Electronic Supplementary Information (ESI)

Structures and photoluminescence of zinc(II) coordination polymers based on in situ generated 1H-tetrazolate-5-propionic acid ligands

Mei-Feng Wu,[a,b] Zhi-Fa Liu,[a,b] Shuai-Hua Wang,[a,b] Jun Chen,[a,b] Gang Xu,[a] Fa-Kun Zheng,*[a] Guo-Cong Guo*[a] and Jin-Shun Huang[a]

[a] *State Key Laboratory of Structural Chemistry, Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, Fuzhou, Fujian 350002, P. R. China.*

[b] *Graduate school, Chinese Academy of Sciences, Beijing 100039, P. R. China.*

E-mail: zfk@fjirsm.ac.cn;Fax: +86 591 83714946.

Table S1 The selected bond distances for **1**–**3**.

1			
Zn(1)-O(2)#1	1.982(3)	Zn(1)-O(1)	1.997(4)
Zn(1)-N(1)#2	1.994(4)	Zn(1)-N(4)#3	2.003(3)
O(2)#1-Zn(1)-N(1)#2	123.39(9)	N(1)#2-Zn(1)-O(1)	98.58(10)
O(2)#1-Zn(1)-O(1)	100.71(12)	O(2)#1-Zn(1)-N(4)#3	109.49(13)
N(1)#2-Zn(1)-N(4)#3	117.62(14)	O(1)-Zn(1)-N(4)#3	101.91(10)
2			
Zn(1)-O(3)	1.905(2)	Zn(1)-N(4)#1	2.016(3)
Zn(1)-O(1)	1.989(2)	Zn(1)-N(7)	2.020(2)
Zn(2)-O(3)	1.9926(19)	Zn(2)-N(6)	2.169(2)
Zn(2)-O(2)	2.132(2)	Zn(2)-N(1)#2	2.190(3)
Zn(2)-N(5)	2.165(2)	Zn(2)-N(7)#3	2.449(3)
O(3)-Zn(1)-O(1)	108.11(8)	O(3)-Zn(2)-O(2)	99.79(8)
O(3)-Zn(1)-N(4)#1	112.10(9)	O(3)-Zn(2)-N(5)	165.53(8)
O(1)-Zn(1)-N(4)#1	106.43(9)	O(2)-Zn(2)-N(5)	90.27(9)
O(3)-Zn(1)-N(7)	114.64(9)	O(3)-Zn(2)-N(6)	92.98(9)
O(1)-Zn(1)-N(7)	106.60(10)	O(2)-Zn(2)-N(6)	165.88(8)
N(4)#1-Zn(1)-N(7)	108.51(11)	N(5)-Zn(2)-N(6)	76.11(9)
O(3)-Zn(2)-N(1)#2	92.02(9)	O(3)-Zn(2)-N(7)#3	85.32(9)
O(2)-Zn(2)-N(1)#2	91.35(8)	O(2)-Zn(2)-N(7)#3	84.14(8)
N(5)-Zn(2)-N(1)#2	98.16(9)	N(5)-Zn(2)-N(7)#3	85.39(9)
N(6)-Zn(2)-N(1)#2	94.21(9)	N(6)-Zn(2)-N(7)#3	90.98(9)
N(1)#2-Zn(2)-N(7)#3	174.29(9)		
3			
Zn(1)-O(1)#1	1.9494(19)	Zn(1)-N(1)	2.019(2)
Zn(1)-N(4)#2	1.990(2)	Zn(1)-N(5)	2.037(2)
O(1)#1-Zn(1)-N(4)#2	108.00(8)	O(1)#1-Zn(1)-N(5)	124.77(10)
O(1)#1-Zn(1)-N(1)	108.47(9)	N(4)#2-Zn(1)-N(5)	100.87(10)
N(4)#2-Zn(1)-N(1)	101.88(10)	N(1)-Zn(1)-N(5)	110.22(9)

[a] Symmetry codes for **1**: (#1) x, –y + 1/2, z – 1/2; (#2) x + 1, y, z; (#3) –x, y – 1/2, – z+ 1/2; for **2**: (#1) x – 1, y, z; (#2) –x + 1, –y, –z + 2; (#3) –x, –y, –z + 1; for **3**: (#1) –x, –y + 1, –z; (#2) x, –y + 3/2, z – 1/2.

Fig. S1 The IR spectra of **1**–**3**.

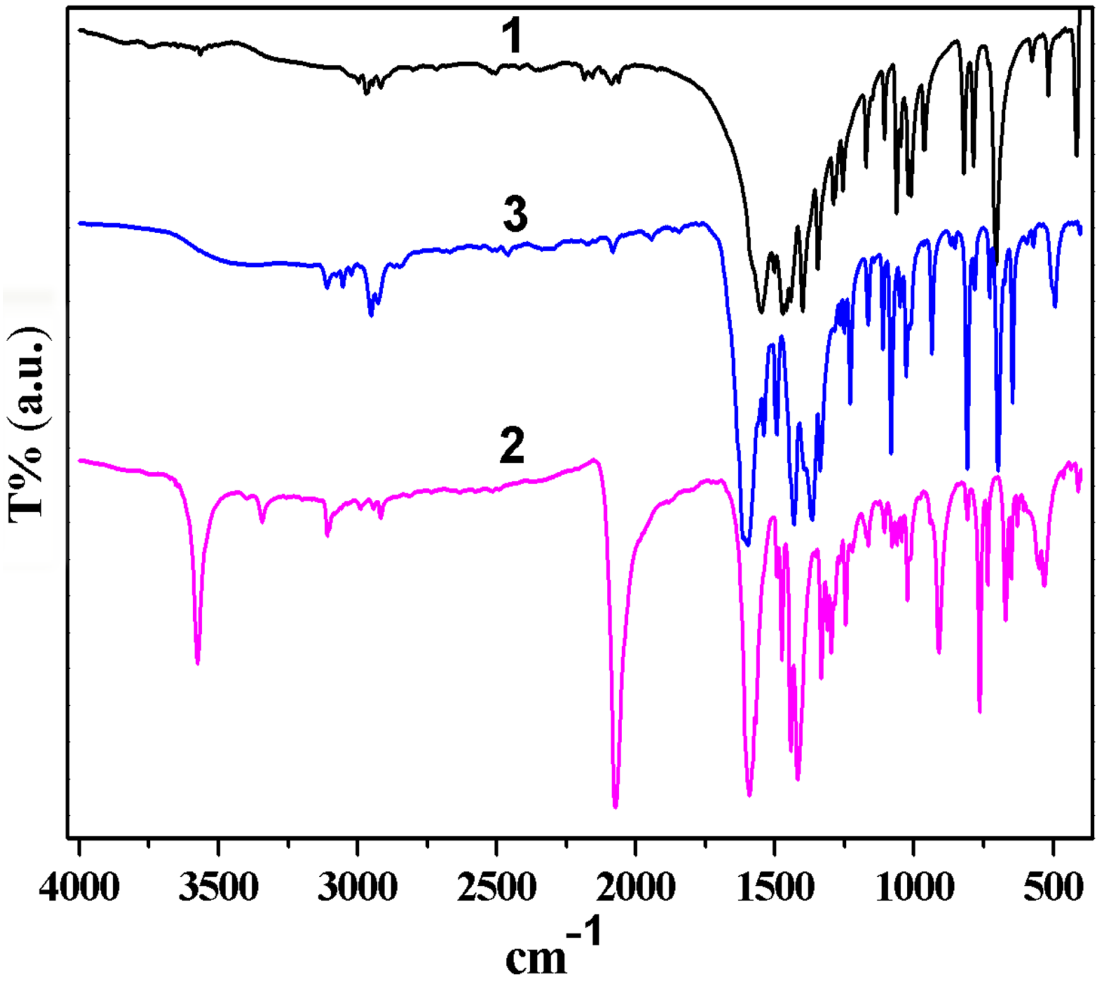

Fig. S2 Powdered *X*-ray diffraction (PXRD) patterns of **1–3**. The black and red lines represent simulated and experimental results, respectively.

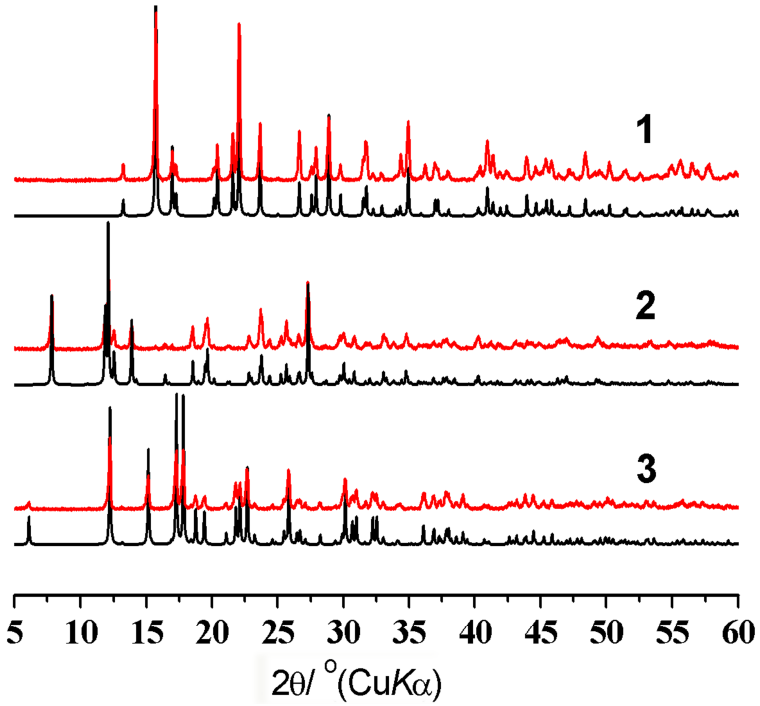

Fig. S3 The 2-D network in **1** constructed by the linkages between Zn(II) atoms and O1, N1 and N4 atoms from μ_4-κO1:κO2:κN1:κN4 tzp^{2-} ligands.

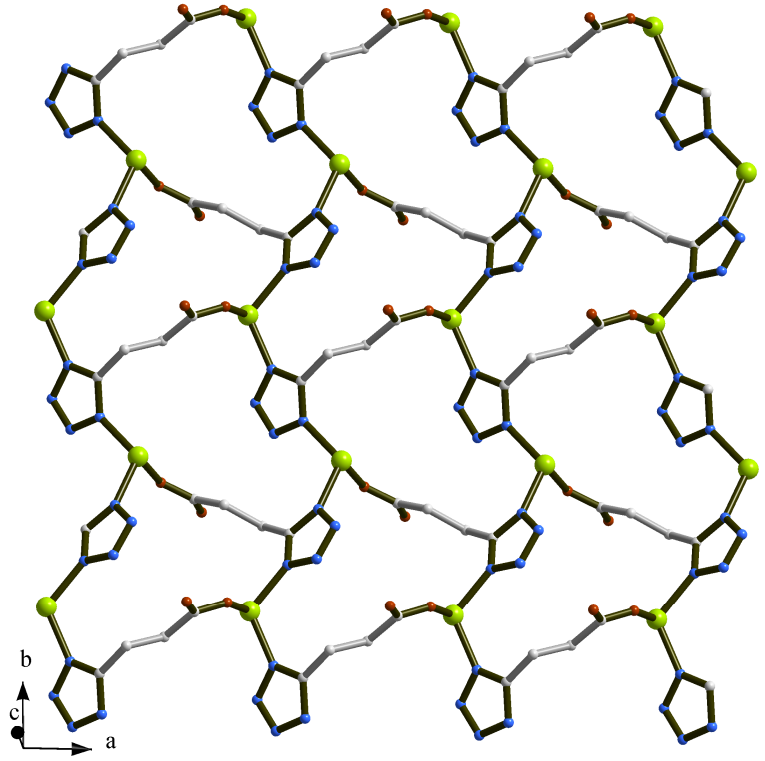

Fig. S4 View of the excited spectra of **1–3** for the strongest maximum emission at 432, 425 and 420nm, respectively.

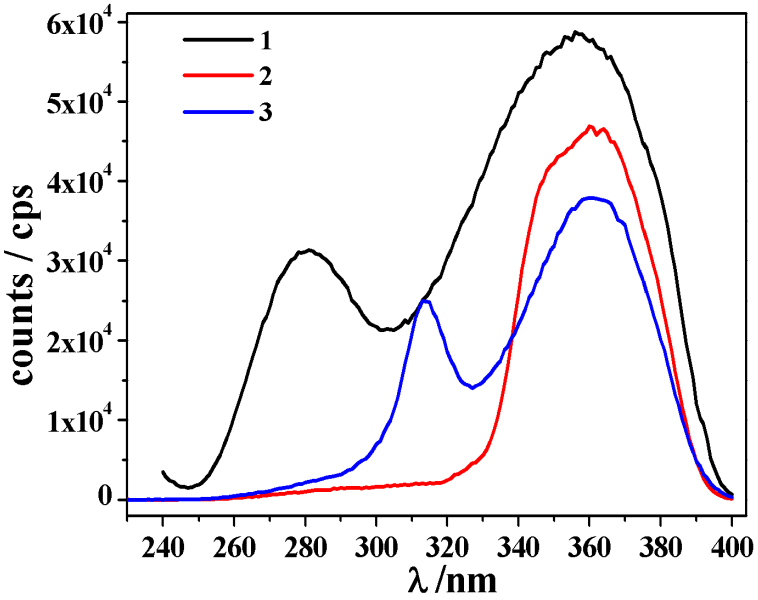

Fig. S5 The TGA curves of **1**–**3**.