Electronic Supplementary Information for

Positional Isomeric Tunable Two Co(II) 6-Connected 3-D Frameworks with Pentanuclear to Binuclear Units: Structures, Ion-Exchange and Magnetic Properties

Min-Le Han,[a,b] Ya-Ping Duan,[a] Dong-Sheng Li, *[,a,b] Hai-Bin Wang,[a] Jun Zhao,[a] and Yao-Yu Wang[b]

[a]*College of Materials and Chemical Engineering, Collaborative Innovation Center for Microgrid of New Energy of Hubei Province, China Three Gorges University, Yichang 443002, P. R. China*

[b]*Key Laboratory of Synthetic and Natural Functional Molecule Chemistry of the Ministry of Education, College of Chemistry & Materials Science, Northwest University, Xi'an 710069, P. R. China*

* Corresponding author: College of Materials and Chemical Engineering, China Three Gorges University, Yichang, P. R. China. Tel./Fax: +86-717- 6397506;

E-mail address: lidongsheng1@126.com (D.-S. Li)

Table S1 Selected bond lengths (Á) and bond angles (°) for complexes **1** and **2**.

1			
Co(1)-O(5)#1	2.078(2)	Co(1)-O(5)	2.078(2)
Co(1)-O(2)	2.077(2)	Co(1)-O(2)#1	2.077(2)
Co(1)-O(7)#1	2.101(2)	Co(1)-O(7)	2.101(2)
Co(2)-O(5)	2.067(2)	Co(2)-O(4)#2	2.071(2)
Co(2)-N(4)#3	2.112(3)	Co(2)-N(8)#1	2.122(3)
Co(2)-O(6)#1	2.154(2)	Co(2)-O(2)#1	2.248(2)
Co(3)-O(3)#2	2.024(3)	Co(3)-O(5)	2.043(2)
Co(3)-N(5)	2.103(3)	Co(3)-N(1)	2.142(3)
Co(3)-O(1)	2.150(2)	Co(3)-O(7)	2.354(2)
O(2)-Co(1)-O(2)#1	180.000(1)	O(2)-Co(1)-O(5)	95.87(8)
O(2)#1-Co(1)-O(5)	84.13(8)	O(2)-Co(1)-O(5)#1	84.13(8)
O(2)#1-Co(1)-O(5)#1	95.87(8)	O(5)-Co(1)-O(5)#1	180.000(1)
O(2)-Co(1)-O(7)	89.87(9)	O(2)#1-Co(1)-O(7)	90.13(9)
O(5)-Co(1)-O(7)	85.30(9)	O(5)#1-Co(1)-O(7)	94.70(9)
O(2)-Co(1)-O(7)#1	90.13(9)	O(2)#1-Co(1)-O(7)#1	89.87(9)
O(5)-Co(1)-O(7)#1	94.70(9)	O(5)#1-Co(1)-O(7)#1	85.30(9)
O(7)-Co(1)-O(7)#1	180.000(1)	O(5)-Co(2)-O(4)#2	94.10(9)
O(5)-Co(2)-N(4)#3	93.08(10)	O(4)#2-Co(2)-N(4)#3	92.52(11)
O(5)-Co(2)-N(8)#1	172.51(10)	O(4)#2-Co(2)-N(8)#1	90.20(11)
N(4)#3-Co(2)-N(8)#1	92.86(11)	O(5)-Co(2)-O(6)#1	87.05(9)
O(4)#2-Co(2)-O(6)#1	176.45(10)	N(4)#3-Co(2)-O(6)#1	90.76(11)
N(8)#1-Co(2)-O(6)#1	88.31(11)	O(5)-Co(2)-O(2)#1	80.22(8)
O(4)#2-Co(2)-O(2)#1	87.58(10)	N(4)#3-Co(2)-O(2)#1	173.29(9)
N(8)#1-Co(2)-O(2)#1	93.85(10)	O(6)#1-Co(2)-O(2)#1	89.31(9)
O(3)#2-Co(3)-O(5)	96.08(9)	O(3)#2-Co(3)-N(5)	90.27(12)

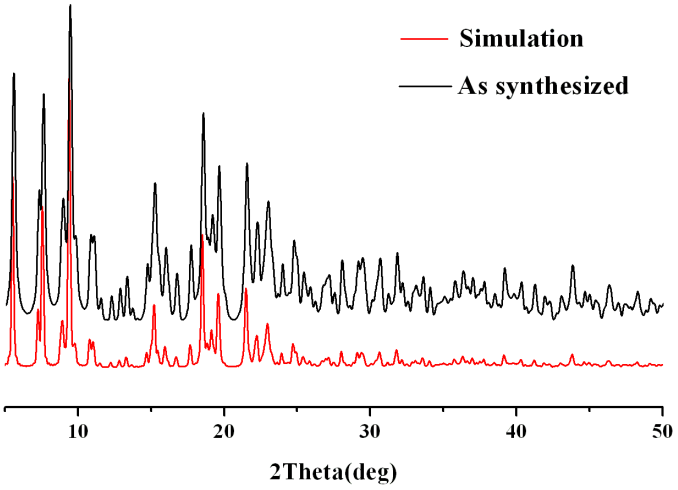
O(5)-Co(3)-N(5)	169.64(10)	O(3)#2-Co(3)-N(1)	97.42(12)
O(5)-Co(3)-N(1)	96.76(10)	N(5)-Co(3)-N(1)	90.49(12)
O(3)#2-Co(3)-O(1)	174.41(11)	O(5)-Co(3)-O(1)	86.16(9)
N(5)-Co(3)-O(1)	86.81(11)	N(1)-Co(3)-O(1)	87.37(10)
O(3)#2-Co(3)-O(7)	88.40(10)	O(5)-Co(3)-O(7)	79.84(9)
N(5)-Co(3)-O(7)	92.20(10)	N(1)-Co(3)-O(7)	173.57(10)
O(1)-Co(3)-O(7)	86.96(9)		

2

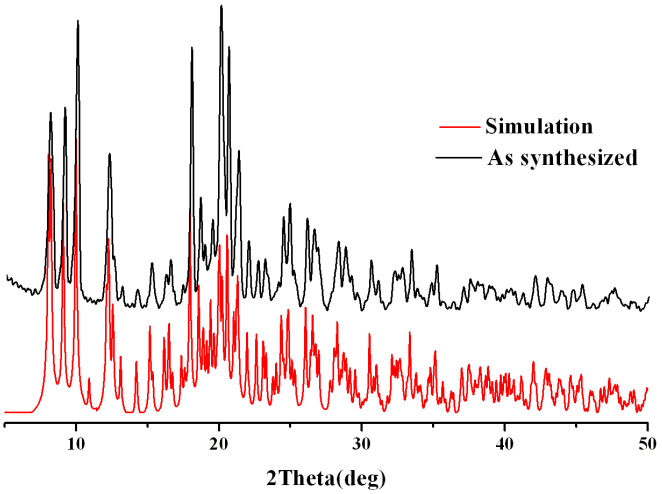
Co(1)-O(7)	2.057(2)	Co(2)-N(4)#3	2.131(3)
Co(1)-O(3)#1	2.102(2)	Co(2)-O(1)	2.068(2)
Co(1)-O(2)	2.101(2)	Co(2)-O(6)	2.066(2)
Co(1)-N(1)	2.119(3)	Co(2)-O(8)#2	2.095(3)
Co(1)-N(5)	2.154(3)	Co(2)-N(8)#3	2.128(3)
Co(1)-O(5)	2.165(2)	Co(2)-O(5)	2.188(2)
O(7)-Co(1)-O(3)#1	177.90(10)	O(7)-Co(1)-O(2)	95.01(10)
O(2)-Co(1)-O(3)#1	84.77(11)	O(7)-Co(1)-N(1)	90.46(10)
O(2)-Co(1)-N(1)	87.31(10)	O(3)#1-Co(1)-N(1)	91.62(11)
O(7)-Co(1)-N(5)	89.17(10)	O(2)-Co(1)-N(5)	173.91(11)
O(3)#1-Co(1)-N(5)	91.22(11)	N(1)-Co(1)-N(5)	88.23(11)
O(7)-Co(1)-O(5)	88.91(9)	O(2)-Co(1)-O(5)	95.71(9)
O(3)#1-Co(1)-O(5)	89.04(9)	N(1)-Co(1)-O(5)	176.96(10)
N(5)-Co(1)-O(5)	88.78(9)	O(6)-Co(2)-O(1)	95.40(10)
O(6)-Co(2)-O(8)#2	89.36(10)	O(1)-Co(2)-O(8)#2	173.97(9)
O(6)-Co(2)-N(8)#3	176.74(11)	O(1)-Co(2)-N(8)#3	87.78(11)
O(8)#2-Co(2)-N(8)#3	87.41(11)	O(6)-Co(2)-N(4)#3	91.23(11)
O(1)-Co(2)-N(4)#3	88.31(10)	O(8)#2-Co(2)-N(4)#3	87.90(10)

N(8)#3-Co(2)-N(4)#3	88.14(11)	O(6)-Co(2)-O(5)	89.15(9)
O(1)-Co(2)-O(5)	94.51(9)	O(8)#2-Co(2)-O(5)	89.24(9)
N(8)#3-Co(2)-O(5)	91.33(10)	N(4)#3-Co(2)-O(5)	177.11(11)

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



1



2

Figure S1 Comparison of the experimental and simulated PXRD patterns.

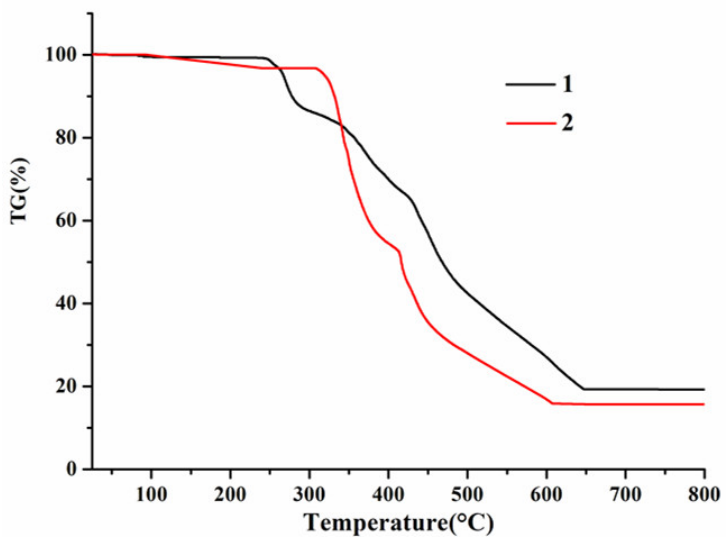


Figure S2 TGA plots of **1** and **2.**