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Electronic supplementary information (ESI)

Bipyridine-triggered modulation of structure and properties of zinc-diphosphonates: coordination role *vs* template rule

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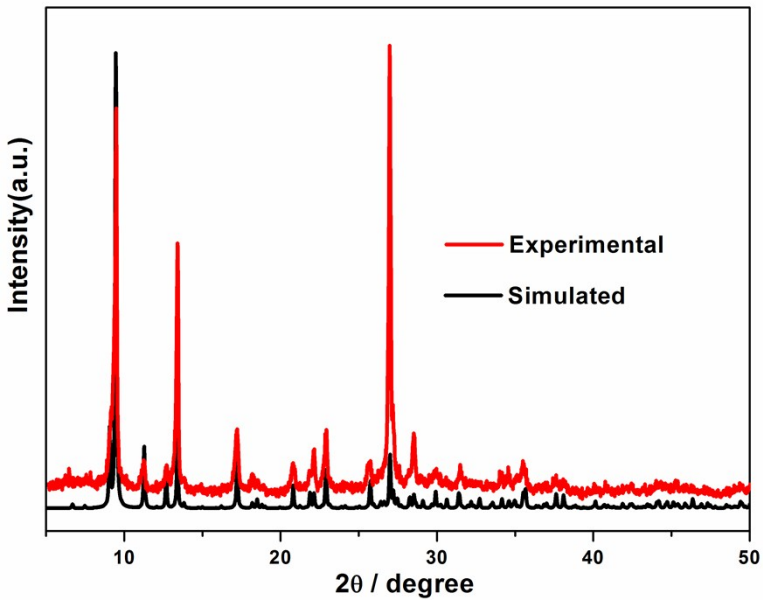

Fig. S1 PXRD patterns of **1**.

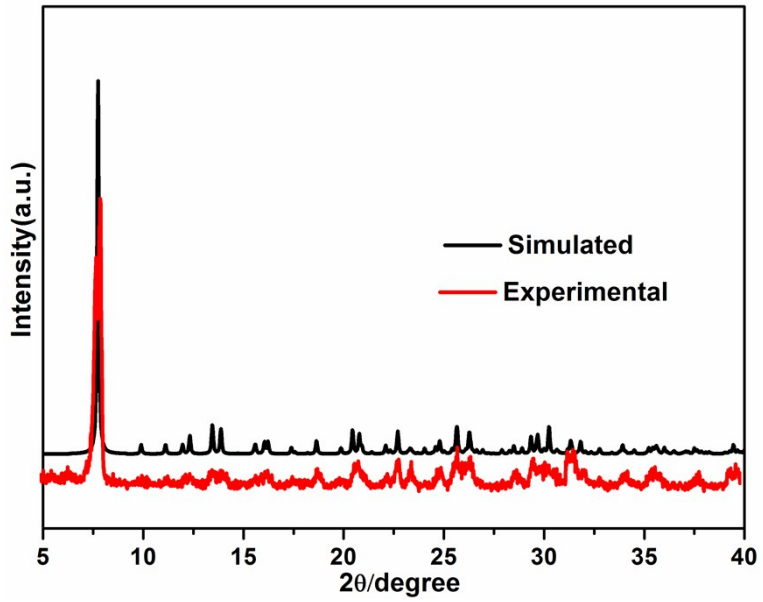

Fig. S2 PXRD patterns of **2**.

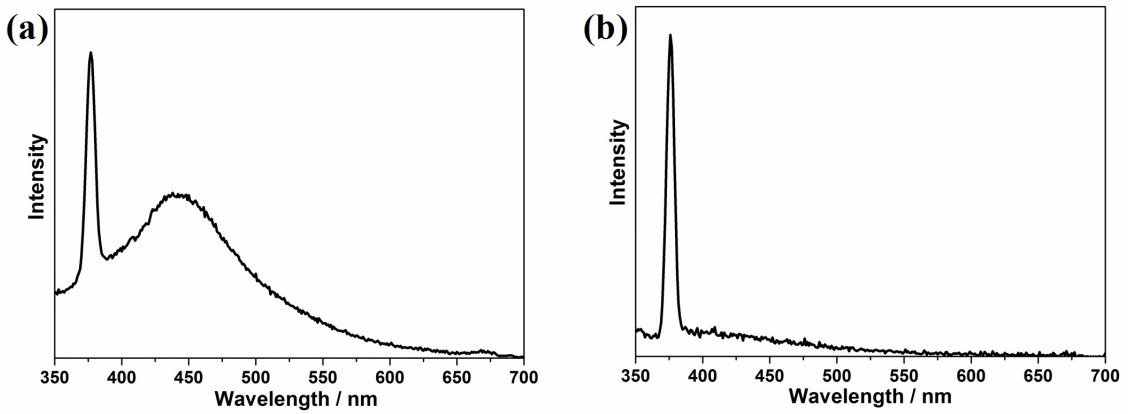

Fig. S3 The emission spectra of 4,4'-bipy (a) and HEDP (b) in water solution upon excitation at 332 nm.

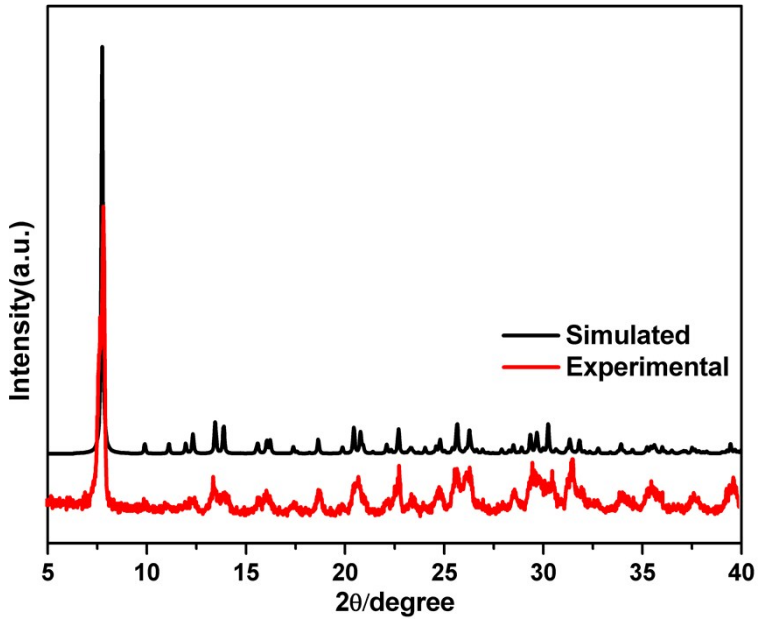

Fig. S4 The PXRD plots of **2** after proton-conducting measurements.

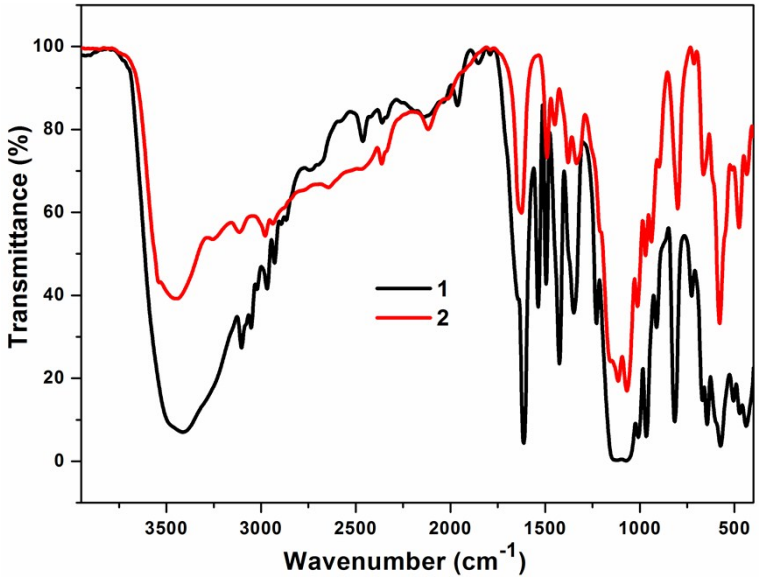

Fig. S5 IR patterns of **1** and **2**.

Table S1. Selected bond lengths (Å) and angles (°) for **1**

N(1)-Zn(1)	2.028(5)	O(5)-Zn(4)	1.972(4)
O(1)-Zn(1)	1.896(4)	O(7)-Zn(4)#3	1.927(4)
O(9)-Zn(1)	1.952(4)	O(2)-P(1)	1.531(5)
O(11)-Zn(1)	1.965(4)	O(1)-P(1)	1.515(5)
N(3)-Zn(2)	2.010(5)	O(3)-P(1)	1.527(4)
O(6)-Zn(2)#2	1.916(4)	O(5)-P(2)	1.517(4)
O(8)-Zn(2)	1.960(4)	O(6)-P(2)	1.524(4)
O(10)-Zn(2)	1.942(4)	O(4)-P(2)	1.517(4)
N(2)-Zn(3)#1	2.022(5)	O(7)-P(3)	1.526(4)
O(3)-Zn(3)	1.950(4)	O(8)-P(3)	1.521(4)
O(4)-Zn(3)	1.938(4)	O(9)-P(3)	1.519(4)
O(12)-Zn(3)	1.913(4)	O(10)-P(4)	1.519(4)
N(4)-Zn(4)#1	2.012(5)	O(11)-P(4)	1.524(4)
O(2)-Zn(4)	1.948(4)	O(12)-P(4)	1.511(5)
O(1)-Zn(1)-O(9)	120.9(2)	O(12)-Zn(3)-O(4)	123.0(2)
O(1)-Zn(1)-O(11)	108.53(2)	O(12)-Zn(3)-O(3)	107.21(2)
O(9)-Zn(1)-O(11)	102.36(2)	O(4)-Zn(3)-O(3)	101.66(2)
O(1)-Zn(1)-N(1)	108.30(2)	O(12)-Zn(3)-N(2)#4	106.4(2)
O(9)-Zn(1)-N(1)	104.90(2)	O(4)-Zn(3)-N(2)#4	104.8(2)
O(11)-Zn(1)-N(1)	111.70(2)	O(3)-Zn(3)-N(2)#4	114.0(2)
O(6)#3-Zn(2)-O(10)	112.20(2)	O(7)#2-Zn(4)-O(2)	111.70(2)
O(6)#3-Zn(2)-O(8)	112.26(2)	O(7)#2-Zn(4)-O(5)	113.59(2)
O(10)-Zn(2)-O(8)	102.60(2)	O(2)-Zn(4)-O(5)	103.01(2)
O(6)#3-Zn(2)-N(3)	108.90(2)	O(7)#2-Zn(4)-N(4)#4	110.50(2)
O(10)-Zn(2)-N(3)	112.60(2)	O(2)-Zn(4)-N(4)#4	111.60(2)
O(8)-Zn(2)-N(3)	108.20(2)	O(5)-Zn(4)-N(4)#4	106.20(2)

Symmetry codes: #1: x-1/2, -y+1/2, z+1/2; #2: x+1, y, z; #3: x-1, y, z; #4: x+1/2, -y+1/2, z-1/2.

Table S2. Selected bond lengths (Å) and angles (°) for **2**

O(1)-Zn(1)	2.012(3)	O(10)-Zn(3)#2	1.962(3)
O(5)-Zn(1)	1.980(4)	O(2)-P(1)	1.517(4)
O(7)-Zn(1)	2.018(3)	O(1)-P(1)	1.522(3)
O(12)-Zn(1)	2.425(4)	O(3)-P(1)	1.519(3)
O(14)-Zn(1)	2.194(4)	O(4)-P(2)	1.512(4)
O(15)-Zn(1)	2.110(4)	O(5)-P(2)	1.502(4)
O(4)-Zn(2)	1.931(4)	O(6)-P(2)	1.574(4)
O(8)-Zn(2)#4	1.925(4)	O(7)-P(3)	1.520(4)
O(11)-Zn(2)#4	1.973(3)	O(8)-P(3)	1.510(3)
O(12)-Zn(2)	1.946(3)	O(9)-P(3)	1.500(3)
O(2)-Zn(3)#2	1.938(4)	O(10)-P(4)	1.523(4)
O(3)-Zn(3)#3	1.937(4)	O(11)-P(4)	1.516(3)
O(9)-Zn(3)	1.915(3)	O(12)-P(4)	1.537(4)
O(5)-Zn(1)-O(1)	96.32(2)	O(14)-Zn(1)-O(12)	77.97(1)
O(5)-Zn(1)-O(7)	94.23(2)	O(8)#4-Zn(2)-O(4)	113.51(2)
O(1)-Zn(1)-O(7)	169.18(2)	O(8)#4-Zn(2)-O(12)	116.08(2)
O(5)-Zn(1)-O(15)	101.75(2)	O(4)-Zn(2)-O(12)	102.43(2)
O(1)-Zn(1)-O(15)	93.87(2)	O(8)#4-Zn(2)-O(11)#4	99.25(1)
O(7)-Zn(1)-O(15)	86.31(2)	O(4)-Zn(2)-O(11)#4	112.15(2)
O(5)-Zn(1)-O(14)	165.24(2)	O(12)-Zn(2)-O(11)#4	113.95(2)
O(1)-Zn(1)-O(14)	88.00(1)	O(9)-Zn(3)-O(3)#3	103.95(2)
O(7)-Zn(1)-O(14)	81.18(1)	O(9)-Zn(3)-O(2)#5	108.08(2)
O(15)-Zn(1)-O(14)	91.99(2)	O(3)#3-Zn(3)-O(2)#5	113.84(2)
O(5)-Zn(1)-O(12)	87.55(1)	O(9)-Zn(3)-O(10)#5	103.65(1)
O(1)-Zn(1)-O(12)	95.71(1)	O(3)#3-Zn(3)-O(10)#5	98.90(2)
O(7)-Zn(1)-O(12)	82.32(1)	O(2)#5-Zn(3)-O(10)#5	126.05(2)
O(15)-Zn(1)-O(12)	165.84(1)		

Symmetry codes: #1: -x+2, -y+1, -z+1; #2: x-1, y, z; #3: -x+1, -y+2, -z+2; #4: -x+1, -y+2, -z+1; #5: x+1, y, z.