

Electronic Supplementary Information

Two eight-connected self-penetrating porous metal-organic frameworks: configurational isomers caused by different linking modes between **terephthalate** and binuclear nickel building units

Guang-Sheng Yang, Ya-Qian Lan, Hong-Ying Zang, Kui-Zhan Shao,

Xin-Long Wang, Zhong-Min Su* and Chun-Jie Jiang*

Institute of Functional Material Chemistry; Department of Chemistry, Northeast
Normal University, Changchun 130024, Jilin, People's Republic of China

* Corresponding author.

E-mail: zmsu@nenu.edu.cn; jiangcj717nenu.edu.cn.

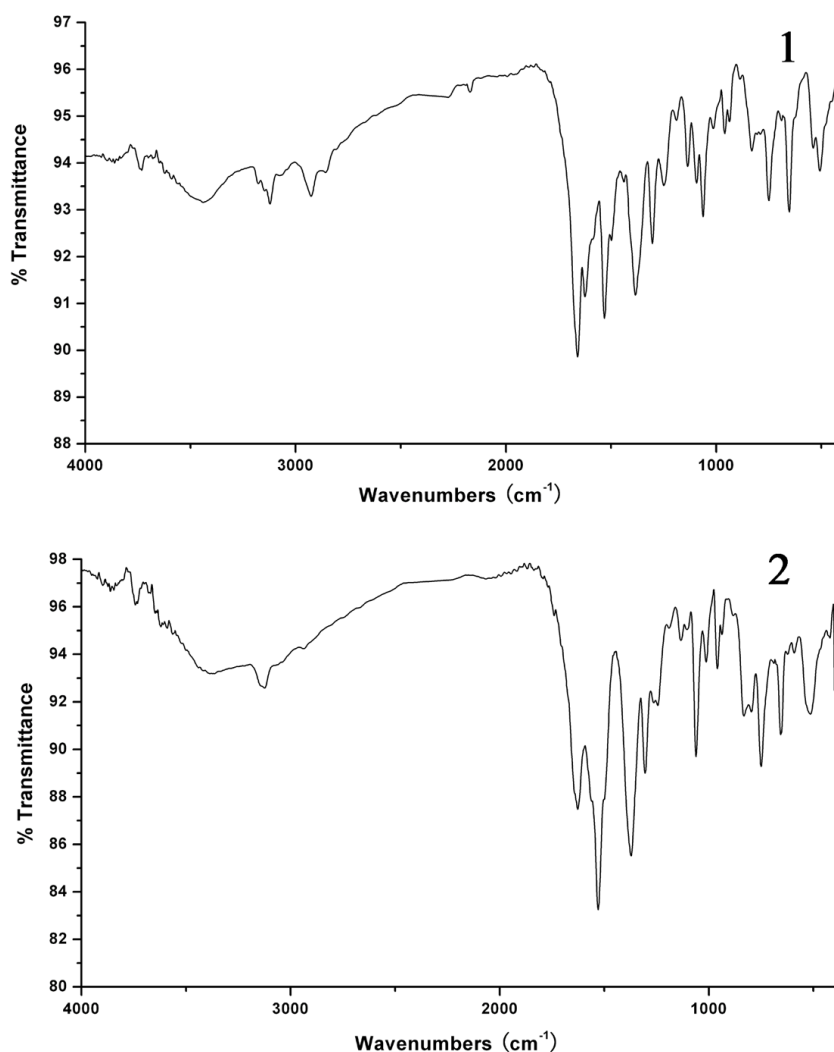


Fig. S1 FT-IR spectra of **1** and **2**.

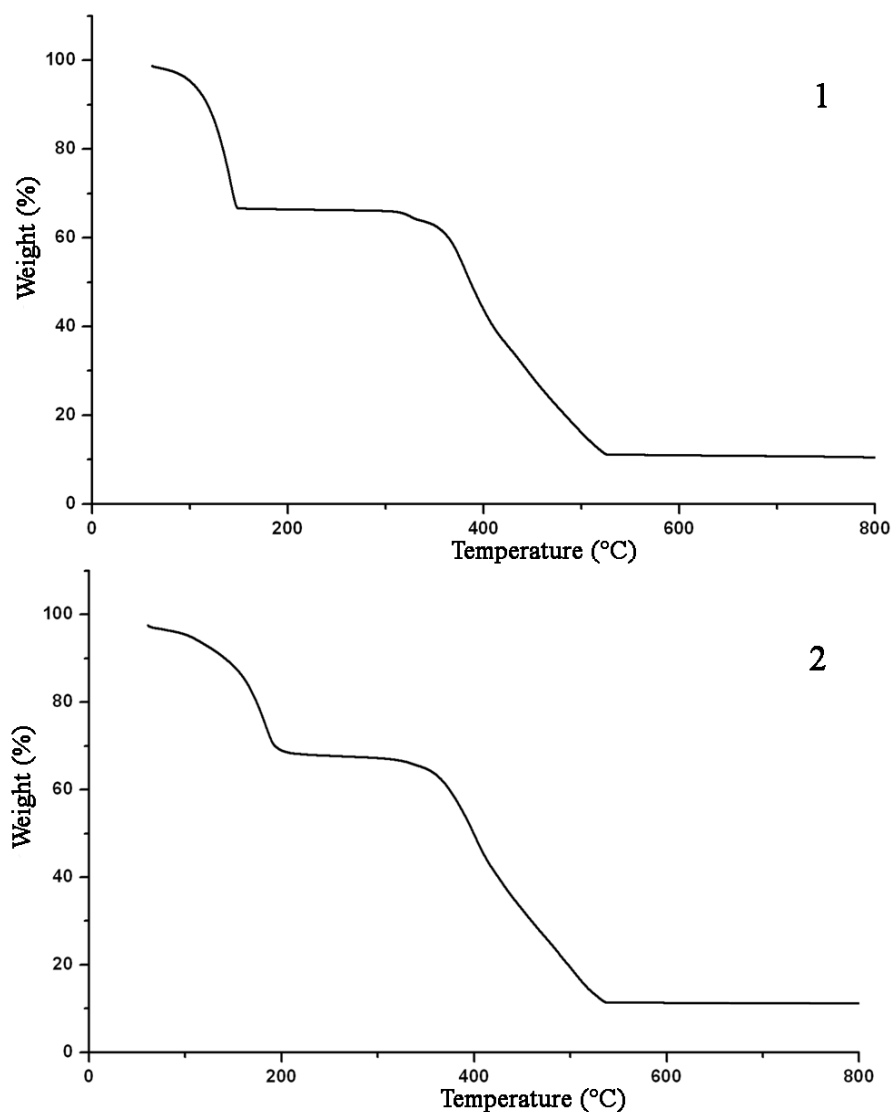


Fig. S2 TGA curves of **1** and **2**.

Table S1 Selected bond lengths (Å) and angles (°) for **1^a** and **2^b**

Complex 1					
Ni(1)-O(2)#1	2.035(4)	Ni(1)-O(1)#2	2.065(4)	Ni(1)-N(1)#3	2.084(6)
Ni(1)-N(4)	2.055(5)	Ni(1)-O(4)	2.069(4)	Ni(1)-O(1W)	2.100(3)
O(2)#1-Ni(1)-N(4)	89.49(19)	O(1)#2-Ni(1)-O(4)	88.04(18)	O(2)#1-Ni(1)-O(1W)	90.18(14)
O(2)#1-Ni(1)-O(1)#2	97.35(18)	O(2)#1-Ni(1)-N(1)#3	87.80(20)	N(4)-Ni(1)-O(1W)	177.30(20)
N(4)-Ni(1)-O(1)#2	85.20(20)	N(4)-Ni(1)-N(1)#3	92.80(20)	O(1)#2-Ni(1)-O(1W)	92.15(15)
O(2)#1-Ni(1)-O(4)	174.26(18)	O(1)#2-Ni(1)-N(1)#3	174.50(20)	O(4)-Ni(1)-O(1W)	91.59(15)
N(4)-Ni(1)-O(4)	88.99(19)	O(4)-Ni(1)-N(1)#3	86.80(20)	N(1)#3-Ni(1)-O(1W)	89.90(20)
Ni(1)#6-O(1W)-Ni(1)	115.10(20)				
Complex 2					
Ni(1)-O(1)	2.043(2)	Ni(1)-O(3)	2.106(2)	Ni(1)-N(3)	2.057(3)
Ni(1)-O(2)#1	2.070(2)	Ni(1)-O(1W)	2.093(2)	Ni(1)-N(1)	2.058(3)

O(1)-Ni(1)-N(3)	173.61(10)	O(1)-Ni(1)-O(2)#1	96.60(8)	O(1)-Ni(1)-O(1W)	92.62(7)
O(1)-Ni(1)-N(1)	85.05(9)	N(3)-Ni(1)-O(2)#1	88.87(10)	N(3)-Ni(1)-O(1W)	90.60(9)
N(3)-Ni(1)-N(1)	91.63(10)	N(1)-Ni(1)-O(2)#1	90.30(9)	N(1)-Ni(1)-O(1W)	177.49(8)
O(2)#1-Ni(1)-O(1W)	90.90(6)	N(3)-Ni(1)-O(3)	85.86(10)	O(2)#1-Ni(1)-O(3)	174.60(8)
O(1)-Ni(1)-O(3)	88.60(8)	N(1)-Ni(1)-O(3)	88.67(9)	O(1W)-Ni(1)-O(3)	90.34(7)
Ni(1)#1-O(1W)-Ni(1)	113.72(12)				

^a Symmetry transformations used to generate equivalent atoms: #1 $x+1/4, -y+9/4, z+1/4$; #2 $-x+1/4, y+1/4, z+1/4$; #3 $x+1/4, -y+7/4, z-1/4$; #6 $-x+1/2, -y+5/2, z$.

^b Symmetry transformations used to generate equivalent atoms: #1 $-x+1, y, -z+1/2$.
