Electronic Supplementary Information (ESI)

Diversified magnetic behaviors in new nickel(II) and copper(II) azido coordination polymers templated by diethyl or triethyl amines

Ying Zeng,[a] Sui-Jun Liu,*[b] Cai-Ming Liu,*[c] Yong-Rong Xie,[a] and Zi-Yi Du*[a]

[a]*Key Laboratory of Jiangxi University for Functional Materials Chemistry, College of Chemistry and Chemical Engineering, Gannan Normal University, Ganzhou 341000, P. R. China*

[b]*School of Metallurgy and Chemical Engineering, Jiangxi University of Science and Technology, Ganzhou 341000, P. R. China*

[c]*Beijing National Laboratory for Molecular Sciences, Center for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing, 100190, P. R. China*

*Corresponding author. E-mail: liusuijun147@163.com; cmliu@iccas.ac.cn; ziyidu@gmail.com.

Table S1. Summary of crystal data and structural refinements for **1** - **3**.

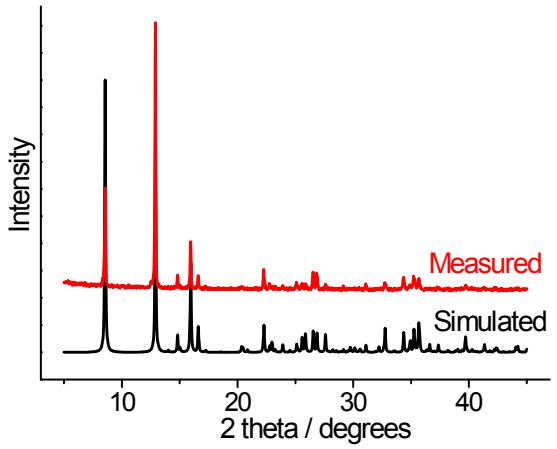
Compound	**1**	**2**	**3**
Empirical formula	$C_6H_{16}N_8Ni_1$	$C_4H_{12}N_{22}Cu_3$	$C_6H_{16}N_{28}Cu_4$
Formula weight	258.98	558.98	734.63
Space group	$P2_1/c$	P-1	P-1
a (Å)	10.4040(8)	6.8322(2)	8.6636(6)
b (Å)	7.9731(6)	11.3756(4)	11.8031(8)
c (Å)	13.523(1)	12.5900(4)	11.9525(8)
α/deg	90	79.412(2)	91.650(1)
β/deg	97.113(1)	89.080(2)	94.884(1)
γ/deg	90	75.553(2)	91.011(1)
V/Å^3	1113.1(2)	930.97(5)	1217.0(2)
Z	4	2	2
D_{calcd}/g cm^{-3}	1.545	1.994	2.005
μ/mm^{-1}	1.727	3.443	3.508
GOF on F^2	1.014	1.014	1.053
R1, wR2 [$I>2\sigma(I)$]	0.0220, 0.0525	0.0252, 0.0650	0.0184, 0.0457
R1, wR2 (all data)	0.0283, 0.0551	0.0275, 0.0665	0.0208, 0.0467

$R1 = \sum||Fo| - |Fc||/\sum|Fo|$, $wR2 = \{\sum w[(Fo)^2 - (Fc)^2]^2/\sum w[(Fo)^2]^2\}^{1/2}$

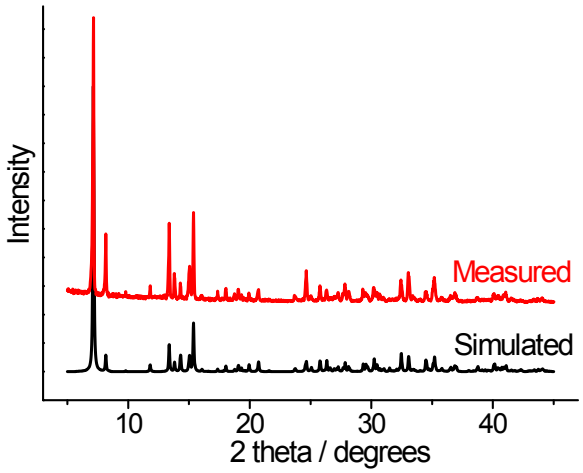
Table S2. Selected bond lengths (Å) in **1-3**.

		1	
Ni(1)–N(7)	2.061(1)	Ni(1)–N(3)#1	2.109(1)
Ni(1)–N(4)#2	2.113(1)	Ni(1)–N(1)	2.123(1)
Ni(1)–N(4)	2.145(1)	Ni(1)–N(8)	2.223(1)
		2	
Cu(1)–N(1)	1.972(2)	Cu(1)–N(7)	1.986(2)
Cu(1)–N(1)#2	1.997(2)	Cu(1)–N(4)	2.015(2)
Cu(1)···N(6)#3	2.659(4)	Cu(2)–N(7)	1.979(2)
Cu(2)–N(10)	1.992(2)	Cu(2)–N(16)	1.998(2)
Cu(2)–N(13)	2.007(2)	Cu(2)···N(13)#4	2.593(2)
Cu(2)···N(15)#5	2.779(3)	Cu(3)–N(19)	1.961(2)
Cu(3)–N(4)#3	2.016(2)	Cu(3)–N(16)	2.024(2)
Cu(3)–N(13)	2.042(2)	Cu(3)···N(10)#4	2.548(3)
Cu(3)···N(12)#5	2.556(2)		
		3	
Cu(1)–N(1)	2.004(2)	Cu(1)–N(7)	2.036(2)
Cu(1)···N(4)#4	2.513(2)	Cu(2)–N(25)	1.977(2)
Cu(2)–N(16)	2.021(2)	Cu(3)–N(10)	1.990(2)
Cu(3)–N(13)	2.000(2)	Cu(3)–N(7)	2.010(2)
Cu(3)–N(22)	2.023(2)	Cu(3)···N(4)#4	2.436(2)
Cu(4)–N(19)	1.993(2)	Cu(4)–N(19)#3	2.000(2)
Cu(4)–N(10)	2.016(2)	Cu(4)–N(16)	2.025(2)
Cu(4)···N(25)#2	2.332(2)	Cu(5)–N(1)#4	1.978(2)
Cu(5)–N(13)	1.998(2)	Cu(5)–N(4)	2.013(2)
Cu(5)–N(22)	2.027(2)	Cu(5)···N(27)	2.491(2)
Cu(5)···N(13)	2.668(2)		

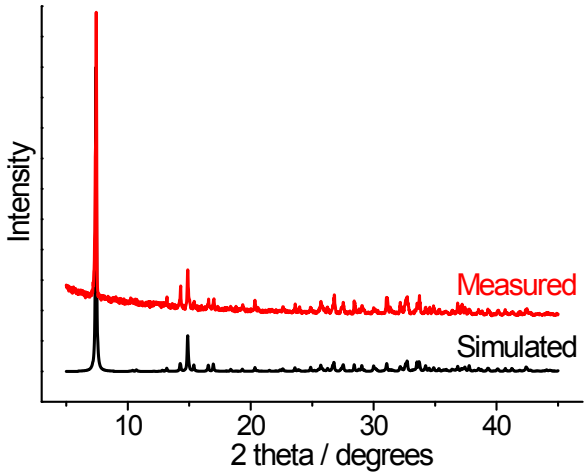
Symmetry codes: #1 $-x + 1, y + 1/2, -z + 1/2$; #2 $-x + 1, -y + 1, -z$; #3. $-x + 2, -y + 1, -z$; #4. $-x + 1, -y + 2, -z$; #5. $-x, -y + 2, -z$.



(a)



(b)



(c)

Fig. S1. Simulated and experimental XRD powder patterns for **1** (a), **2** (b), and **3** (c), respectively.

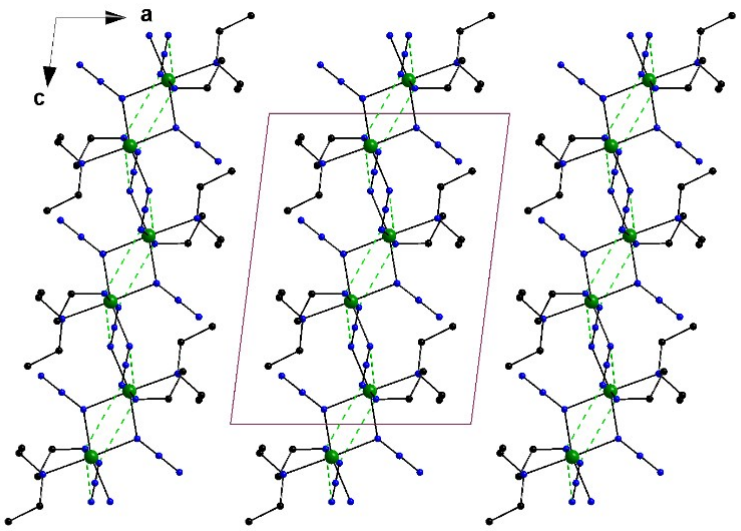


Fig. S2. View of the structure of **1** down the *b*-axis. the N···N hydrogen bonds are drawn as green dashes. For other display details, see the caption for Fig. 1.

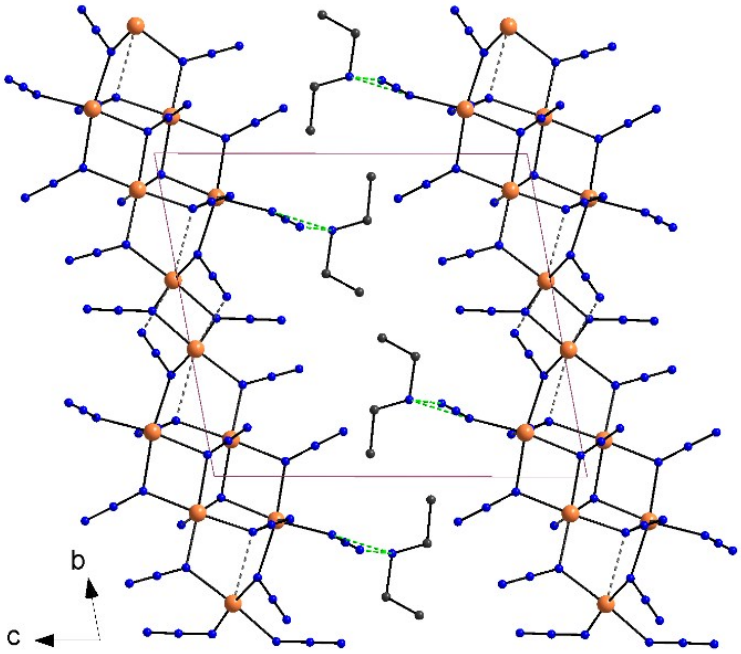


Fig. S3. View of the structure of **2** down the *a*-axis. The weak Cu–N bonds with the bond lengths longer than 2.40 Å and the N···N hydrogen bonds are drawn as dark grey and green dashes, respectively. For other display details, see the caption for Fig. 2.

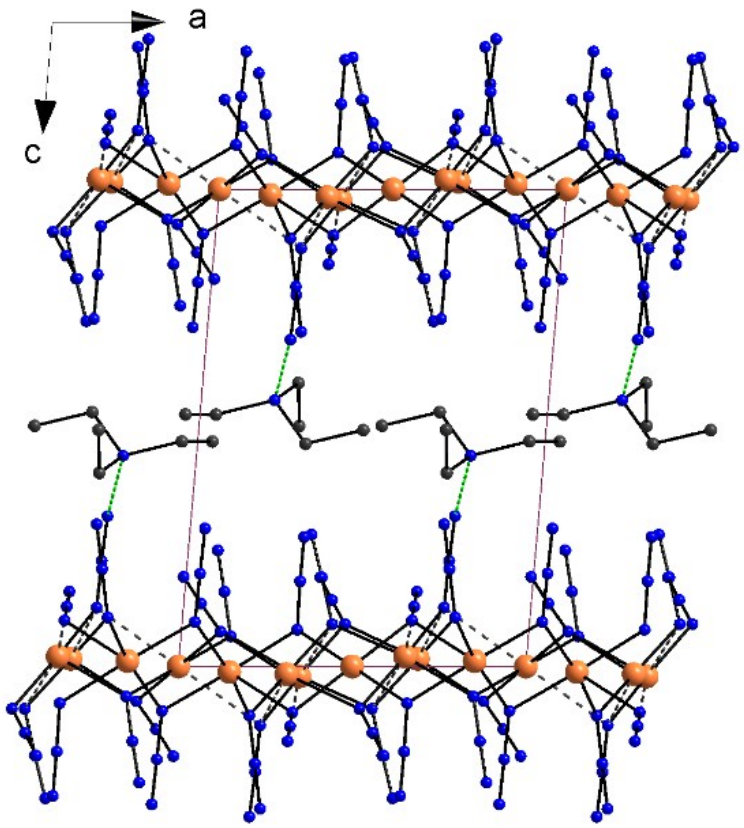


Fig. S4. View of the structure of **3** down the *b*-axis. For display details, see the caption for Fig. S3.

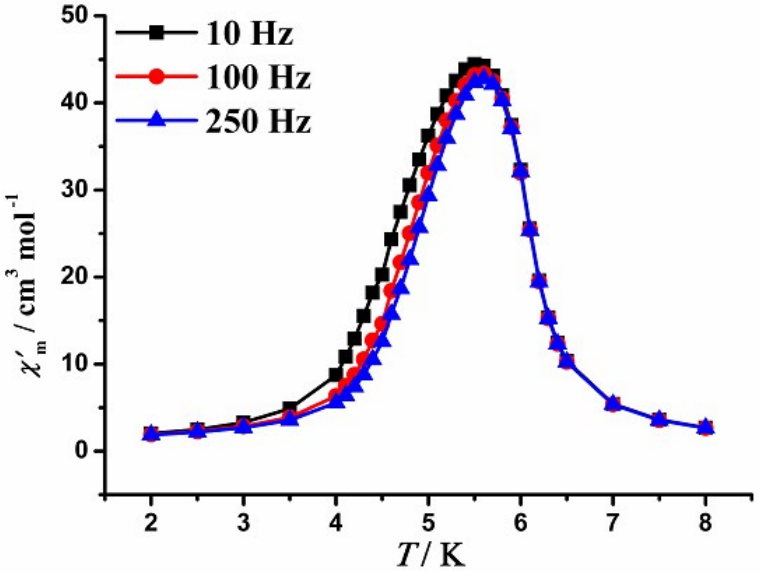
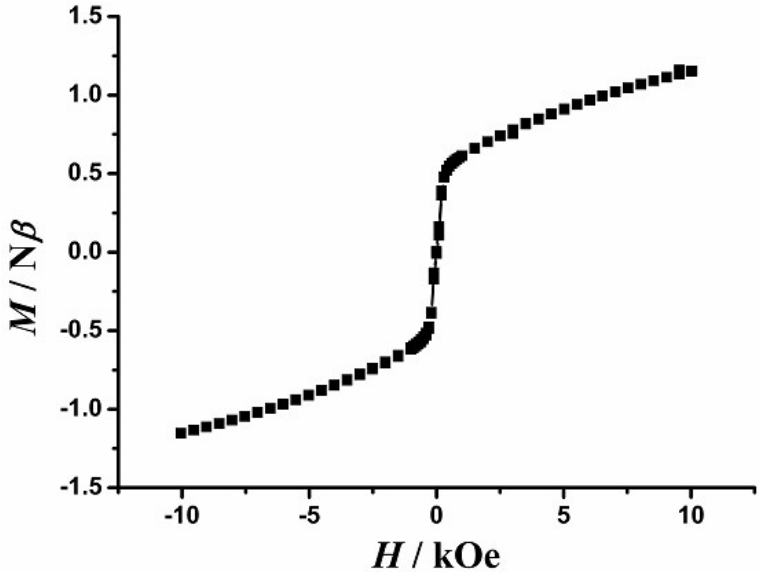
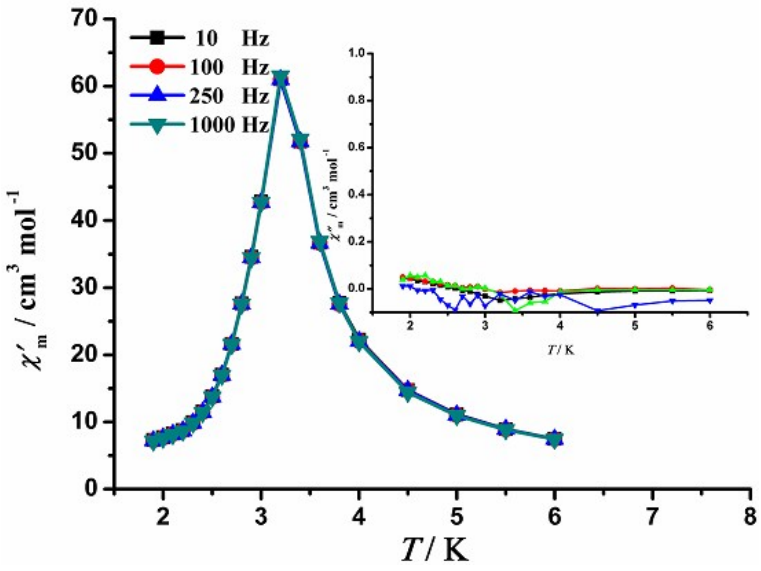


Fig. S5. The in-phase signals with H_{dc} = 0 Oe for **2**.



(a)



(b)

Fig. S6. Field dependence of the magnetization of **3** measured at 2 K (a), and temperature dependence of the ac χ_m at different frequencies for **3** with H_{dc} = 0 Oe (b).