## Supplementary Information

## A three-dimensional coordination polymer constructed from linear trinuclear copper(II) clusters with a ferromagnetic exchange coupling

Qilong Zhu,<sup>*a,b*</sup> Chongbin Tian,<sup>*a,b*</sup> Chaojun Shen,<sup>*a*</sup> Tianlu Sheng,<sup>*a*</sup> Shengmin Hu<sup>*a*</sup> and Xintao Wu<sup>\**a*</sup>

 <sup>a</sup> State Key Laboratory of Structure Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, 350002, China.
<sup>b</sup> Graduate School of the Chinese Academy of Sciences, Beijing, 100049, China.

 Corresponding author: E-mail: *wxt@ fjirsm.ac.cn.* Tel: +86-591-83719238; Fax: +86-591-83719238



Fig. S1 The trinuclear copper(II) cluster in compound 1.



**Fig. S2** View of the 3-D framework along *b* axis with the highlighted 1-D inorganic hybrid chain in compound **1**.



Fig. S3 IR spectrum of compound 1.



Fig. S4 Powder X-ray diffractions for simulated and experimental 1.



Fig. S5 TG and DTA curves of compound 1.

Cu1-O5	1.899(3)	Cu1-O3b	2.445(4)	
Cu1-O2a	1.939(3)	Cu2-O5	1.895(3)	
Cu1-O4c	1.951(3)	Cu2-O1a	1.948(3)	
Cu1-N3	2.077(4)			
O5-Cu1-O2a	90.05(14)	N3-Cu1-O3b	102.70(12)	
O5-Cu1-O4c	93.98(14)	O5e-Cu2-O5	180	
O2a-Cu1-O4c	174.58(14)	O5e-Cu2-O1a	90.54(15)	
O5-Cu1-N3	159.72(15)	O5-Cu2-O1a	89.46(15)	
O2a-Cu1-N3	85.73(14)	O5e-Cu2-O1d	89.46(15)	
O4c-Cu1-N3	89.24(13)	O5-Cu2-O1d	90.54(15)	
O5-Cu1-O3b	96.76(13)	O1a-Cu2-O1d	180	
O2a-Cu1-O3b	85.87(14)	Cu2-O5-Cu1	111.00(17)	
O4c-Cu1-O3b	97.22(13)			

**Table S1.** Selected Bond Lengths [Å] and Angles [°] for **1**<sup>a</sup>

<sup>a</sup>Symmetry transformations used to generate equivalent atoms: (a) -x+3/2,y-1/2,-z+1/2; (b) x+1/2,-y+1/2,z+1/2; (c) -x+3/2,y+1/2,-z-1/2; (d) x+1/2,-y+1/2,z-1/2; (e) -x+2,-y,-z.