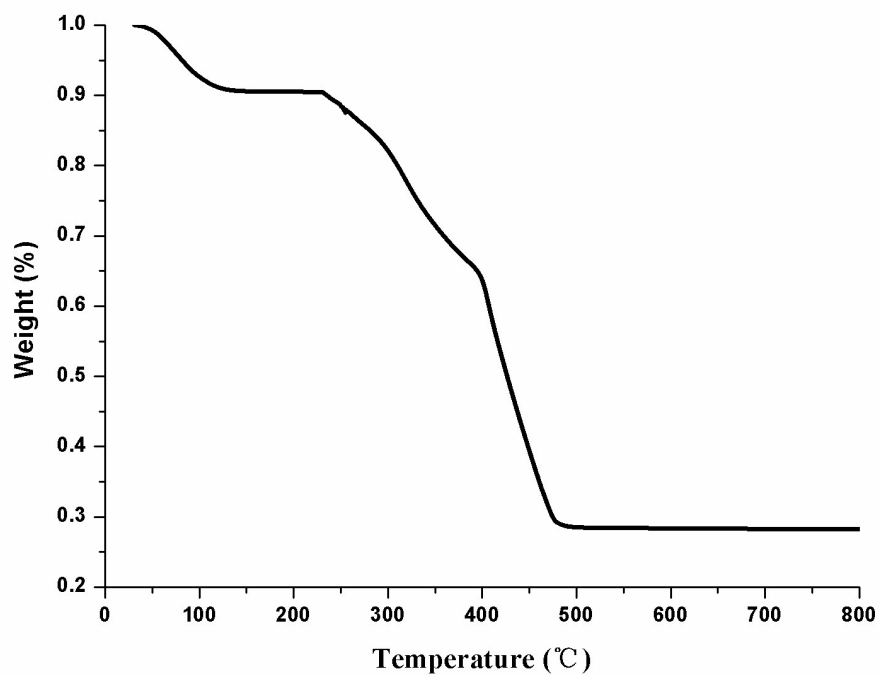Figure S4: XRD of complex **3** (simulated, experimental)
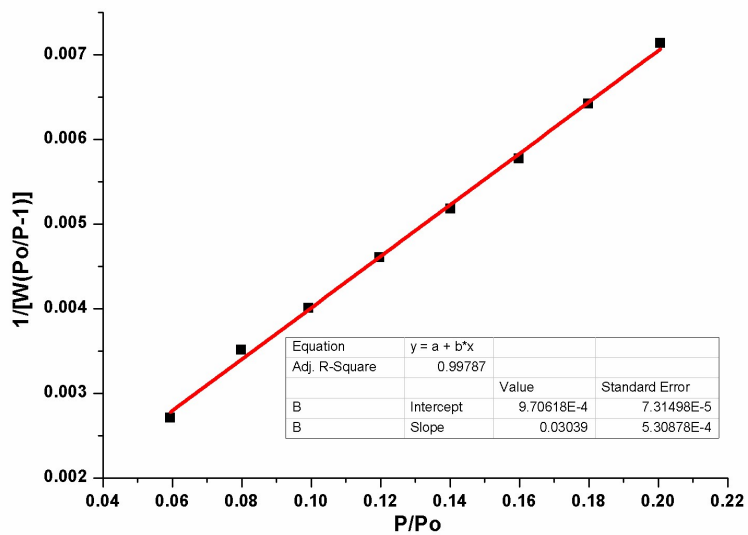
Figure S5: TGA of complex **1**;

Equation	y = a + b*x		
Adj. R-Square	0.99787		
		Value	Standard Error
B	Intercept	9.70618E-4	7.31498E-5
B	Slope	0.03039	5.30878E-4

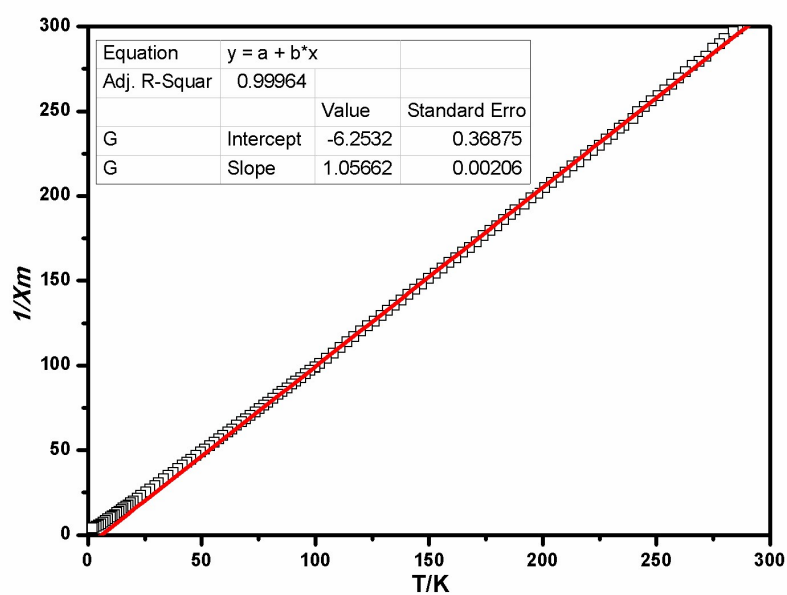Figure S6: BET plot for **1d**.

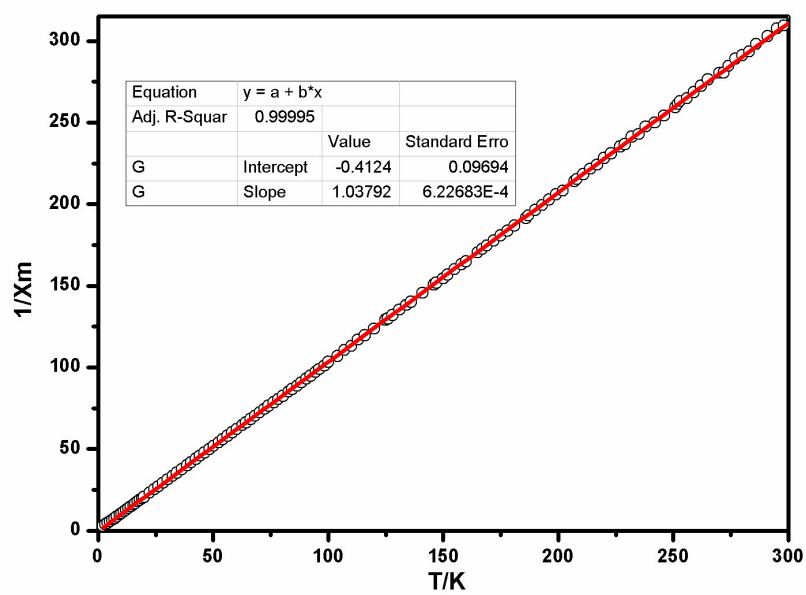Figure S7: The fitting to the Curie-Weiss law of complex **1**;

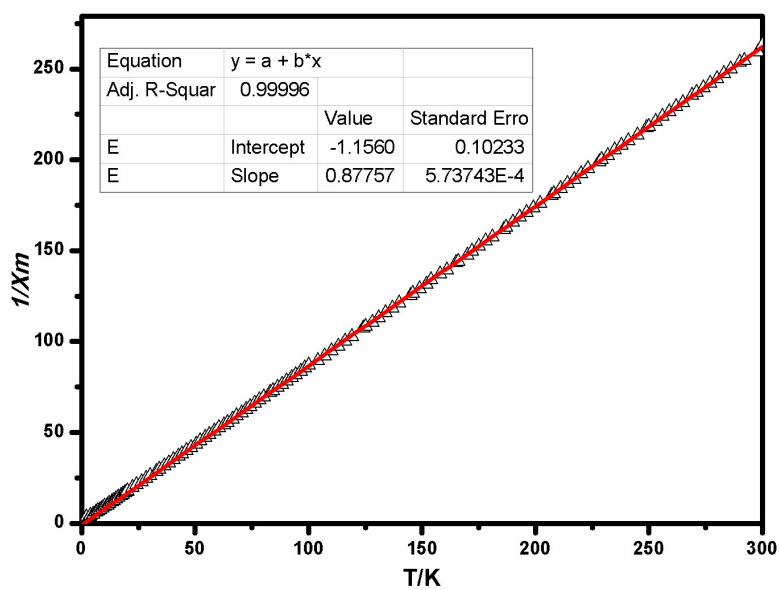Figure S8: The fitting to the Curie-Weiss law of complex **2**;

Figure S9: The fitting to the Curie-Weiss law of complex **3**;