Electronic Supplementary Information (ESI)

Zinc-diphosphonates with extended dipyridine units: synthesis, structures, in situ reaction, and photochromism

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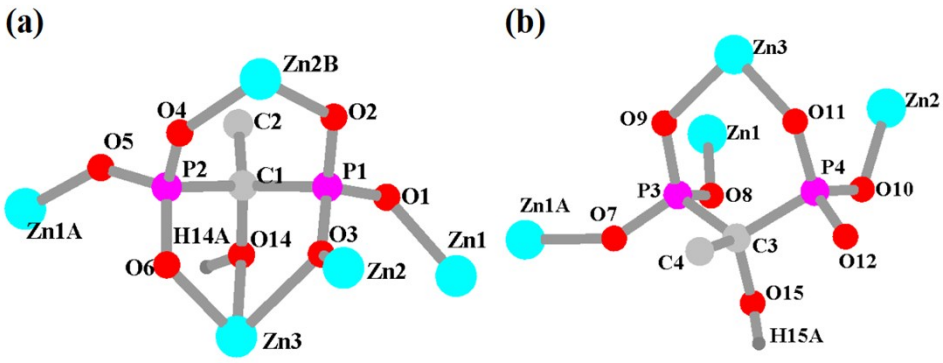

Fig. S1 The coordination mode of diphosphonate ligand in **1** (H atoms for CH_3 group are omitted for clarity).

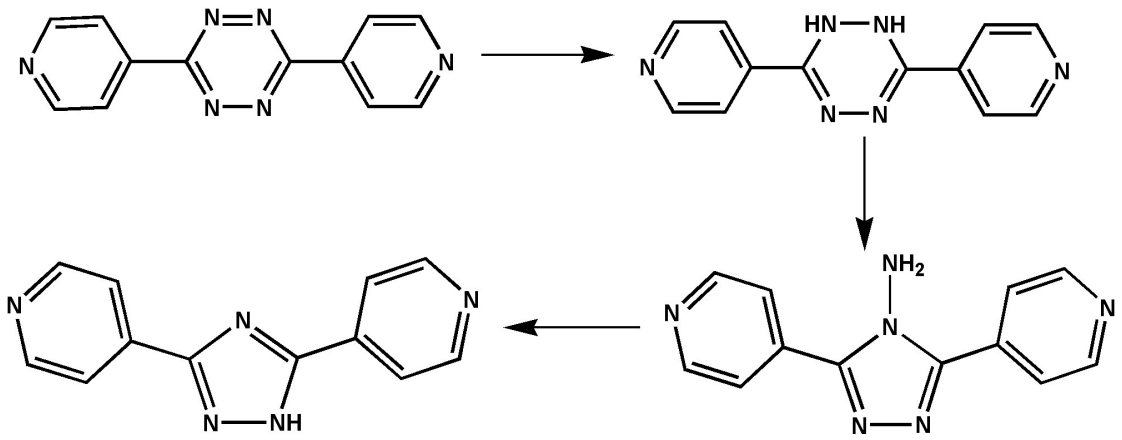

Fig. S2 The possible formation routines of the in situ generated Hdpt from dipytz.

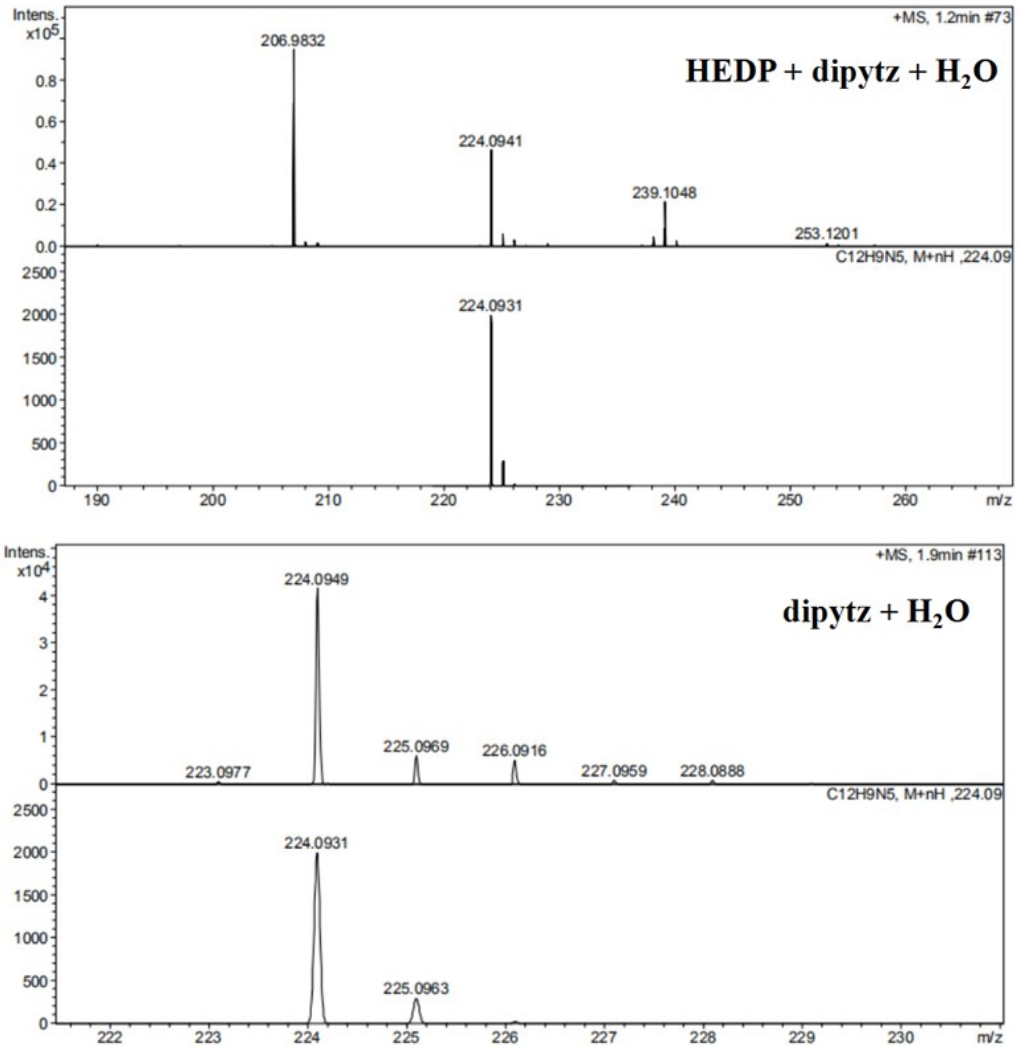

Fig. S3 The high resolution mass spectrometry of the reactant liquors.

Table S1. Reactant liquors for mass spectrum determination

Sequence	H_2O/mL	dipytz/g	HEDP/mL	Temp/°C	Time/days
I	5	0.4	0.5	145	7
II	5	0.4	0	145	7

Table S2. Reactant liquors for ammonium ion determination

Sequence	H_2O/mL	dipytz/g	HEDP/mL	ZnO/g	LiF/g	Temp/°C	Time/days
I	5	0.4	0.5	0	0	145	7
II	5	0.4	0.5	0.08	0.1	145	7

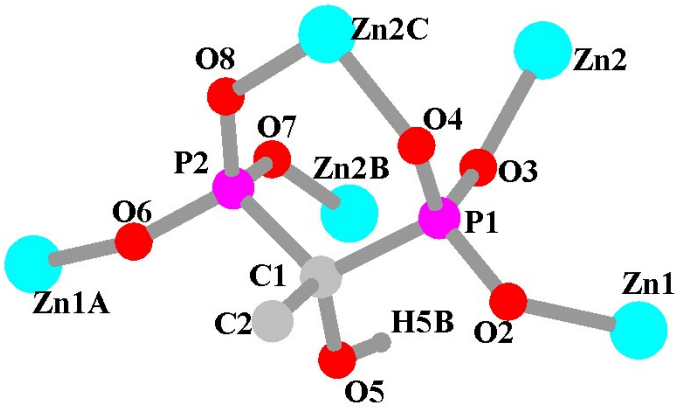

Fig. S4 The coordination mode of diphosphonate ligand in **2** (H atoms for CH_3 group are omitted for clarity).

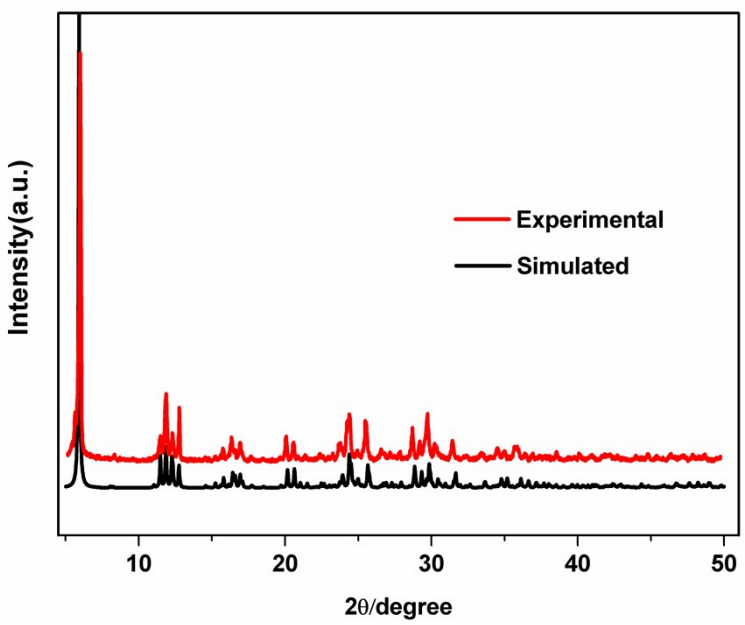

Fig. S5 PXRD pattern of **1**

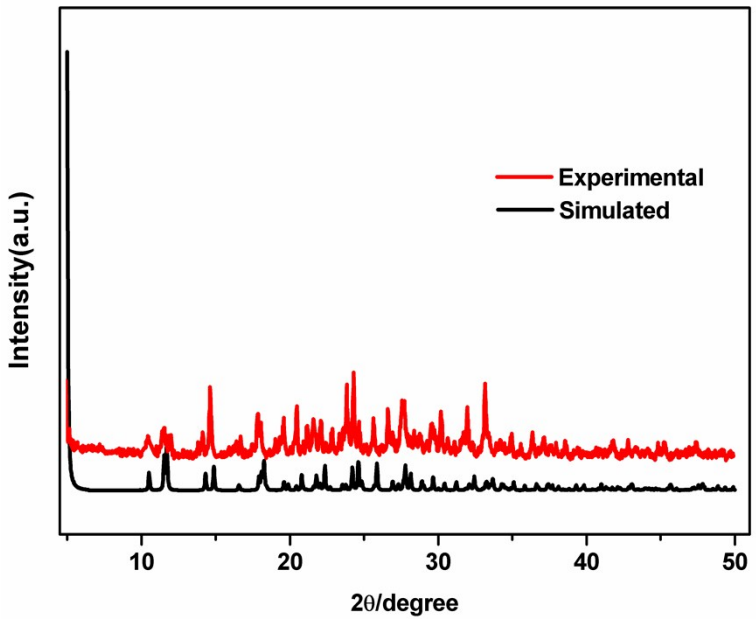

Fig. S6 PXRD patterns of **2**.

Table S3. Selected bond lengths (Å) and angles (°) for **1**

Zn(1)-O(1)	1.965(2)	Zn(3)-O(14)	2.202(3)
Zn(1)#2-O(5)	1.903(2)	O(1)-P(1)	1.523(2)
Zn(1)#3-O7	1.932(2)	O(2)-P(1)	1.514(2)
Zn(1)-O(8)	1.915(3)	O(3)-P(1)	1.530(3)
Zn(2)#1-O(2)	1.980(2)	O(4)-P(2)	1.509(2)
Zn(2)-O(3)	1.954(2)	O(5)-P(2)	1.501(2)
Zn(2)#1-O(4)	1.908(2)	O(6)-P(2) O(7)-	1.522(3)
Zn(2)-O(10)	1.931(3)	P(3)	1.512(2)
Zn(3)-O(3)	2.378(2)	O(8)-P(3)	1.515(3)
Zn(3)-O(6)	2.029(2)	O(9)-P(3) O(10)-	1.527(2)
Zn(3)-O(9)	2.016(2)	P(4)	1.508(3)
Zn(3)-O(11)	1.983(3)	O(11)-P(4) O(12)-	1.513(3)
Zn(3)-O(13)	2.123(2)	P(4)	1.553(3)
O(5)#4-Zn(1)-O(8)	109.85(11)	O(11)-Zn(3)-O(6) O(9)-	94.72(10)
O(5)#4-Zn(1)-O(7)#3	104.51(11)	Zn(3)-O(6)	168.52(11)
O(8)-Zn(1)-O(7)#3	111.03(11)	O(11)-Zn(3)-O(13)	99.61(11)
O(5)#4-Zn(1)-O(1)	103.62(10)	O(9)-Zn(3)-O(13)	94.55(10)
O(8)-Zn(1)-O(1)	125.49(10)	O(6)-Zn(3)-O(13)	86.98(10)
O(7)#3-Zn(1)-O(1)	100.21(11)	O(11)-Zn(3)-O(3) O(9)-	90.68(10)
O(4)#1-Zn(2)-O(10)	113.23(12)	Zn(3)-O(3) O(6)-Zn(3)-	94.76(9)
O(4)#1-Zn(2)-O(3)	114.13(11)	O(3) O(13)-Zn(3)-O(3)	81.67(9)

O(10)-Zn(2)-O(3)	103.19(10)	O(11)-Zn(3)-O(14)	165.28(10)
O(4)#1-Zn(2)-O(2)#1	99.01(10)	O(9)-Zn(3)-O(14)	168.71(12)
O(10)-Zn(2)-O(2)#1	113.61(12)	O(6)-Zn(3)-O(14)	86.69(11)
O(3)-Zn(2)-O(2)#1	114.19(10)	O(13)-Zn(3)-O(14)	81.89(11)
O(11)-Zn(3)-O(9)	96.24(10)		91.00(12)

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

Table S4. Selected bond lengths (Å) and angles (°) for **2**

	1.8990(14)		1.9429(14)
Zn(1)#1-O(6) Zn(1)-	2.0315(17)	Zn(2)#3-O(4) O(2)-	1.5202(14)
N(1) Zn(1)-O(1)	1.9621(15)	P(1) O(3)-P(1)	1.5114(15)
Zn(1)-O(2) Zn(2)#3-	1.9102(13)	O(4)-P(1) O(6)-	1.5285(14)
O(8) Zn(2)-O(3)	1.9725(13)	P(2) O(7)-P(2)	1.5151(14)
Zn(2)#4-O(7)	1.9000(14)	O(8)-P(2)	1.5192(14)
	1.9260(13)		1.5319(14)
O(6)#5-Zn(1)-O(2)	112.29(6)	O(3)-Zn(2)-O(7)#4	100.54(7)
O(6)#5-Zn(1)-O(1)	115.41(7)	O(3)-Zn(2)-O(4)#3	114.12(7)
O(2)-Zn(1)-O(1)	117.27(6)	O(7)#4-Zn(2)-O(4)#3	119.87(6)
O(6)#5-Zn(1)-N(1)	105.50(7)	O(3)-Zn(2)-O(8)#3	118.09(7)
O(2)-Zn(1)-N(1)	103.72(7)	O(7)#4-Zn(2)-O(8)#3	103.38(6)
O(1)-Zn(1)-N(1)	100.30(7)	O(4)#3-Zn(2)-O(8)#3	101.32(6)

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