

Syntheses, characterizations, and properties of five coordination compounds based on ligand tetrakis (4-pyridyloxymethylene)methane

Zemin Ju, Dapeng Cao, Ling Qin, Chuanlei Zhang, Mingdao Zhang, Zhiqiang Shi and Hegen Zheng*

*Fax: 86-25-83314502. E-mail: zhenghg@nju.edu.cn.

State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing National Laboratory of Microstructures, Nanjing University, Nanjing 210093, P. R. China

Table S1. Selected bond lengths (Å) and angles (deg) for compounds **1-5**.

Compound 1			
Cu1 – O2	1.943(4)	Cu1 – O2	2.709(5)
Cu1 – N1	2.014(4)	Cu1 – O2_e	1.943(4)
O2 – Cu1 – O2_e	180.00(1)	O2_e – Cu1 – N1_e	89.59(18)
O2 – Cu1 – N1_e	90.41(18)	O2 – Cu1 – N1	89.59(18)
O2_e – Cu1 – N1	90.41(18)	N1 – Cu1 – N1_e	180.00
Symmetry code: e = 1 - x, 1 - y, -z.			
Compound 2			
Zn1 – O2	1.993(4)	Zn1 – O4	2.030(3)
Zn1 – N1	2.057(3)	Zn1 – N2	2.062(3)
O2- Zn1 -O4	142.97(15)	O2- Zn1- N1	103.24(16)
O4- Zn1- N1	100.02(13)	O2- Zn1- N2	104.22(15)
O4 -Zn1- N2	101.01(13)	N1 -Zn1- N2	97.11(13)
C10- N2- Zn1	120.7(3)	C6 -N2 -Zn1	123.7(3)
C14- O2- Zn1	104.9(3)	C18- O4- Zn1	98.3(3)
C1- N1- Zn1	121.0(3)	C5- N1- Zn1	123.0(3)
Compound 3			
Cd1-O4	2.317(4)	Cd1 – O7	2.272(3)
Cd1 – N1	2.321(4)	Cd1 – O4_b	2.317(4)
Cd1 –O7_b	2.272(3)	Cd1 – N1_b	2.321(4)
Cd2-O2	2.269(2)	Cd2-O3	2.279(4)

Cd2-N2	2.361(4)	Cd2-O2_c	2.269(2)
Cd2-O3_c	2.279(4)	Cd2-N2_c	2.361(4)
O4-Cd1-O7	87.23(12)	O4-Cd1-N1	87.67(13)
O4-Cd1-O4_b	97.59(13)	O4-Cd1-O7_b	86.94(12)
O4-Cd1-N1_b	174.69(13)	O7-Cd1-N1	92.54(12)
O4_b-Cd1-O7	86.94(12)	O7-Cd1-O7_b	171.15(14)
O7-Cd1-N1_b	93.88(12)	O4_b-Cd1-N1	174.69(13)
O7_b-Cd1-N1	93.88(12)	N1-Cd1-N1_b	87.09(13)
O4_b-Cd1-O7_b	87.23(12)	O4_b-Cd1-N1_b	87.67(13)
O7_b-Cd1-N1_b	92.54(12)	O2-Cd2-O3	89.83(12)
O2-Cd2-N2	90.91(11)	O2-Cd2-O2_c	180.00
O2-Cd2-O3_c	90.17(12)	O2-Cd2-N2_c	89.10(11)
O3-Cd2-N2	94.92(13)	O2_c-Cd2- -O3	90.17(12)
O3-Cd2- -O3_c	180.00	O3-Cd2- -N2_c	85.08(13)
O2_c-Cd2- N2	89.10(11)	O3_c-Cd2- N2	85.08(13)
N2-Cd2- N2_c	180.00	O2_c-Cd2-O3_c	89.83(12)
O2_c -Cd2-N2_c	90.91(11)	O3_c-Cd2-N2_c	94.92(13)

Symmetry codes: b = 1-x, y, 0.5-z; c = -x, -y, 1-z.

Compound 4

Ni1-O1	2.0690(16)	Ni1-O3	2.0988(15)
Ni1 - N1	2.1075(19)	Ni1 - O1_f	2.0690(16)
Ni1 -O3_f	2.0988(15)	Ni1 - N1_f	2.1075(19)
O1 -Ni1 - O3	89.14(7)	O1 -Ni1 - N1	89.69(8)
O1 -Ni1 - O1_f	180.00	O1 -Ni1 - O3_f	90.86(7)
O1 -Ni1 -N1_f	90.31(8)	O3 -Ni1 - N1	87.83(7)
O1_f -Ni1 - O3	90.86(7)	O3 -Ni1 - O3_f	180.00
O3 -Ni1 - N1_f	92.17(7)	O1_f -Ni1 -N1	90.31(8)
O3_f -Ni1- N1	92.17(7)	N1 -Ni1 -N1_f	180.00
O1_f -Ni1 -O3_f	89.14(7)	O1_f -Ni1 -N1_f	89.69(8)
O3_f -Ni1 -N1_f	87.83(7)		

Symmetry code: f = 0.5 - x, 2.5 - y, 1 - z.

Compound 5

N(1)-Zn(1)#3	2.035(4)	C(11)-N(3)-Zn(1)	123.7(2)
N(2)-Zn(2)	2.048(3)	C(11)#1-N(3)-Zn(1)	123.7(2)
N(3)-Zn(1)	2.045(4)	C(12)-O(4)-Zn(1)	129.3(2)
O(4)-Zn(1)	1.916(2)	N(4)-O(6)-Zn(2)	129.7(3)
O(6)-Zn(2)	2.046(3)	O(4)-Zn(1)-O(4)#1	121.06(16)
C(19)-N(1)-C(19)#1	117.1(4)	O(4)-Zn(1)-N(1)#3	114.19(8)
C(19)#1-N(1)-Zn(1)#3	121.2(2)	O(4)#1-Zn(1)-N(1)#3	114.19(8)

C(5)-N(2)-Zn(2)	119.3(2)	O(4)-Zn(1)-N(3)	100.41(10)
C(6)-N(2)-Zn(2)	124.0(2)	O(4)#1-Zn(1)-N(3)	100.41(10)
N(1)#3-Zn(1)-N(3)	102.08(16)	O(6)-Zn(2)-N(2)	117.34(12)
O(6)-Zn(2)-O(6)#2	108.79(17)	O(6)#2-Zn(2)-N(2)	107.96(12)
O(6)-Zn(2)-N(2)#2	107.96(12)	N(2)#2-Zn(2)-N(2)	97.51(16)
O(6)#2-Zn(2)-N(2)#2	117.34(12)		

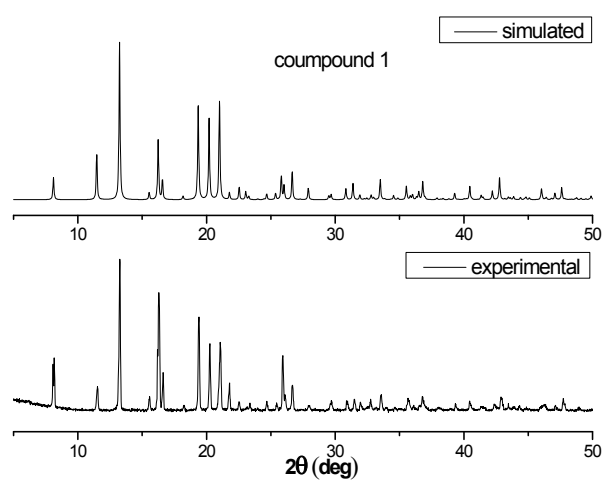


Figure S1. Powder x-ray diffraction patterns of compound 1

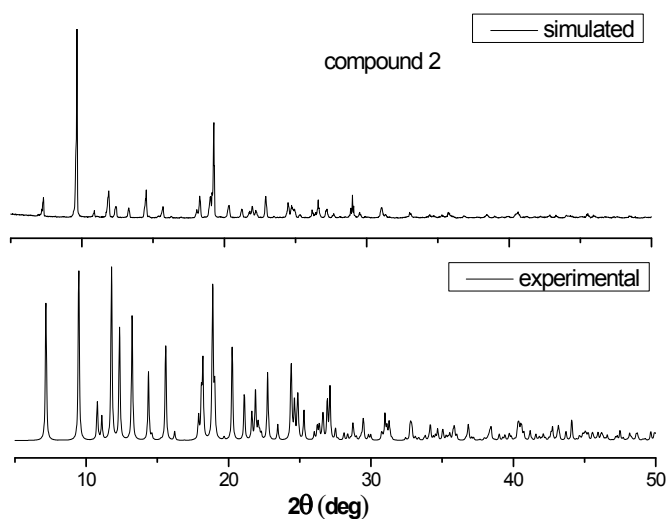


Figure S2. Powder x-ray diffraction patterns of compound 2

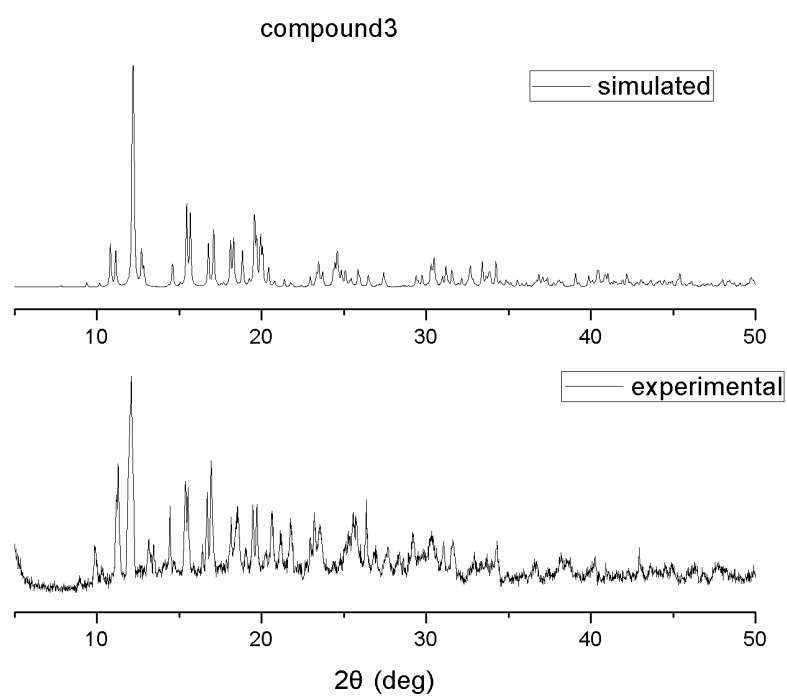


Figure S3. Powder x-ray diffraction patterns of compound 3

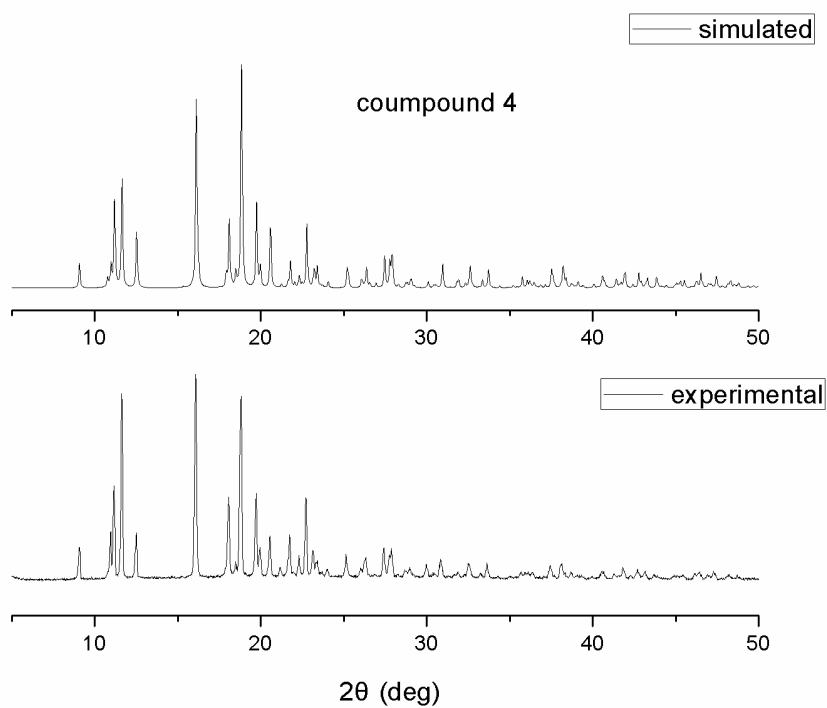


Figure S4. Powder x-ray diffraction patterns of compound4

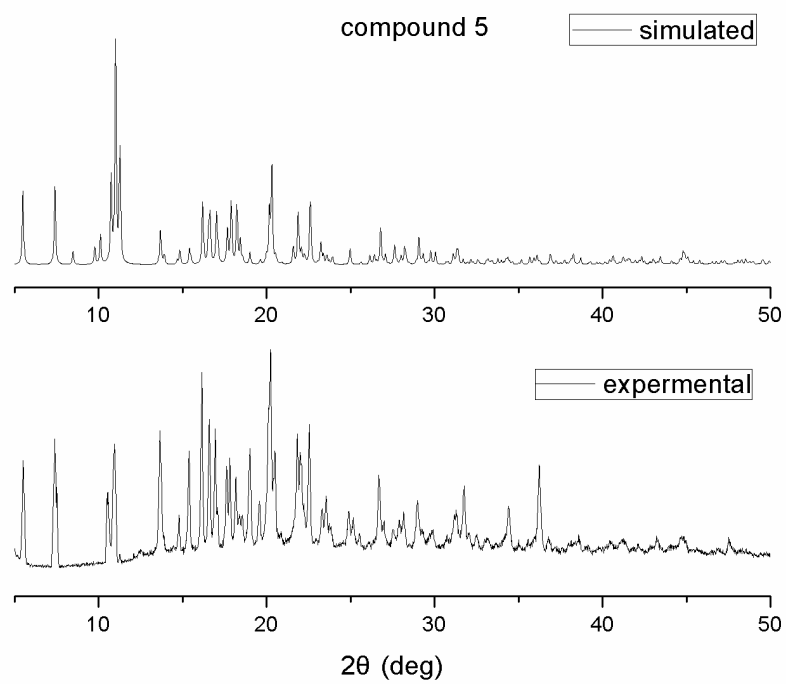


Figure S5. Powder x-ray diffraction patterns of compound 5