Charge-controlled Formation of Zn(II) Coordination Polymers from 1D to 3D with Triazole-carboxylate Ligands: Syntheses, Structures, and Luminescent Properties

Shao-Bin Miao, Xiao-Juan Sun, Ke-Xin Wang, Chun-Ying Xu, Zhao-Hao Li, Zhi-Qiang, Wang*

[†]Henan Key Laboratory of Function-Oriented Porous Materials, and College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471934, China

*(Z.-Q. Wang) Email: wzq197811@163.com

Table S1. Selected Bond Lengths (Å) and Bond Angles (°) for **1**–**3**

Bond lengths (Å)		Bond angles (°)	
Compound **1**			
Zn01–O3#1	2.1400(18)	O3#1–Zn01–O3	180.0
Zn01–O3	2.1400(18)	O3–Zn01–N3#2	90.93(8)
Zn01–N3#3	2.159(2)	O3–Zn01–N3#2	89.07(8)
Zn01–N3#2	2.159(2)	O3–Zn01–N3#3	89.07(8)
Zn01–N6#1	2.148(2)	O3–Zn01–N3#3	90.93(8)
Zn01–N6	2.148(2)	O3–Zn01–N6#1	91.18(8)
		O3–Zn01–N6	91.18(8)
		O3–Zn01–N6#1	88.82(8)
		O3–Zn01–N6	88.82(8)
		N3#2–Zn01–N3#3	180.00(6)
		N6–Zn01–N3#3	87.68(8)
		N6–Zn01–N3#2	92.32(8)
		N6–Zn01–N3#2	87.68(8)
		N6–Zn01–N3#3	92.32(8)
		N6–Zn01–N6	180.0
Symmetry transformations used to generate equivalent atoms: #1 – *x*, 1 – *y*, 1 – *z*; #2 1/2 – *x*, 1/2 – *y*, *z*; –1/2 + *x*, 1/2 + *y*, 1 – *z*.			
Compound **2**			
Zn01–O1	1.975(3)	O1–Zn01–O3#1	121.39(14)
Zn01–O3#1	2.132(3)	O1–Zn01–O4#1	176.86(16)
Zn01–O4#1	2.304(4)	O1–Zn01–O5	92.76(16)
Zn01–O5	2.155(4)	O1–Zn01–O6	89.19(15)
Zn01–O6	2.157(4)	O1–Zn01–N3#2	94.40(16)
Zn01–N3#2	2.117(4)	O3#1–Zn01–O4#1	58.87(13)
		O3#1–Zn01–O5	87.49(15)
		O3#1–Zn01–O6	88.79(14)
		O5–Zn01–O4#1	90.38(16)
		O5–Zn01–O6	176.27(14)
		O6–Zn01–O4#1	87.69(15)
		N3#2–Zn01–O3#1	144.07(15)
		N3#2–Zn01–O4#1	85.57(15)
		N3#2–Zn01–O5	87.85(17)
		N3#2–Zn01–O6	95.18(16)
Symmetry transformations used to generate equivalent atoms: #1 *x*, 1/2 – *y*, –1/2 + *z*; #2 *x*, –1 + *y*, *z*.			
Compound **3**			
Zn1–O6#3	2.137(3)	O6#5–Zn1–O6#3	161.5(2)
Zn1–O6#5	2.137(3)	O7–Zn1–O6#5	102.8(3)
Zn1–O7	2.039(9)	O7–Zn1–O6#3	95.3(3)
Zn1–N6	2.069(4)	O7–Zn1–N6	89.1(3)

Zn1–N6#4	2.069(4)	O7–Zn1–N6#4	112.0(3)
Zn2–O1	1.948(3)	N6–Zn1–O6#3	92.17(15)
Zn2–O3	1.942(4)	N6#4–Zn1–O6#3	84.45(15)
Zn2–O5#2	1.968(4)	N6#4–Zn1–O6#5	92.17(15)
Zn2–N3#1	2.064(4)	N6–Zn1–O6#5	84.45(15)
		N6–Zn1–N6#4	158.9(3)
		O1–Zn2–O5#2	103.81(16)
		O1–Zn2–N3#1	96.60(15)
		O3–Zn2–O1	136.52(18)
		O3–Zn2–O5#2	108.55(19)
		O3–Zn2–N3#1	98.15(19)
		O5#2–Zn2–N3#1	110.88(17)

Symmetry transformations used to generate equivalent atoms: #1 –1/2 + *x*, 1/2 + *y*, *z*; *x*, 1 + *y*, *z*; *x*, 1 – *y*, –1/2 + *z*; 1 – *x*, *y*, 1/2 – *z*; 1 – *x*, 1 – *y*, 1 – *z*.

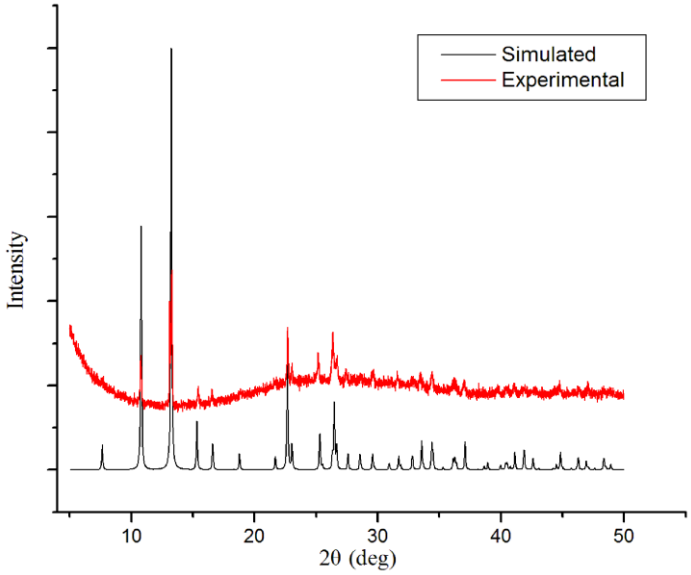

Fig. S1. Experimental (red) and simulated (black) PXRD patterns of compound **1**.

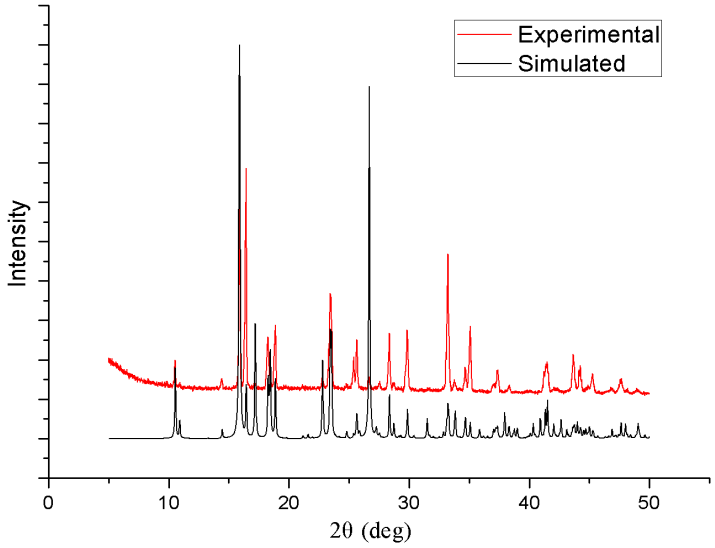

Fig. S2. Experimental (red) and simulated (black) PXRD patterns of compound **2**.

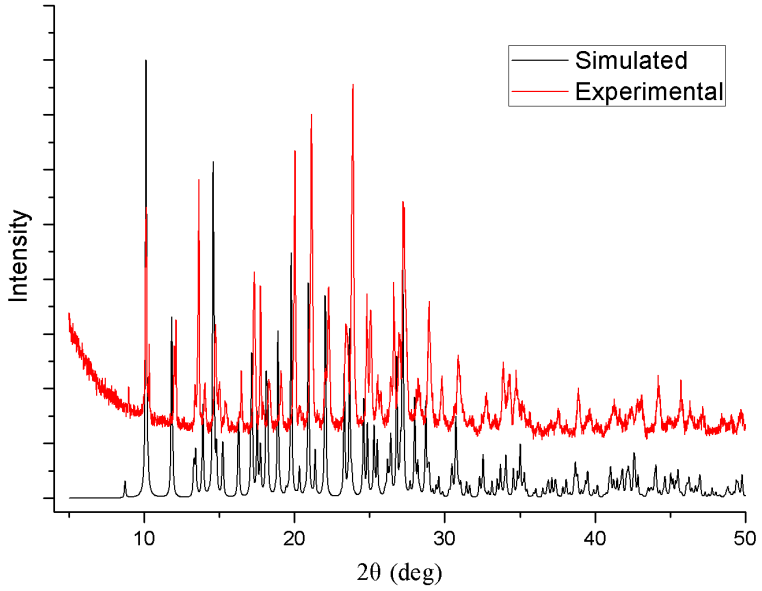

Fig. S3. Experimental (red) and simulated (black) PXRD patterns of compound **3**.