

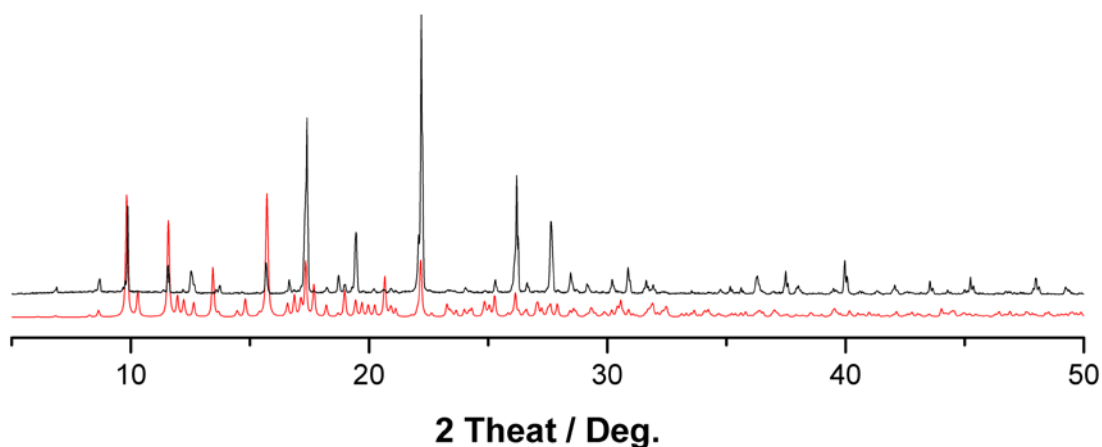
## Spontaneous resolution of a homochiral helix built from tetra-nuclear nickel cluster

Wenxu Zheng,<sup>ab</sup> Yongqin Wei,<sup>a</sup> Chong-Bin Tian,<sup>ab</sup> Xueying Xiao,<sup>ab</sup> and Kechen Wu<sup>a\*</sup>

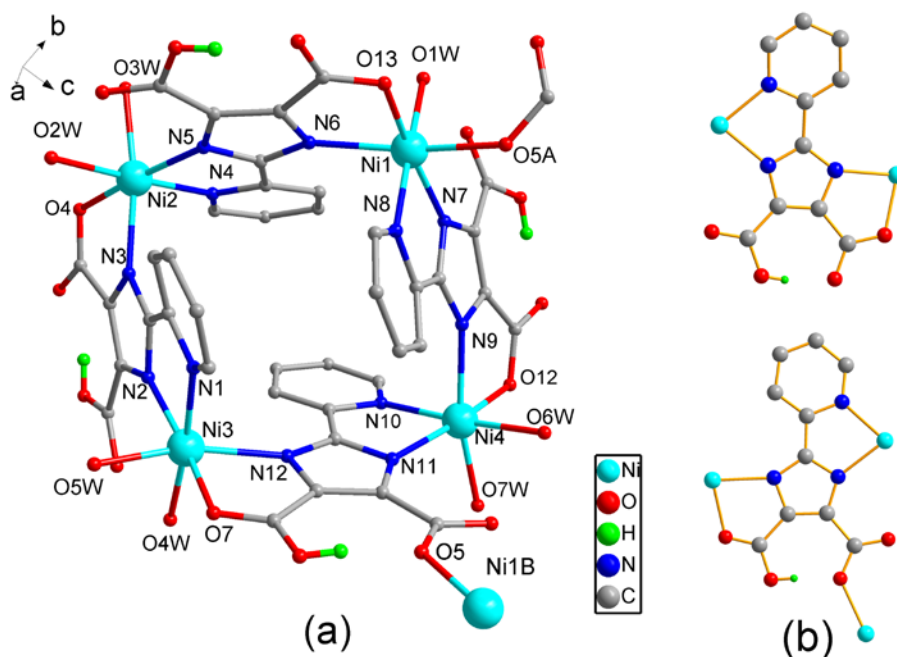
<sup>a</sup> State Key Laboratory of Structure Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China

<sup>b</sup> Graduate School of Chinese Academy of Sciences, Beijing 100039, P. R. China.

\* The corresponding author, Tel: (+86)- 591-83792600; E-mail: [wkc@fjirsm.ac.cn](mailto:wkc@fjirsm.ac.cn)



**Fig. S1.** XPRD patterns for **1** (top, black) experimental at room temperature; (bottom, red) calculated on the basis of the structure determined by single-crystal X-ray diffraction.



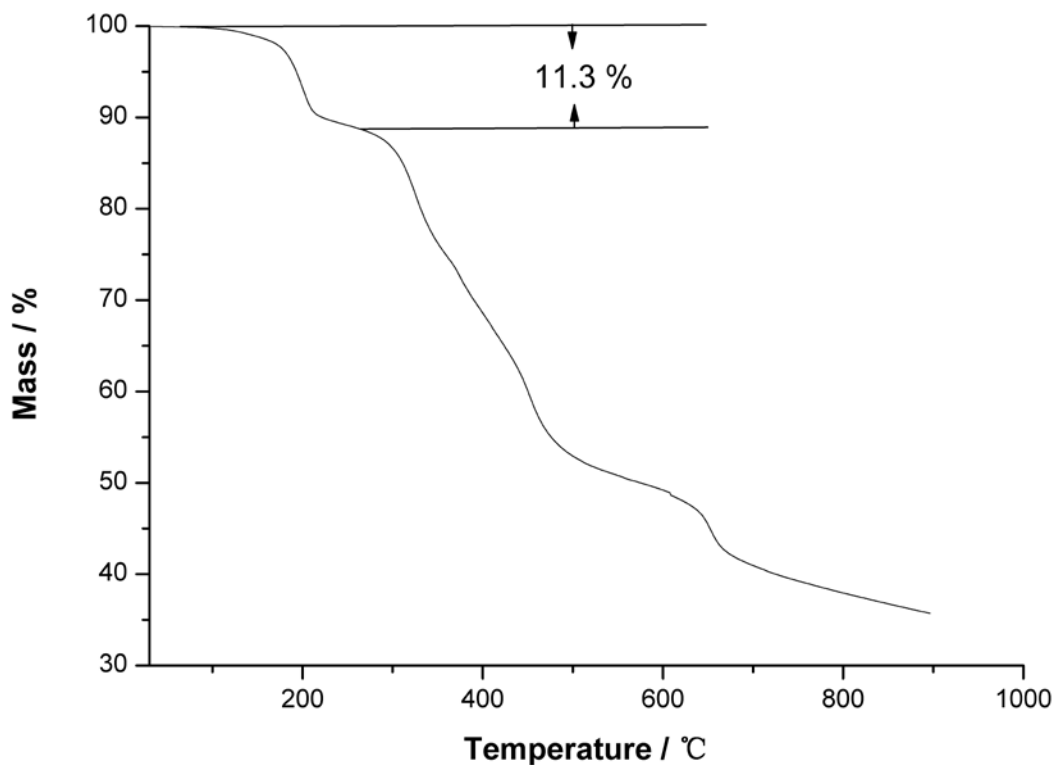
**Fig. S2.** Coordination environment of Ni(II) (a) and bonding mode of **L** (b) in compound **1P**. The

bond length of Ni1—O5A is 2.152(2) Å. Symmetry code: A  $-x, 0.5+y, -0.5-z$ ; B  $1-x, -0.5+y, 0.5-z$ . Guest water molecular and hydrogen atoms in pyridyl rings and coordination water molecules are omitted for clarity.

**Table S1** Geometrical parameters of hydrogen bonds in **1P**.

D-H...A	D-H/ Å	H...A/ Å	D...A/ Å	<DHA/°
O(1W)-H(1WA)...O(4)#1	0.82	2.05	2.864(3)	174.8
O(2W)-H(2WA)...O(1)#2	0.82	2.08	2.868(4)	162.1
O(3W)-H(3WA)...O(13)#3	0.82	2.01	2.788(3)	159.0
O(3W)-H(3WB)...O(6)#4	0.82	1.94	2.701(3)	153.0
O(4W)-H(4WA)...O(12)#5	0.82	1.87	2.663(3)	162.2
O(5W)-H(5WB)...O(3)#2	0.82	2.04	2.800(3)	154.2
O(5W)-H(5WA)...O(16)#6	0.82	1.90	2.718(3)	178.5
O(6W)-H(6WB)...O(2W)#7	0.82	2.22	3.000(3)	158.9
O(7W)-H(7WA)...O(10)#7	0.82	2.08	2.886(3)	169.4
O(7W)-H(7WB)...O(4W)#8	0.82	2.27	2.848(3)	128.2
O(8W)-H(8WA)...O(7)#9	0.82	2.31	2.995(4)	141.8

Symmetry code: #1  $x-1/2, -y+3/2, -z$  #2  $x-1/2, -y+1/2, -z$  #3  $x+1/2, -y+3/2, -z$  #4  $-x+3/2, -y+1, z-1/2$   
#5  $-x+2, y-1/2, -z+1/2$  #6  $x+1/2, -y+1/2, -z$  #7  $-x+3/2, -y+1, z+1/2$  #8  $-x+2, y+1/2, -z+1/2$   
#9  $-x+1, y+1/2, -z+1/2$



**Fig. S3.** The TGA diagram of **1**. The weight of 11.3 % is corresponding to the loss of guest and coordinated water molecules.