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The impact of positional isomerism on electronic and photochromic properties of 1-D zinc-based naphthalene diimide coordination polymers

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Content

1. **Figures**

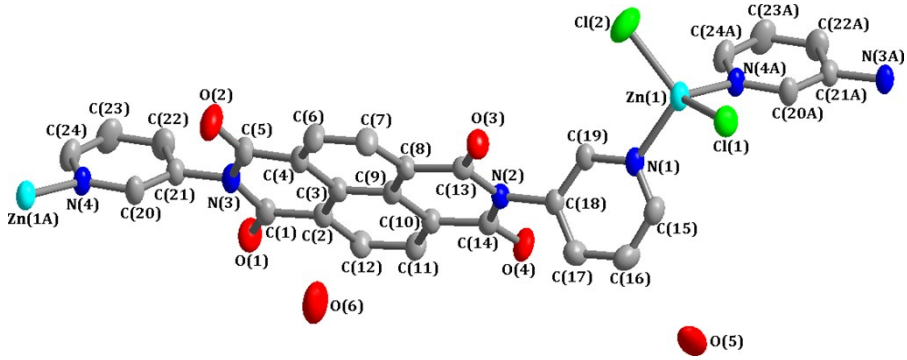

Fig. S1. The asymmetric unit of **1** (symmetry codes: A: -1+x, -1+y, 1+z).

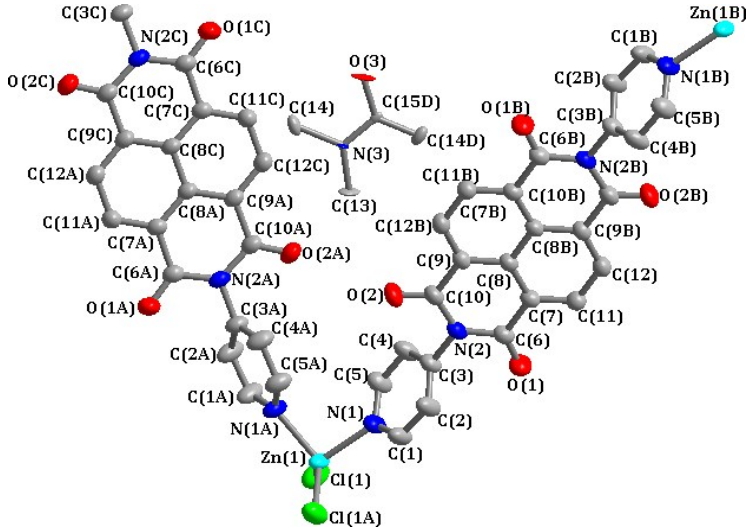

Fig. S2. View of the coordination modes of zinc ions and ligands in **2** (symmetry codes: A: 1-x, y, 3/2-z; B: -x, 1-y, 2-z; C: 1+x, 1-y, -1/2+z; D: 1-x, y 1/2-z).

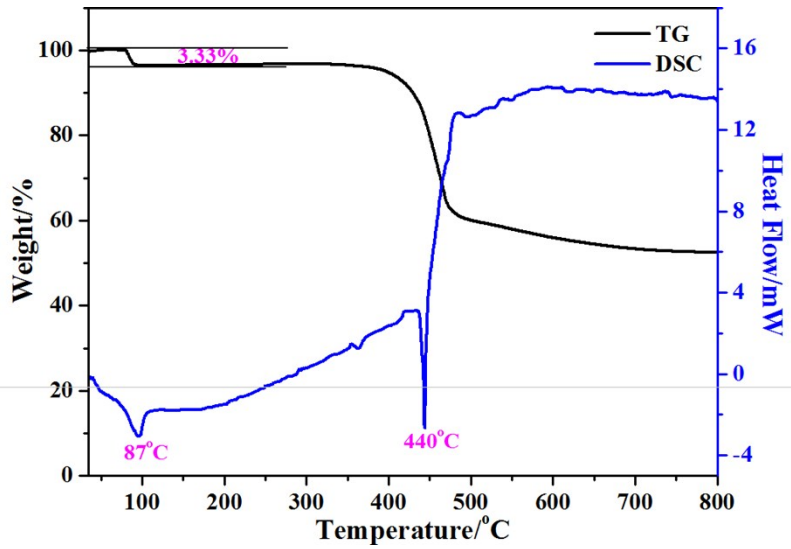

Fig. S3. Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **1**.

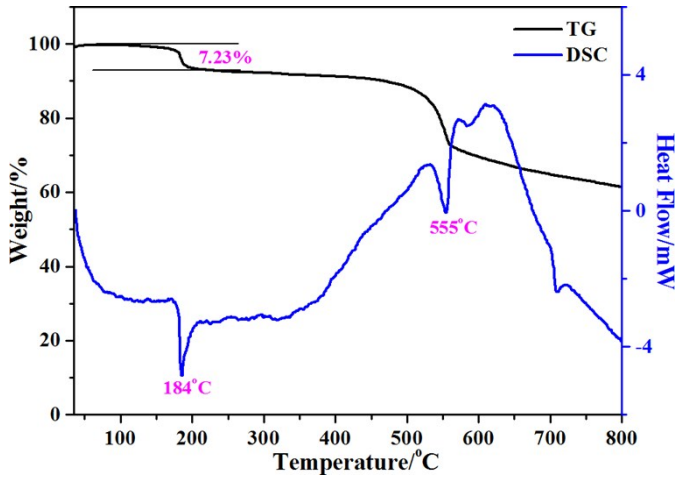

Fig. S4. Thermo-gravimetric (TG) and Differential scanning calorimetry (DSC) curves of **2**.

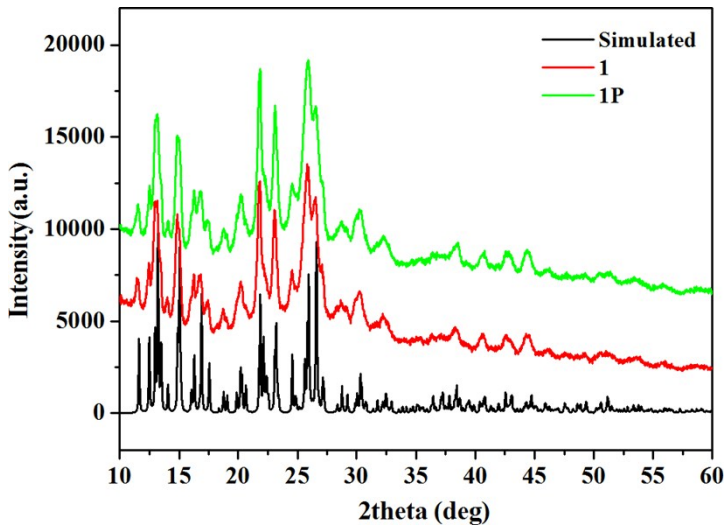

Fig. S5. Powder X-ray diffraction (PXRD) patterns for **1** and **1P** at room temperature.

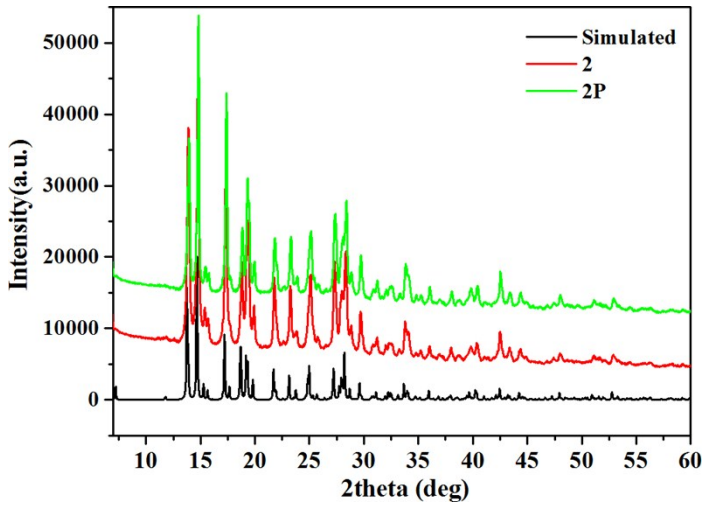

Fig. S6. Powder X-ray diffraction (PXRD) patterns for **2** and **2P** at room temperature.

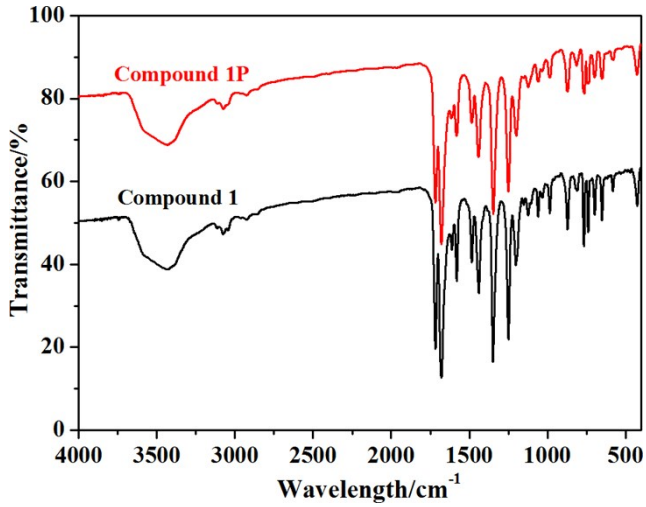

Fig. S7. IR spectra of **1**.

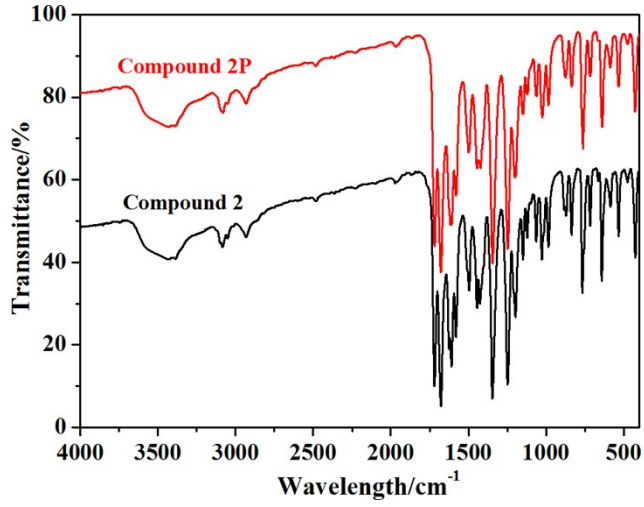

Fig. S8. IR spectra of **2**.

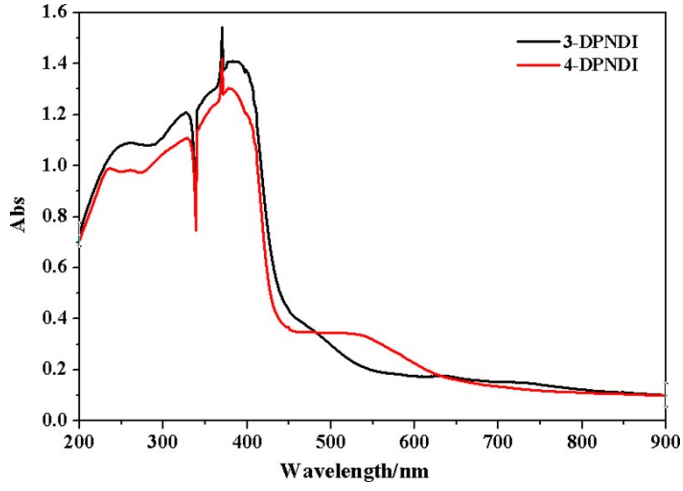

Fig. S9. UV-vis absorption spectra of free 3-DPNDI and 4-DPNDI.

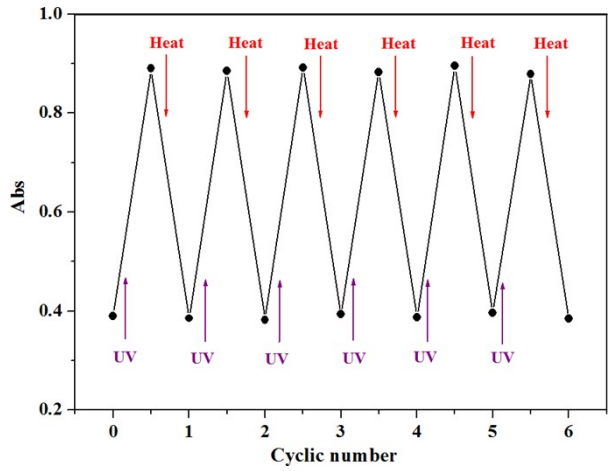

Fig. S10. The switching cycles of coloration-decoloration processes of **1** upon alternating UV light illumination and thermal treatment.

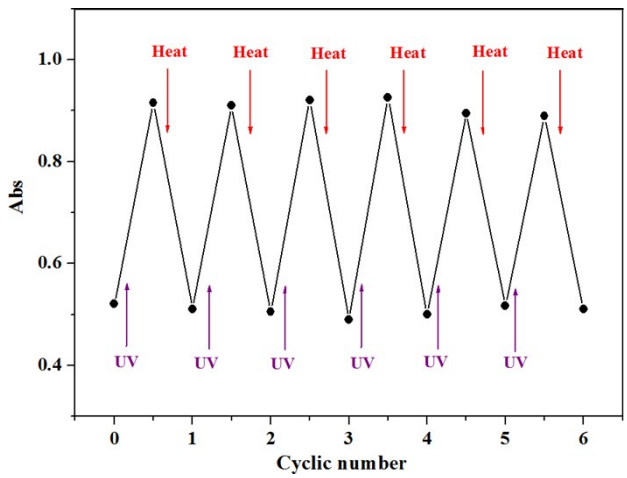

Fig. S11. The switching cycles of coloration-decoloration processes of **2** upon alternating UV light illumination and thermal treatment.

2. Tables

Table S1. Crystallographic data and refinement of compounds **1** and **2**.

Compounds	**1**	**2**
Empirical formula	$C_{24}H_{12}Cl_2N_4O_5Zn$	$C_{28}H_{21}Cl_2N_5O_5Zn$
Formula weight	572.65	643.77
Crystal system	Triclinic	Monoclinic
Space group	*P*-1	*P*2/c
a (Å)	7.2372(11)	7.5740(8)
b (Å)	12.7860(19)	12.2366(12)
c (Å)	14.237(2)	15.0059(15)
α (°)	68.774(3)	90
β (°)	78.572(4)	93.741(3)
γ (°)	81.970(4)	90
V (Å^3)	1200.4(3)	1387.8(2)
μ(mm^{-1})	1.290	1.126
R_{int}	0.0546	0.0221
Goodness-of-fit on F^2	1.093	1.046
R_1/wR_2, [$I \geq 2\sigma(I)$][a,b]	0.0700/0.1670	0.0320/0.0839
R_1/wR_2, (all data)	0.1390/0.1936	0.0392/0.0879

[a] $R_1 = \sum||F_o|-|F_c||/\sum|F_o|$ [b] $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$

Table S2. Selected bond lengths (Å) and angles (°) for compounds **1** and **2**.

Compound **1**			
Zn(1)-Cl(2)	2.2071(17)	Zn(1)-Cl(1)	2.2226(15)
N(1)-Zn(1)	2.029(4)	Zn(1)-N(4)#2	2.047(4)
C(1)-O(1)	1.202(6)	C(1)-N(3)	1.402(6)
C(1)-C(2)	1.492(6)	C(2)-C(12)	1.376(7)
C(2)-C(3)	1.402(7)	C(3)-C(9)	1.408(6)
C(3)-C(4)	1.417(6)	C(4)-C(6)	1.365(7)
C(4)-C(5)	1.471(7)	C(5)-O(2)	1.212(6)
C(5)-N(3)	1.396(7)	C(6)-C(7)	1.378(7)
C(7)-C(8)	1.376(7)	C(8)-C(9)	1.405(7)
C(8)-C(13)	1.476(6)	C(9)-C(10)	1.420(6)
C(10)-C(11)	1.368(7)	C(10)-C(14)	1.482(6)
C(11)-C(12)	1.416(7)	C(13)-O(3)	1.194(6)
C(13)-N(2)	1.408(6)	C(14)-O(4)	1.203(6)
C(14)-N(2)	1.397(6)	C(15)-N(1)	1.322(7)
C(15)-C(16)	1.367(8)	C(16)-C(17)	1.379(7)
C(17)-C(18)	1.381(8)	C(18)-C(19)	1.373(7)
C(18)-N(2)	1.445(6)	C(19)-N(1)	1.349(6)
C(20)-N(4)	1.339(6)	C(20)-C(21)	1.366(7)
C(21)-C(22)	1.371(8)	C(21)-N(3)	1.442(6)
C(22)-C(23)	1.387(8)	C(23)-C(24)	1.373(8)
C(24)-N(4)	1.332(7)		
N(4)#2-Zn(1)-Cl(2)	108.10(14)	N(1)-Zn(1)-Cl(1)	106.96(13)
N(4)#2-Zn(1)-Cl(1)	106.10(12)	Cl(2)-Zn(1)-Cl(1)	119.32(6)
C(24)-N(4)-Zn(1)#1	122.6(3)	C(20)-N(4)-Zn(1)#1	118.9(4)
N(1)-Zn(1)-N(4)#2	107.27(18)	N(1)-Zn(1)-Cl(2)	108.52(13)
O(1)-C(1)-N(3)	120.9(4)	O(1)-C(1)-C(2)	123.5(5)
N(3)-C(1)-C(2)	115.6(4)	C(12)-C(2)-C(3)	120.1(4)
C(12)-C(2)-C(1)	119.7(4)	C(3)-C(2)-C(1)	120.2(4)
C(2)-C(3)-C(9)	120.0(4)	C(2)-C(3)-C(4)	121.3(4)
C(9)-C(3)-C(4)	118.7(4)	C(6)-C(4)-C(3)	120.0(4)
C(6)-C(4)-C(5)	120.3(4)	C(3)-C(4)-C(5)	119.7(5)
O(2)-C(5)-N(3)	120.5(5)	O(2)-C(5)-C(4)	122.6(5)
N(3)-C(5)-C(4)	116.9(4)	C(4)-C(6)-C(7)	121.0(5)
C(8)-C(7)-C(6)	120.4(5)	C(7)-C(8)-C(9)	120.2(4)
C(7)-C(8)-C(13)	119.4(4)	C(9)-C(8)-C(13)	120.4(4)
C(8)-C(9)-C(3)	119.4(4)	C(8)-C(9)-C(10)	121.2(4)
#1 x+1,y+1,z-1; #2 x-1,y-1,z+1			

Compound **2**			
Zn(1)-N(1)	2.0680(15)	Zn(1)-Cl(1)	2.2068(6)
C(1)-N(1)	1.339(2)	C(1)-C(2)	1.377(2)
C(2)-C(3)	1.367(2)	C(2)-H(2)	0.9300
C(3)-C(4)	1.375(3)	C(3)-N(2)	1.4413(19)
C(4)-C(5)	1.377(2)	C(5)-N(1)	1.334(2)
C(6)-O(1)	1.210(2)	C(6)-N(2)	1.400(2)
C(6)-C(7)	1.479(2)	C(7)-C(11)	1.376(2)
C(7)-C(8)	1.410(2)	C(8)-C(9)	1.410(2)
C(9)-C(10)	1.479(2)	C(10)-O(2)	1.208(2)
C(10)-N(2)	1.402(2)	C(11)-C(12)	1.401(2)
C(14)-C(15)	1.463(4)	C(14)-N(3)	1.581(4)
C(15)-O(3)	1.292(4)		
N(1)#1-Zn(1)-N(1)	94.72(9)	N(1)-Zn(1)-Cl(1)#1	103.55(5)
N(1)-Zn(1)-Cl(1)	113.59(5)	Cl(1)#1-Zn(1)-Cl(1)	124.16(4)
N(1)-C(1)-C(2)	122.83(17)	C(1)-C(2)-C(3)	118.37(17)
C(4)-C(3)-C(2)	119.85(15)	C(4)-C(3)-N(2)	119.29(14)
C(2)-C(3)-N(2)	120.85(16)	C(3)-C(4)-C(5)	118.07(16)
N(1)-C(5)-C(4)	123.06(17)	O(1)-C(6)-N(2)	120.58(15)
O(1)-C(6)-C(7)	123.44(16)	N(2)-C(6)-C(7)	115.97(14)
C(11)-C(7)-C(8)	120.38(13)	C(11)-C(7)-C(6)	119.33(14)
C(8)-C(7)-C(6)	120.28(14)	C(7)-C(8)-C(9)	121.48(13)
C(8)-C(9)-C(10)	119.70(14)	O(2)-C(10)-N(2)	120.63(14)
N(2)-C(10)-C(9)	116.47(14)	O(2)-C(10)-C(9)	122.90(16)
C(7)-C(11)-C(12)	120.05(15)	C(15)-C(14)-N(3)	37.51(17)
O(3)-C(15)-C(14)	133.3(3)	C(5)-N(1)-C(1)	117.61(15)
C(6)-N(2)-C(10)	126.08(13)	C(6)-N(2)-C(3)	117.27(14)
C(10)-N(2)-C(3)	116.52(14)		
#1 -x+1,y,-z+3/2			

Table S3. Hydrogen bonds of for compounds **1**, and **2** (Å and °).

Compound **1**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(15)-H(15)...O(3)#3	0.93	2.56	3.100(7)	117.2
C(15)-H(15)...Cl(2)#4	0.93	2.84	3.513(5)	130.6
C(16)-H(16)...O(3)#4	0.93	2.52	3.307(7)	142.1
C(19)-H(19)...O(1)#5	0.93	2.61	3.067(7)	110.9
C(20)-H(20)...O(5)#6	0.93	2.56	3.349(10)	143.4
C(20)-H(20)...Cl(1)#1	0.93	2.85	3.448(5)	122.8
C(23)-H(23)...Cl(2)#7	0.93	2.72	3.638(6)	170.2
#1 x+1,y+1,z-1; #3 -x+1,-y+1,-z+2;#4 x-1,y,z;#5 –x+2,-y+1,-z+1;#6 x+1,y+1,z;#7 -x+3,-y+1,-z+1				
Compound **2**				
D-H···A	d(D-H)	d(H···A)	d(D···A)	<(DHA)
C(11)-H(11)...Cl(1)#1	0.93	3.00	3.7107(19)	134.2
C(4)-H(4)...O(3)#4	0.93	2.47	3.235(3)	139.7
#1 x-1, 2-y, 1/2+z; #4 -x,-y+1,-z+1				

Table S4. π-π interactions for compound **1**.

Cg	Cg	Distances (Å)	Dihedral angles (°)	Ring-slippage (Å)
C20 C21 C22 C23 C24 N4	C20A C21A C22A C23A C24A N4A	3.9530(5)	0	1.705
C15 C16 C17 C18 C19 N1	C15B C16B C17B C18B C19B N1B	3.9668(4)	0	0.791
C2 C3 C9 C10 C11 C12	C8C C9C C10C C13C C14C N2C	3.8946(4)	1.581	1.868
C2 C3 C9 C10 C11 C12	C2C C3C C9C C10C C11C C12C	3.6616(5)	0	1.320
A 2-x, 2-y, -z; B -x+1,-y+1,-z+2; B 1-x, 1-y, 2-z; C 2-x, 1-y, 1-z;				