

Supporting Information for

Syntheses, crystal structures and luminescent properties of four Zn(II) coordination polymers with pyrazolone derivatives and 4,4'-bipyridine

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Table S1. Selected bond lengths (Å) and angles (°) for the complexes **1-4**.

Complex 1			
Zn-O1	2.010(3)	Zn-O2	2.078(3)
Zn-N3	1.993(4)	Zn-N6	2.078(4)
Zn-N7A	2.066(5)		
N3-Zn-O1	92.78(16)	N3-Zn-N7A	139.84(18)
O1-Zn-N7A	92.20(16)	N3-Zn-N6	113.76(17)
O1-Zn-N6	94.78(15)	N7A-Zn-N6	105.47(18)
N3-Zn-O2	78.87(14)	O1-Zn-O2	169.02(16)
N7A-Zn-O2	89.74(15)	N6-Zn-O2	95.11(15)
Complex 2			
Zn-O1	2.022(3)	Zn-O2	2.027(3)
Zn-N3	2.051(3)	Zn-N6	2.061(3)
Zn-N7A	2.138(3)		
O1-Zn-O2	164.30 (11)	O1-Zn-N3	90.40(12)
O2-Zn-N3	79.10(12)	O1-Zn-N6	91.84(12)
O2-Zn-N6	94.00(12)	N3-Zn-N6	159.37(13)
O1-Zn-N7A	92.02(12)	O2-Zn-N7A	100.49(12)
N3-Zn-N7A	95.32(13)	N6-Zn-N7A	105.09(12)
Complex 3			
Zn1-O1	1.985(3)	Zn1-O2	2.147(3)
Zn1-N3	1.982(4)	Zn1-O4	2.033(3)
Zn1-N16	2.031(4)		
Zn2-O2	2.112(3)	Zn2-O3	1.959(3)
Zn2-O4	2.093(3)	Zn2-N8	2.068(4)
Zn2-N15A	2.094(4)		
Zn3-O5	2.013(3)	Zn3-O6	2.077(3)
Zn3-N10	2.064(4)	Zn3-N13	2.018(4)
Zn3-N5B	2.081(4)		
N3-Zn1-O1	93.55(15)	N16-Zn1-O4	113.45(16)
N3-Zn1-N16	137.89(17)	N3-Zn1-O2	79.11(14)
O1-Zn1-N16	90.42(16)	O1-Zn1-O2	172.48(14)

N3-Zn1-O4	107.40(14)	N16-Zn1-O2	96.13(14)
O1-Zn1-O4	98.26(14)	O4-Zn1-O2	82.54(12)
O3-Zn2-N8	90.48(14)	O4-Zn2-N15A	94.26(14)
O3-Zn2-O4	166.97(13)	O3-Zn2-O2	105.13(13)
N8-Zn2-O4	76.52(13)	N8-Zn2-O2	116.62(14)
O3-Zn2-N15A	96.31(15)	O4-Zn2-O2	82.00(12)
N8-Zn2-N15A	147.53(15)	N15A-Zn2-O2	92.20(14)
Zn1-O2-Zn2	95.38(12)	Zn1-O4-Zn2	99.55(13)
O5-Zn3-N13	92.02(14)	N10-Zn3-O6	95.09(14)
O5-Zn3-N10	92.02(14)	O5-Zn3-N5B	92.35(14)
N13-Zn3-N10	111.22(15)	N13-Zn3-N5B	138.49(15)
O5-Zn3-O6	169.78(12)	N10-Zn3-N5B	109.84(15)
N13-Zn3-O6	78.58(14)	O6-Zn3-N5B	92.12(14)
Complex 4			
Zn-O1	2.0552(18)	Zn-O2	2.0962(18)
Zn-N3	2.092(2)	Zn-N5A	2.127(2)
Zn-N6	2.233(2)	Zn-N7B	2.280(10)
O1-Zn-N3	88.03(8)	O2-Zn-N6	91.23(9)
O1-Zn-O2	166.65(7)	N5A-Zn-N6	86.44(8)
N3-Zn-O2	78.88(8)	O1-Zn-N7B	90.5(5)
O1-Zn-N5A	91.80(8)	N3-Zn-N7B	92.2(4)
N3-Zn-N5A	177.69(9)	O2-Zn-N7B	87.2(6)
O2-Zn-N5A	101.39(8)	N5A-Zn-N7B	91.1(4)
O1-Zn-N6	91.79(8)	N6-Zn-N7B	176.73(17)
N3-Zn-N6	91.26(8)		

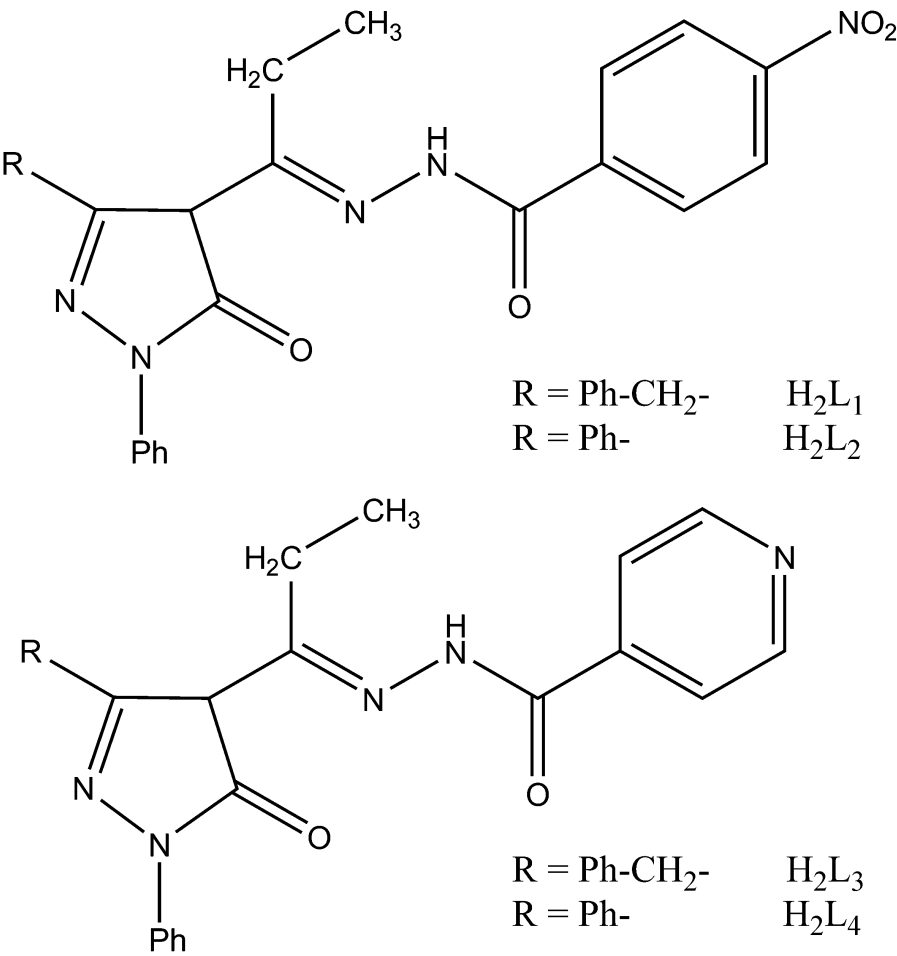
Symmetry mode: For **1**, A: -x+1/2, y+1/2, -z+1/2; For **2**, A: -x+1/2, y-1/2, -z+1/2; For **3**, A: -x+3/2, y-1/2, -z+3/2,
B: x+1/2, -y+1/2, z+1/2; For **4**, #1: x, -y+3/2, z+1/2; #2: x+1, y, z.

Table S2. Distance (Å) and angles (°) of hydrogen bonds for the complexes **1-4**.

D-H...A	Distance (H...A)	Distance (D...A)	Angle (D-H-A)
Complex 1			
O5-H5D...O2#1	1.9800	2.826(10)	179.00
C25-H25...O5#2	2.4900	3.324(12)	150.00
Complex 2			
C19-H19B...O3#1	2.5500	3.511(5)	165.00
O5-H5D...O4	2.0200	2.866(7)	178.00
Complex 3			
C22-H22...O6#1	2.4600	3.046(6)	120.00
C24-H24A...O3	2.5800	3.245(6)	127.00
C76-H76A...N7#2	2.6100	3.483(7)	152.00
Complex 4			
C27-H27...O3	2.5000	3.354(5)	151.00

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

1/2-z. For **2**: #1: 1/2+x, 1/2-y, -1/2+z. For **3**: #1: -1/2+x, 1/2-y, -1/2+z. #2: x, 1+y, z.



Scheme S1. The structure of ligands H_2L_1 - H_2L_4 .

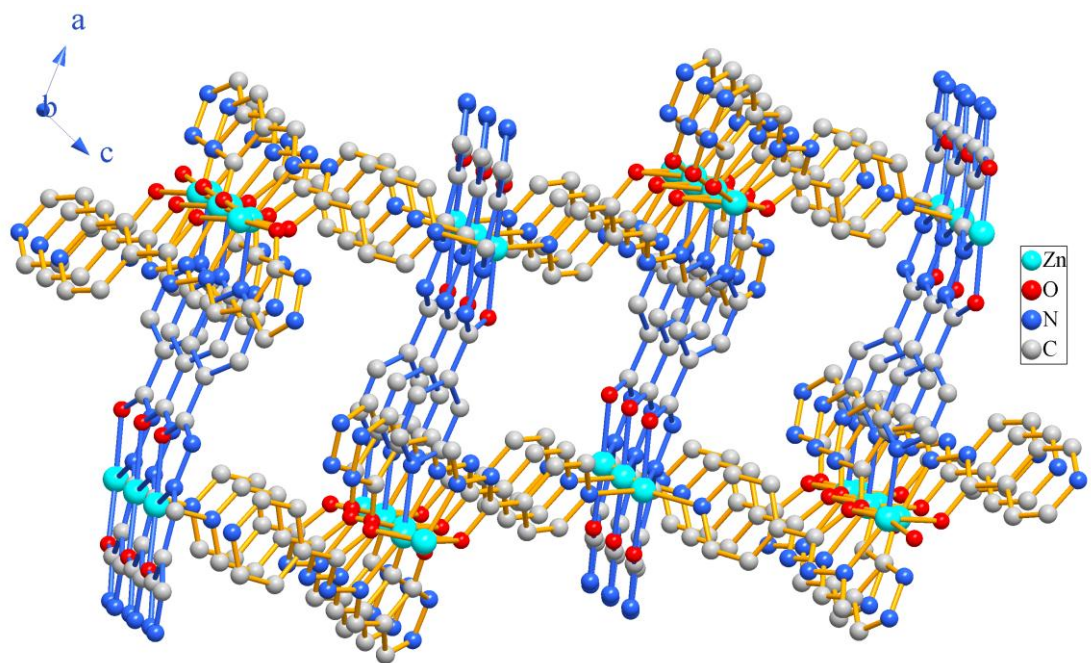


Figure S1. Perspective view of the 2D network structure of **3** formed by the coordination of the ligand and Zn(II) atom along the *b*-axis. The ligands C are indicated by the blue line.

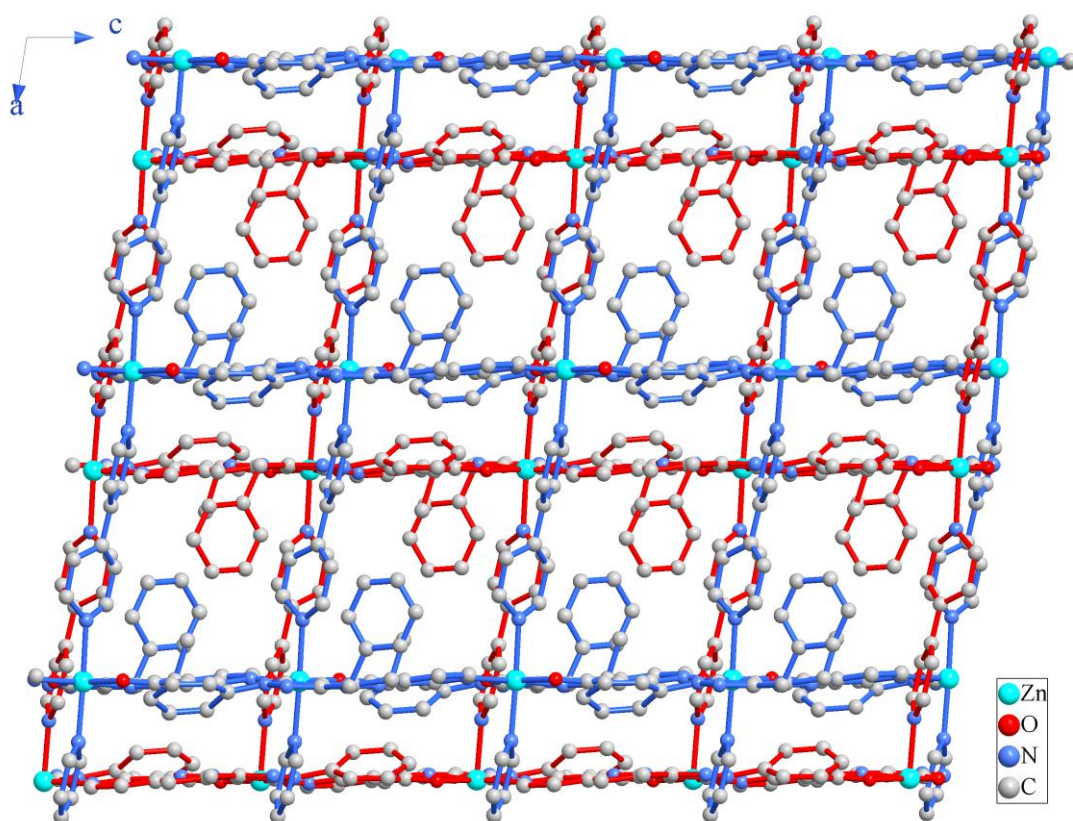


Figure S2. The crystal packing diagram of **4**.