Electronic supplementary information

Homo-chiral helical coordination polymer constructed by achiral ligand with excellent photo-physical properties and cell imaging application

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Table S1 Crystallographic data and structural refinement data for polymer **1**.

Crystal data for polymer **1**			
Empirical formula	$C_{20}H_{16}C_{l2}N_2Zn$		
Formula weight	420.62		
Temperature	296(2)		
Wavelength	0.71073 Å		
Crystal system	Tetragonal		
Space group	P4(3)2(1)2		
Unit cell dimensions	a = 8.7877(6) Å	α= 90°	□
	b = 8.7877(6) Å	β= 90°	□
	c = 24.203(3) Å	γ= 90°	□
Volume	1869.1(3) Å3		
Z	4		
Density (calculated)	1.495 Mg/m^3		
Absorption coefficient	1.604 mm^{-1}		
F(000)	856		
Crystal size	0.31 x 0.28 x 0.19 mm^3		
Theta range for data collection	2.47 to 26.43°		
Index ranges	-10<=h<=9, -10<=k<=7, -29<=l<=21		
Reflections collected	1743		
Independent reflections	0.0302		
Completeness to theta = 25.48°	99.58%		
Absorption correction	Semi-empirical from equivalents		
Refinement method	Full-matrix least-squares on F2		
Data / restraints / parameters	1743 / 0 / 115		
Goodness-of-fit on F2	1.107		
Final R indices [I>2sigma(I)]	R1 = 0.0226, wR2 = 0.0578		
R indices (all data)	R1 = 0.0245, wR2 = 0.0585		
Extinction coefficient	0.049		
Largest diff. peak and hole	0.256 and -0.166 e.Å-3		
Flack	0.013(7)		

[*a*] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$; $wR_2 = [\Sigma w(F_o^2 - F_c^2)_2/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected bond lengths [Å] and angles [°] for polymer **1**.

Bond lengths	
Zn1—N1	2.0425(18)
Zn1—N1#1	2.0425(18)
Zn1—Cl1	2.2148(6)
Zn1—Cl1#2	2.2148(7)
Angles	
N1—Zn1—N1#1	110.98(11)
N1—Zn1—Cl1	105.15(6)
N1—Zn1—Cl1#2	106.28(5)
N1#1—Zn1—Cl1	106.28(5)
N1#1—Zn1—Cl1#2	105.15(6)
Cl1—Zn1—Cl1#2	122.89(4)

Symmetry transformations used to generate equivalent atoms:

#1-1+y,1+x,1-z #2 -1+y,1+x,1-z

Table S3 Hydrogen bonding data for polymer 1

D-H···A	d(D-H) (Å)	d(H···A) (Å)	d(D···A) (Å)
C4-H4…Cl1#	0.93	2.83	3.451(3)

Symmetry transformations used to generate equivalent atoms:

#x, -1+y, z

Table S4 The torsion angle for **1**

1			
Zn1-N1-C1-C2	-179.1(3)	C4-C3-C6-C7	12.0(5)
Zn1-N1-C5-C4	178.6(2)	C5-N1-C1-C2	-1.5(5)
N1-C1-C2-C3	0.5(5)	C6-C3-C4-C5	177.0(3)
C1-N1-C5-C4	1.0(4)	C6-C7-C9-C8	12.8(4)
C1-C2-C3-C4	1.0(5)	C6-C7-C9-C10	-167.2(3)
C1-C2-C3-C6	-177.6(3)	C7-C9-C10-C11	179.2(2)
C2-C3-C4-C5	-1.5(4)	C8-C9-C10-C11	-0.8(4)
C2-C3-C6-C7	-169.6(3)	C9-C8-C9-C7	-179.6(3)
C3-C4-C5-N1	0.6(5)	C9-C8-C9-C10	0.4(2)
C3-C6-C7-C9	-177.3(3)	C9-C10-C11-C10	0.4(2)

Table S5 The dihedral angle between the various sides in the polymer **1**.

dihedral angle (°)	**Polymer 1**
P1-M	11.84
M-P2	12.78
P1-P2	24.62
P2-N	11.84
N-P3	12.78
P2-P3	24.62

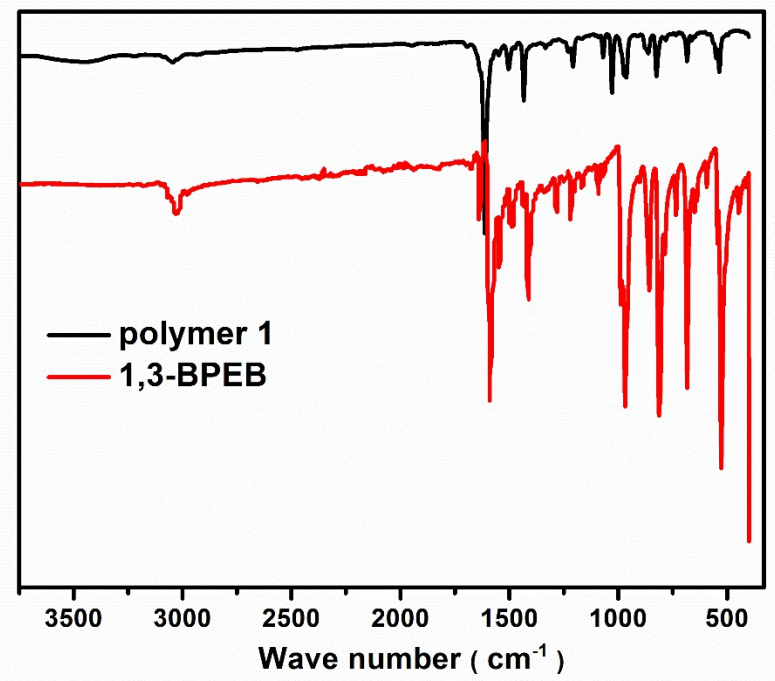

Fig. S1 The IR spectra of polymer **1** and ligand (1,3-BPEB) in solid state.

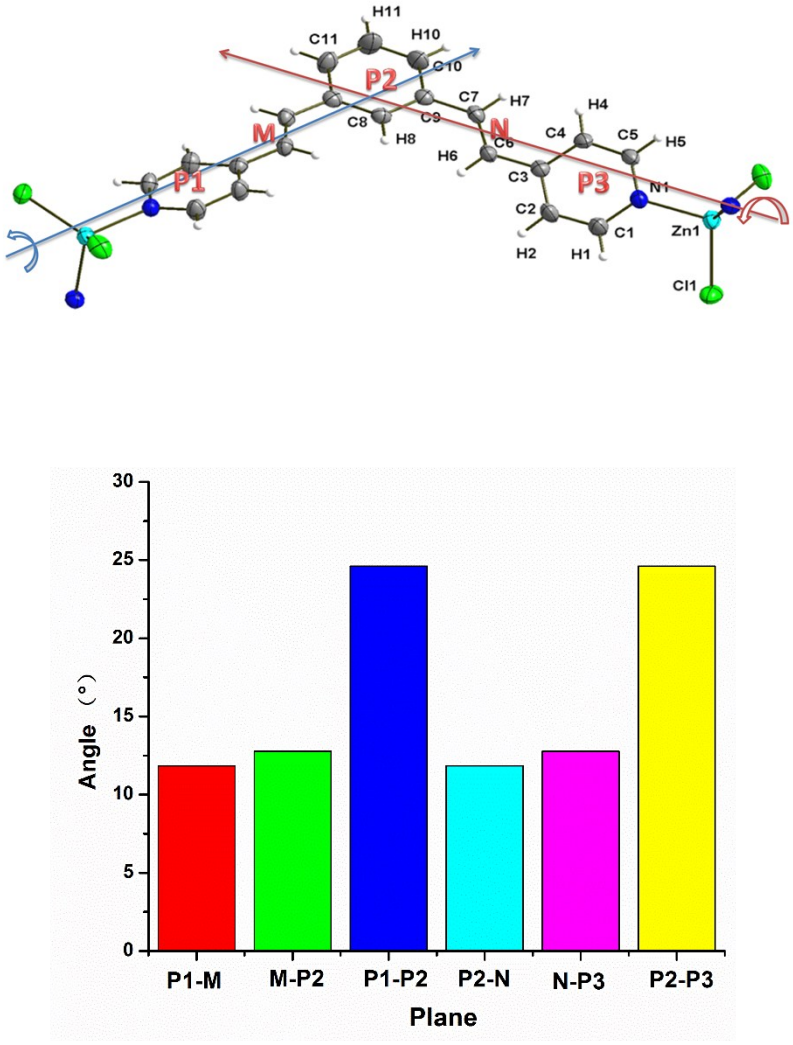

Fig. S2 The dihedral angles between the various planes in the polymer **1**.