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Supporting Information

Influence of Noncovalent Intermolecular Interactions on Crystal Packing: Syntheses and Crystal Structures of Three Layered Zn(II)/1, 2, 4-Triazole/Carboxylate Coordination Polymers

Zhe Song, Hongze Gao, Guanghua Li, Yang Yu, Zhan Shi*, and Shuohua Feng

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun 130012, People's Republic of China.

*To whom correspondence should be addressed. Fax: +86-431-85168624.

E-mail: zshi@mail.jlu.edu.cn.

Table S1. Selected bond distances /Å and bond angles /° for **1- 3**

Compound 1			
Zn(1)-O(2)	1.9886(13)	Zn(1)-N(1)#1	2.0026(12)
Zn(1)-N(3)	2.0106(13)	Zn(1)-N(2)#2	2.0231(13)
N(1)-Zn(1)#3	2.0026(12)	N(2)-Zn(1)#4	2.0231(13)
O(2)-Zn(1)-N(1)#1	127.63(6)	O(2)-Zn(1)-N(3)	102.89(5)
N(1)#1-Zn(1)-N(3)	112.21(6)	O(2)-Zn(1)-N(2)#2	100.99(5)
N(1)#1-Zn(1)-N(2)#2	103.74(5)	N(3)-Zn(1)-N(2)#2	107.63(6)
Compound 2			
Zn(1)-O(1)	1.960(6)	Zn(1)-N(4)	2.001(5)
Zn(1)-N(3)	2.016(5)	Zn(1)-N(5)#1	2.035(5)
Zn(2)-O(3)	1.943(5)	Zn(2)-N(2)#2	1.998(5)
Zn(2)-N(6)#3	2.019(5)	Zn(2)-N(1)	2.047(5)
Zn(3)-O(5)	1.956(5)	Zn(3)-N(11)#4	2.002(5)
Zn(3)-N(9)	2.013(5)	Zn(3)-N(10)	2.041(5)
Zn(4)-O(8)	1.953(6)	Zn(4)-N(7)	1.987(5)
Zn(4)-N(12)#5	2.017(5)	Zn(4)-N(8)#6	2.050(5)
O(1)-Zn(1)-N(4)	119.2(2)	O(1)-Zn(1)-N(3)	115.3(2)
N(4)-Zn(1)-N(3)	110.5(2)	O(1)-Zn(1)-N(5)#1	100.4(2)
N(4)-Zn(1)-N(5)#1	107.4(2)	N(3)-Zn(1)-N(5)#1	101.5(2)
O(3)-Zn(2)-N(2)#2	121.4(2)	O(3)-Zn(2)-N(6)#3	111.4(2)
N(2)#2-Zn(2)-N(6)#3	113.3(2)	O(3)-Zn(2)-N(1)	98.3(2)
N(2)#2-Zn(2)-N(1)	106.73(19)	N(6)#3-Zn(2)-N(1)	102.6(2)
O(5)-Zn(3)-N(11)#4	119.6(2)	O(5)-Zn(3)-N(9)	111.8(2)
N(11)#4-Zn(3)-N(9)	113.9(2)	O(5)-Zn(3)-N(10)	100.8(2)
N(11)#4-Zn(3)-N(10)	106.0(2)	N(9)-Zn(3)-N(10)	102.0(2)
O(8)-Zn(4)-N(7)	119.6(2)	O(8)-Zn(4)-N(12)#5	118.3(2)
N(7)-Zn(4)-N(12)#5	110.3(2)	O(8)-Zn(4)-N(8)#6	97.3(2)
N(7)-Zn(4)-N(8)#6	107.4(2)	N(12)#5-Zn(4)-N(8)#6	100.4(2)

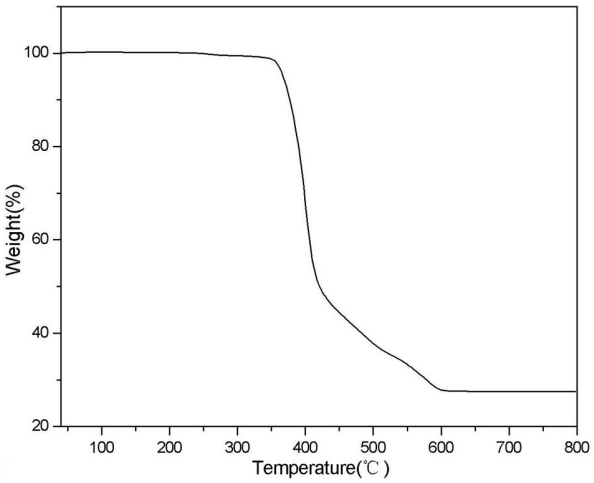
Compound 3

Zn(1)-O(1)	1.947(13)	Zn(1)-N(1)	1.983(13)
Zn(1)-N(9)	2.012(15)	Zn(1)-N(4)	2.054(11)
Zn(2)-O(3)	1.966(14)	Zn(2)-N(5)	1.980(13)
Zn(2)-N(12)	2.026(13)	Zn(2)-N(2)	2.030(11)
Zn(3)-O(6)	1.938(14)	Zn(3)-N(8)#1	1.959(13)
Zn(3)-N(3)	2.005(12)	Zn(3)-N(10)#2	2.051(11)
Zn(4)-O(8)	1.962(14)	Zn(4)-N(11)#3	2.009(13)
Zn(4)-N(7)	2.019(11)	Zn(4)-N(6)#2	2.029(12)
O(1)-Zn(1)-N(1)	122.1(5)	O(1)-Zn(1)-N(9)	115.5(6)
N(1)-Zn(1)-N(9)	110.7(5)	O(1)-Zn(1)-N(4)	96.6(6)
N(1)-Zn(1)-N(4)	107.1(5)	N(9)-Zn(1)-N(4)	101.0(5)
O(3)-Zn(2)-N(5)	120.9(6)	O(3)-Zn(2)-N(12)	114.4(6)
N(5)-Zn(2)-N(12)	111.9(5)	O(3)-Zn(2)-N(2)	97.3(5)
N(5)-Zn(2)-N(2)	107.6(5)	N(12)-Zn(2)-N(2)	101.4(5)
O(6)-Zn(3)-N(8)#1	118.9(6)	O(6)-Zn(3)-N(3)	116.8(6)
N(8)#1-Zn(3)-N(3)	112.0(5)	O(6)-Zn(3)-N(10)#2	96.9(6)
N(8)#1-Zn(3)-N(10)#2	107.7(5)	N(3)-Zn(3)-N(10)#2	101.1(5)
O(8)-Zn(4)-N(11)#3	122.0(5)	O(8)-Zn(4)-N(7)	98.7(5)
N(11)#3-Zn(4)-N(7)	105.9(5)	O(8)-Zn(4)-N(6)#2	116.0(6)
N(11)#3-Zn(4)-N(6)#2	109.9(5)	N(7)-Zn(4)-N(6)#2	100.6(5)

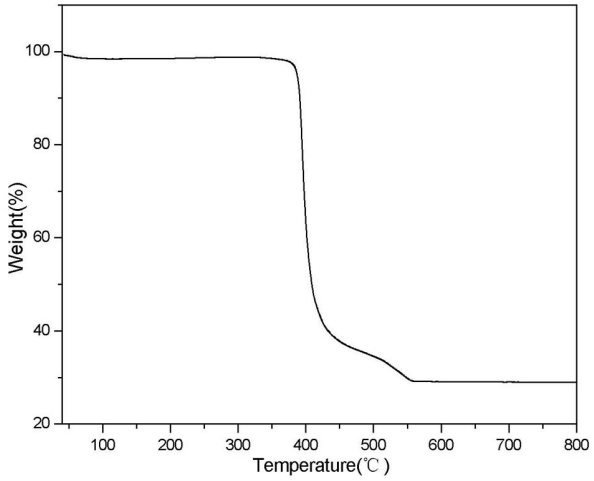
Symmetry codes for **1**: #1 (x,-y+1/2,z+1/2), #2 (-x-1,y+1/2,-z-1/2), #3 (x,-y+1/2,z-1/2), #4 (-x-1,y-1/2,-z-1/2); for **2**: #1 (-x+1,-y+3,-z), #2 (-x+2,-y+2,-z), #3 (-x+1,-y+2,-z), #4 (-x,-y+1,-z+1), #5 (-x,-y,-z+1), #6 (-x-1,-y,-z+1); for **3**: #1 (x-1/2,y+1/2,z), #2 (x+1/2,y+1/2,z), #3 (x+1,y,z).

Figure S1. TGA plots of compound **1** (a), **2** (b) and **3** (c).

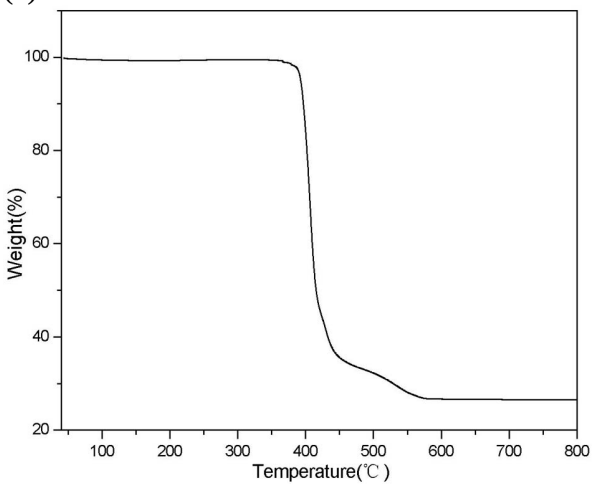
(a)



(b)



(c)



TG analysis. TGA of each compound was performed using a Netzsch STA 449C instrument. Each sample was heated from room temperature to 800 °C in air with a heating rate of 10.0 °C /min. The TGA curve of compound **1** displays one continuous events between 40 and 800 °C. The structure of compound **1** is stable up to 350 °C. The event occurred at 350 – 600 °C where the organic linkers got destroyed (observed, 72.47 %; calculated, 72.68 %) (Figure S1 a). TGA of **2** first shows a weight loss (found 0.83 %) from 40 to 120 °C, which is attributed to the loss of guest water molecules (calcd 0.82 %). The structure is stable up to 385 °C. A sharp weight loss observed between 385 and 540 °C. The total weight loss was 70.17 %, which corresponds to the loss of organic linker groups (calcd 69.55 %) (Figure S1 b). The TGA curve of compound **3** is similar to compound **1** and **2**. It is stable up to 400 °C. The event occurred at 400 – 580 °C where the organic linkers got destroyed (observed, 73.48 %; calculated, 71.84 %) (Figure S1 c).

Figure S2. The coordination environment of compounds **1** (a), **2** (b) and **3** (c).