Electronic Supplementary Information

Assembly of Co(II)/Cu(II)-Azide Polynuclear Polymers: Structural Diversity and Magnetic Behavior

Shuai-Hua Wang[ab], Fa-Kun Zheng[*a], Mei-Feng Wu[c], Zhi-Fa Liu[ab], Jun Chen[ab], Yu Xiao[ab], Guo-Cong Guo[a] and A-Qing Wu[a]

[a] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China*

[b] *University of Chinese Academy of Sciences, Beijing 100039, P. R. China*

[c] *School of Environmental and Chemical Engineering, Nanchang Hangkong University, Nanchang, Jiangxi 330063, P. R. China*

Table S1 The selected bond distances and angles for **1**–**3**.

Polymer 1			
Co(1)-O(4)	1.948(2)	Co(2)-O(3)	2.024(2)
Co(1)-O(6)#1	1.959(2)	Co(2)-N(3)	2.150(3)
Co(1)-N(7)	2.017(3)	Co(2)-O(1)	2.163(2)
Co(1)-N(4)	2.122(3)	Co(2)-N(4)	2.185(3)
Co(1)-N(7)#2	2.207(3)	Co(2)-O(2)	2.219(2)
Co(2)-O(5)#1	2.007(2)	N(7)-Co(1)-N(4)	98.01(12)
O(4)-Co(1)-O(6)#1	121.1(1)	O(4)-Co(1)-N(7)#2	86.59(11)
O(4)-Co(1)-N(7)	115.1(1)	O(6)#1-Co(1)-N(7)#2	88.97(11)
O(6)#1-Co(1)-N(7)	121.7(1)	N(7)-Co(1)-N(7)#2	79.78(12)
O(4)-Co(1)-N(4)	95.8(1)	N(4)-Co(1)-N(7)#2	177.31(11)
O(6)#1-Co(1)-N(4)	90.9(1)	O(5)#1-Co(2)-O(3)	111.20(10)

Symmetry transformations used to generate equivalent atoms:

#1 x + 1/2, y – 1/2, z; #2 – x + 3/2, – y + 3/2, – z.

[*] Corresponding author. Tel: +86 591 83704827; fax: +86 591 83714946.

E-mail address: zfk@fjirsm.ac.cn (F.-K. Zheng)

Polymer 2			
Co(1)-O(5)#1	1.955(3)	Co(2)-O(6)#1	2.023(3)
Co(1)-O(3)	1.957(3)	Co(2)-N(3)	2.132(3)
Co(1)-N(7)	2.016(3)	Co(2)-N(4)	2.169(3)
Co(1)-N(4)	2.123(3)	Co(2)-O(1)	2.167(2)
Co(1)-N(7)#2	2.196(3)	Co(2)-O(2)	2.208(3)
Co(2)-O(4)	2.014(2)	N(7)-Co(1)-N(4)	97.2(1)
O(5)#1-Co(1)-O(3)	121.4(1)	O(5)#1-Co(1)-N(7)#2	86.8(1)
O(5)#1-Co(1)-N(7)	113.2(1)	O(3)-Co(1)-N(7)#2	89.4(1)
O(3)-Co(1)-N(7)	123.6(1)	N(7)-Co(1)-N(7)#2	80.3(1)
O(5)#1-Co(1)-N(4)	96.0(1)	N(4)-Co(1)-N(7)#2	176.8(1)
O(3)-Co(1)-N(4)	90.5(2)	O(4)-Co(2)-O(6)#1	110.9(1)

Symmetry transformations used to generate equivalent atoms:

#1 x – 1/2, y + 1/2, z; #2 – x + 1/2, – y + 1/2, – z.

Polymer 3			
Cu(1)-N(7)	1.982(4)	Cu(3)-N(18)#1	1.975(4)
Cu(1)-N(13)	2.011(3)	Cu(3)-N(19)	2.023(3)
Cu(1)-N(19)	2.015(3)	Cu(3)-N(4)#2	2.049(3)
Cu(1)-N(22)	2.025(3)	Cu(3)-N(22)	2.071(3)
Cu(1)-N(16)	2.347(4)	Cu(3)-N(13)#2	2.344(4)
Cu(2)-N(10)	1.973(4)	Cu(1)-N(19)#1	2.688(4)
Cu(2)-N(7)	2.026(3)	Cu(2)-N(4)	2.067(4)
Cu(2)-N(3)	2.060(4)	N(22)-Cu(3)-N(13)#2	94.48(13)
N(7)-Cu(1)-N(13)	86.68(14)	N(10)-Cu(2)-N(4)	88.85(15)
N(7)-Cu(1)-N(19)	169.66(15)	N(7)-Cu(2)-N(4)	89.00(14)
N(13)-Cu(1)-N(19)	95.14(14)	N(3)-Cu(2)-N(4)	168.64(14)
N(7)-Cu(1)-N(22)	95.45(14)	N(18)#1-Cu(3)-N(19)	172.26(14)
N(13)-Cu(1)-N(22)	170.43(15)	N(18)#1-Cu(3)-N(4)#2	95.52(14)
N(19)-Cu(1)-N(22)	81.14(13)	N(19)-Cu(3)-N(4)#2	90.82(13)

N(7)-Cu(1)-N(16)	95.31(14)	N(18)#1-Cu(3)-N(22)	93.94(14)
N(13)-Cu(1)-N(16)	93.49(14)	N(19)-Cu(3)-N(22)	79.85(13)
N(19)-Cu(1)-N(16)	94.74(14)	N(4)#2-Cu(3)-N(22)	170.47(13)
N(22)-Cu(1)-N(16)	95.59(14)	N(18)#1-Cu(3)-N(13)#2	95.34(14)
N(10)-Cu(2)-N(7)	177.08(14)	N(19)-Cu(3)-N(13)#2	89.78(13)
N(10)-Cu(2)-N(3)	92.94(14)	N(4)#2-Cu(3)-N(13)#2	83.45(14)
N(7)-Cu(2)-N(3)	88.78(14)		

Symmetry transformations used to generate equivalent atoms:

#1 – x, – y + 1, – z; #2 – x + 1, – y + 1, – z.

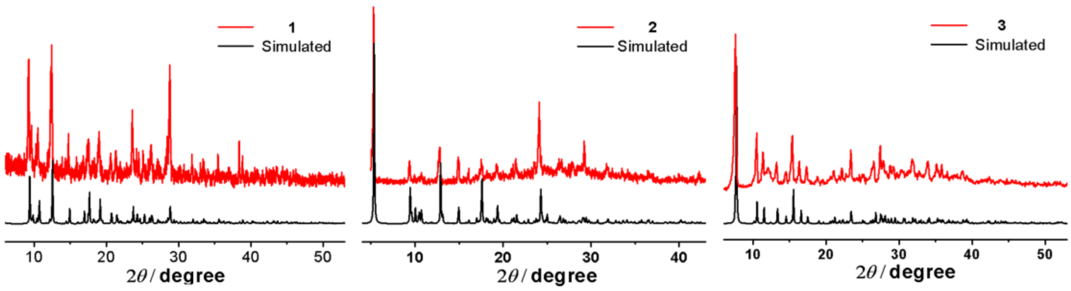

Fig. S1 PXRD patterns of **1**–**3**.

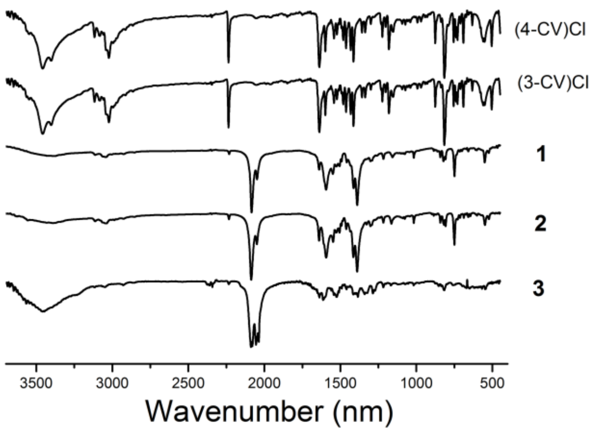

Fig. S2 IR of (4-CV)Cl, (3-CV)Cl and **1**–**3**.

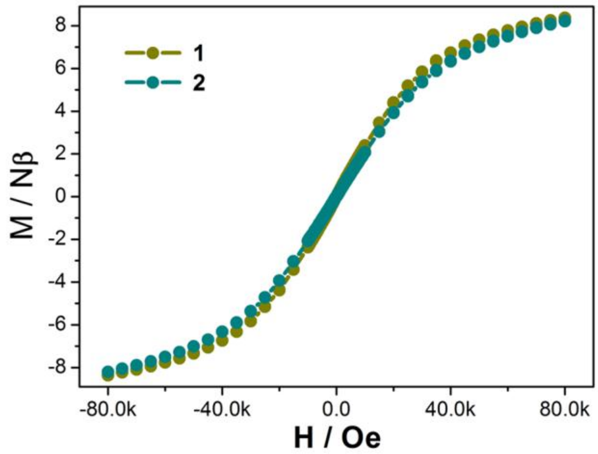

Fig. S3 Field dependence of magnetization up to H = 80 kOe at T = 2K for **1** and **2**.

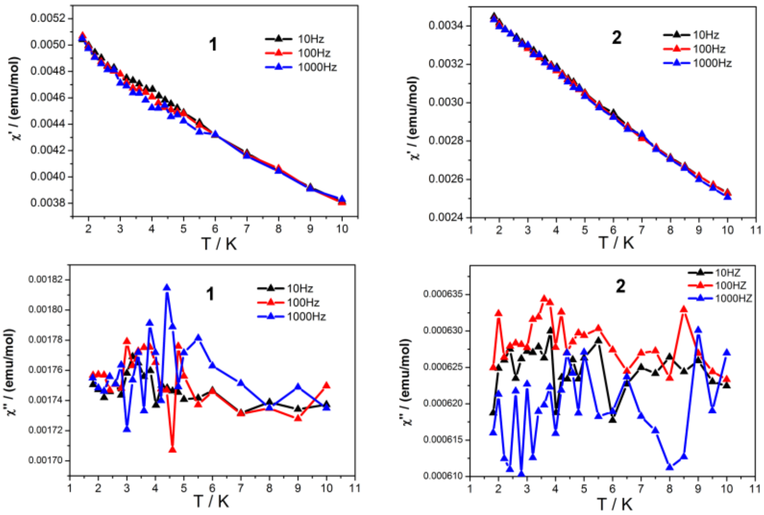

Fig. S4 Temperature dependence of in-phase (χ') and out-of-phase (χ'') *ac* magnetic susceptibility for **1** and **2** at zero external magnetic field under three different frequencies of 10 Hz, 100 Hz and 1000 Hz.

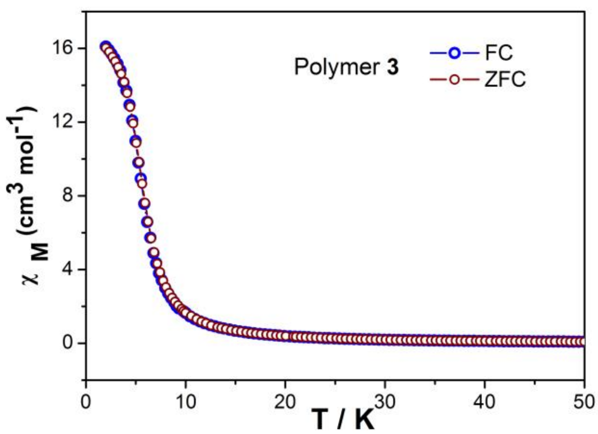

Fig. S5 Zero-filed-cooling (ZFC) and field-cooling (FC) magnetization versus *T* measured under 1000 Oe for **3**.

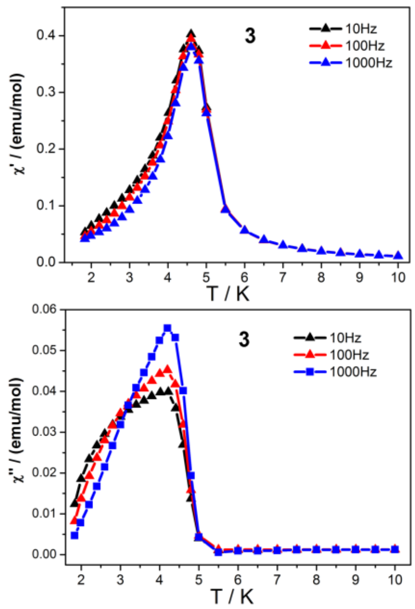

Fig. S6 Temperature dependence of in-phase (χ') and out-of-phase (χ'') *ac* magnetic susceptibility for **3** at zero external magnetic field with three different frequencies of 10 Hz, 100 Hz and 1000 Hz.