Supplementary Material (ESI) for CrystEngComm

Homochiral Coordination Polymers of Metallosalen Complexes with Tunable Helical Pitches

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1. **Materials and General Procedures**.

All of the chemicals are commercial available, and used without further purification. Elemental analyses of C, H and N were performed with an EA1110 CHNS-0 CE elemental analyzer. The IR (KBr pellet) spectrum was recorded (400 - 4000 cm^{-1} region) on a Nicolet Magna 750 FT-IR spectrometer. UV-visible absorption spectrum was measured at room temperature with a PE Lambda 900 UV-Visible spectrophotometer in 400-2000 nm. BaSO4 plate was used as a standard (100 % reflectance) for the measurement of the optical diffuse reflectance spectrum. The solid state CD spectra were recorded on a J-800 spectropolarimeter (Jasco, Japan). Thermogravimetric analyses (TGA) were carried out in an air atmosphere with a heating rate of 10 ºC min^{-1} on a STA449C integration thermal analyzer. Powder X-ray diffraction (PXRD) data were collected on a DMAX2500 diffractometer using Cu Kα radiation. The calculated PXRD patterns were produced using the SHELXTL-XPOW program and single crystal reflection data.

X-ray Crystallography. Single-crystal XRD data for the compounds was collected on a Bruker Smart 1000 CCD diffractometer with Mo-Kα radiation (λ = 0.71073 Å) at room temperature. The empirical absorption correction was applied by using the SADABS program (G. M. Sheldrick, SADABS, program for empirical absorption correction of area detector data; University of Göttingen, Göttingen, Germany, 1996). The structure was solved using direct method, and refined by full-matrix least-squares on *F*2 (G. M. Sheldrick, SHELXTL97, program for crystal structure refinement, University of Göttingen, Germany, 1997). Crystal data and details of the data collection are given in Table S1. The selected bond distances and angles are presented in Tables S2-S5.

Table S1. Selected bond lengths [Å] and angles [º] for **1**.

Zn(1)-O(2)	1.953(3)
Zn(1)-O(1)	1.965(3)
Zn(1)-N(2)	2.085(4)
Zn(1)-N(1)	2.094(3)
Zn(1)-N(3)#1	2.107(4)
Zn(2)-O(3)	1.949(3)
Zn(2)-O(4)	1.966(3)
Zn(2)-N(6)	2.088(4)
Zn(2)-N(5)	2.094(4)
Zn(2)-N(8)#2	2.108(4)
O(2)-Zn(1)-O(1)	95.16(12)
O(2)-Zn(1)-N(2)	145.38(17)
O(1)-Zn(1)-N(2)	89.32(14)
O(2)-Zn(1)-N(1)	88.16(13)
O(1)-Zn(1)-N(1)	163.63(18)
N(2)-Zn(1)-N(1)	79.07(14)
O(2)-Zn(1)-N(3)#1	110.35(17)
O(1)-Zn(1)-N(3)#1	97.86(16)
N(2)-Zn(1)-N(3)#1	102.95(15)
N(1)-Zn(1)-N(3)#1	95.98(15)
O(3)-Zn(2)-O(4)	94.96(12)
O(3)-Zn(2)-N(6)	157.23(16)
O(4)-Zn(2)-N(6)	88.30(13)
O(3)-Zn(2)-N(5)	88.44(13)
O(4)-Zn(2)-N(5)	153.05(16)
N(6)-Zn(2)-N(5)	78.90(14)
O(3)-Zn(2)-N(8)#2	107.16(16)
O(4)-Zn(2)-N(8)#2	101.28(15)
N(6)-Zn(2)-N(8)#2	94.21(15)
N(5)-Zn(2)-N(8)#2	103.22(15)

Symmetry transformations used to generate equivalent atoms:
#1:-x,y+1/2,-z+1; #2:-x+1,y-1/2,-z+2;
#3:-x,y-1/2,-z+1;#4 -x+1,y+1/2,-z+2

Table S2. Selected bond lengths [Å] and angles [º] for **2**.

Co(1)-N(3)	1.866(8)
Co(1)-O(2)	1.871(6)
Co(1)-O(1)	1.877(8)
Co(1)-N(2)	1.896(7)
Co(1)-N(1)#1	2.118(9)
Co(2)-N(7)	1.857(9)
Co(2)-N(6)	1.859(7)
Co(2)-O(3)	1.882(7)
Co(2)-O(4)	1.899(6)
Co(2)-N(5)#2	2.118(9)
N(3)-Co(1)-O(2)	92.7(3)
N(3)-Co(1)-O(1)	173.1(4)
O(2)-Co(1)-O(1)	86.2(3)
N(3)-Co(1)-N(2)	86.3(3)
O(2)-Co(1)-N(2)	168.8(4)
O(1)-Co(1)-N(2)	93.3(3)
N(3)-Co(1)-N(1)#1	95.9(4)
O(2)-Co(1)-N(1)#1	96.5(3)
O(1)-Co(1)-N(1)#1	90.9(3)
N(2)-Co(1)-N(1)#1	94.7(4)
N(7)-Co(2)-N(6)	86.1(4)
N(7)-Co(2)-O(3)	176.1(4)
N(6)-Co(2)-O(3)	92.8(3)
N(7)-Co(2)-O(4)	93.6(3)
N(6)-Co(2)-O(4)	165.9(4)
O(3)-Co(2)-O(4)	86.6(3)
N(7)-Co(2)-N(5)#2	91.9(4)
N(6)-Co(2)-N(5)#2	96.5(4)
O(3)-Co(2)-N(5)#2	91.9(3)
O(4)-Co(2)-N(5)#2	97.5(3)

Symmetry transformations used to generate equivalent atoms:
#1: -x+1,y+1/2,-z+1; #2: -x+2,y-1/2,-z+2;
#3 -x+1,y-1/2,-z+1; #4 -x+2,y+1/2,-z+2

Table S3. Selected bond lengths [Å] and angles [º] for **3**.

Ni(1)-O(2)	1.966(5)
Ni(1)-O(1)	1.968(5)
Ni(1)-N(2)	2.079(6)
Ni(1)-N(3)	2.089(7)
Ni(1)-N(5)	2.112(5)
Ni(2)-O(4)	1.954(5)
Ni(2)-O(3)	1.965(5)
Ni(2)-N(6)	2.079(6)
Ni(2)-N(7)	2.100(6)
Ni(2)-N(1)#1	2.114(6)

O(2)-Ni(1)-O(1)	94.6(2)
O(2)-Ni(1)-N(2)	88.4(2)
O(1)-Ni(1)-N(2)	160.0(2)
O(2)-Ni(1)-N(3)	146.8(2)
O(1)-Ni(1)-N(3)	88.3(2)
N(2)-Ni(1)-N(3)	78.6(2)
O(2)-Ni(1)-N(5)	105.7(2)
O(1)-Ni(1)-N(5)	100.0(2)
N(2)-Ni(1)-N(5)	98.1(2)
N(3)-Ni(1)-N(5)	106.3(2)
O(4)-Ni(2)-O(3)	94.1(2)
O(4)-Ni(2)-N(6)	149.0(2)
O(3)-Ni(2)-N(6)	89.2(2)
O(4)-Ni(2)-N(7)	88.4(2)
O(3)-Ni(2)-N(7)	159.2(2)
N(6)-Ni(2)-N(7)	78.3(2)
O(4)-Ni(2)-N(1)#1	105.5(2)
O(3)-Ni(2)-N(1)#1	100.7(2)
N(6)-Ni(2)-N(1)#1	104.2(2)
N(7)-Ni(2)-N(1)#1	98.5(2)

Symmetry transformations used to generate equivalent atoms:
#1: x-1,y,z-1; #2: x+1,y,z+1

Table S4. Selected bond lengths [Å] and angles [º] for **4**.

Mn(1)-O(1)	1.852(8)
Mn(1)-O(2)	1.891(7)
Mn(1)-N(2)	1.962(10)
Mn(1)-N(1)	1.994(9)
Mn(1)-O(3)	2.111(8)
Mn(2)-O(6)	1.884(7)
Mn(2)-O(5)	1.896(8)
Mn(2)-N(5)	1.982(9)
Mn(2)-N(6)	1.997(10)
Mn(2)-O(7)	2.095(9)
Mn(2)-N(8)#1	2.514(10)
O(1)-Mn(1)-O(2)	94.2(3)
O(1)-Mn(1)-N(2)	174.7(4)
O(2)-Mn(1)-N(2)	90.4(4)
O(1)-Mn(1)-N(1)	92.7(3)
O(2)-Mn(1)-N(1)	168.2(4)
N(2)-Mn(1)-N(1)	82.3(4)
O(1)-Mn(1)-O(3)	93.4(3)
O(2)-Mn(1)-O(3)	97.9(3)
N(2)-Mn(1)-O(3)	88.5(3)
N(1)-Mn(1)-O(3)	91.3(3)
O(6)-Mn(2)-O(5)	93.6(4)
O(6)-Mn(2)-N(5)	169.9(4)
O(5)-Mn(2)-N(5)	91.8(4)
O(6)-Mn(2)-N(6)	92.0(3)
O(5)-Mn(2)-N(6)	173.9(4)
N(5)-Mn(2)-N(6)	82.3(4)
O(6)-Mn(2)-O(7)	97.3(4)
O(5)-Mn(2)-O(7)	93.0(4)
N(5)-Mn(2)-O(7)	90.9(4)
N(6)-Mn(2)-O(7)	88.8(4)
O(6)-Mn(2)-N(8)#1	83.6(3)
O(5)-Mn(2)-N(8)#1	89.9(4)
N(5)-Mn(2)-N(8)#1	87.9(4)
N(6)-Mn(2)-N(8)#1	88.2(3)
O(7)-Mn(2)-N(8)#1	176.9(4)

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

Table S5. A comparison of helical pitch and turning angles of 1D polymer.

	Adjacent M···M separation (Å)	Helical pitch (Å)	Turning angle (°)	Chain diameter (Å)
1	10.237(1) 10.067(1)	10.430(1)	61.257(5) 62.402(4)	29.69
2	10.590(3) 10.604(3)	12.656(2)	73.388(12) 73.283(12)	29.50
3	10.790(3) 10.807(3)	18.798(6)	121.004(9)	16.64
4	11.509(4) 11.360(4)	12.191(5)	63.959(14) 64.903(15)	28.37

Table S6. A comparison of twisted angles of M**L** ligands.

	Twisted angles (°)	Dihedral angles of pyridine and N2O2 planes (°)	Dihedral angles of coordinated pyridine and adjacent phenylic ring (°)	Dihedral angles of two pyridines (°)
1	167.078(3) 167.232(3)	78.64 78.96	9.46 16.46	19.22 11.85
2	147.351(5) 147.503(5)	88.38 89.10	40.90 37.88	46.23 47.08
3	159.782(4) 159.199(4)	88.06 89.83	43.95 38.96	70.81 69.94
4	158.061(8) 171.065(8)	61.03 75.59	25.16 3061	13.24 5.26

Figure S1. Ball-and-stick (top) and space-filling (bottom) representations of a 1D zigzag chain of **1**.

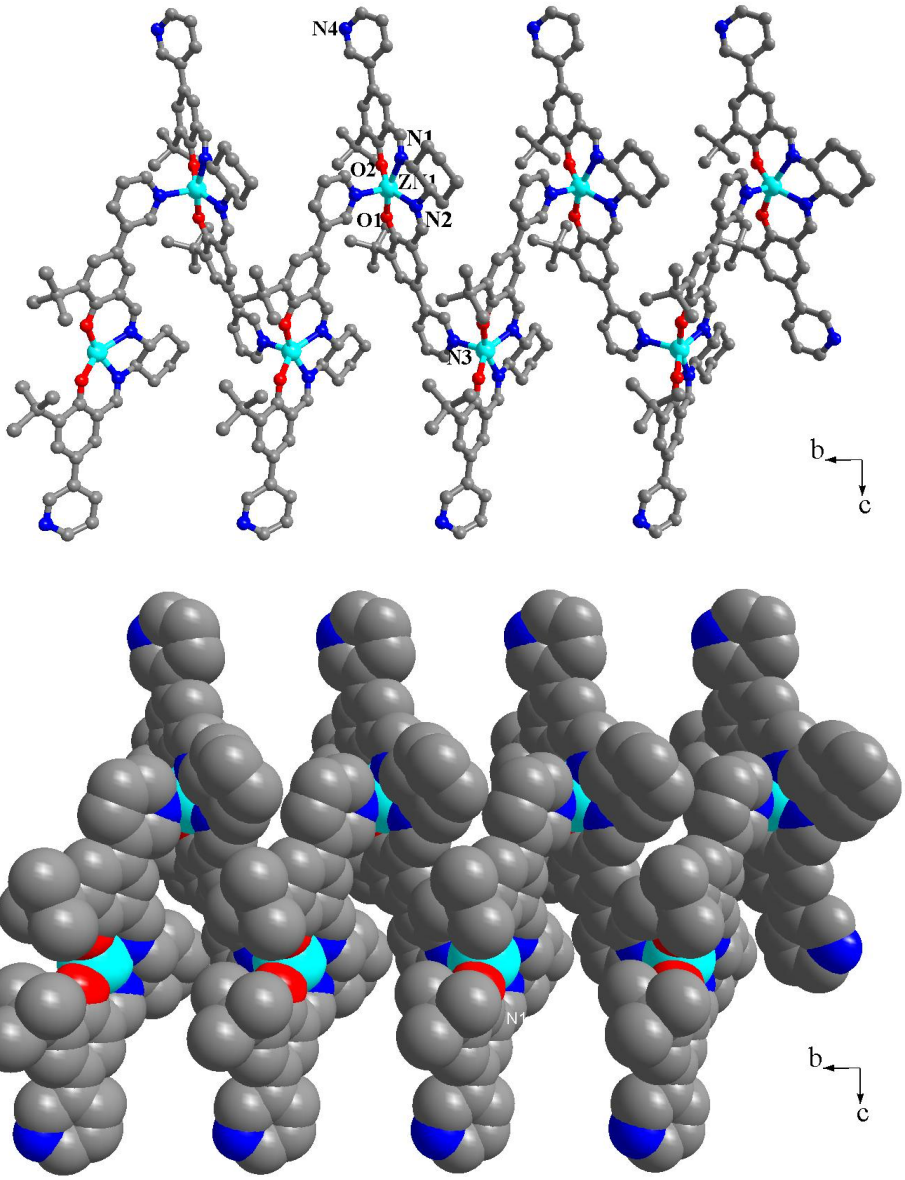

Figure S2. Ball-and-stick representations of a 1D zigzag chain of **2**.

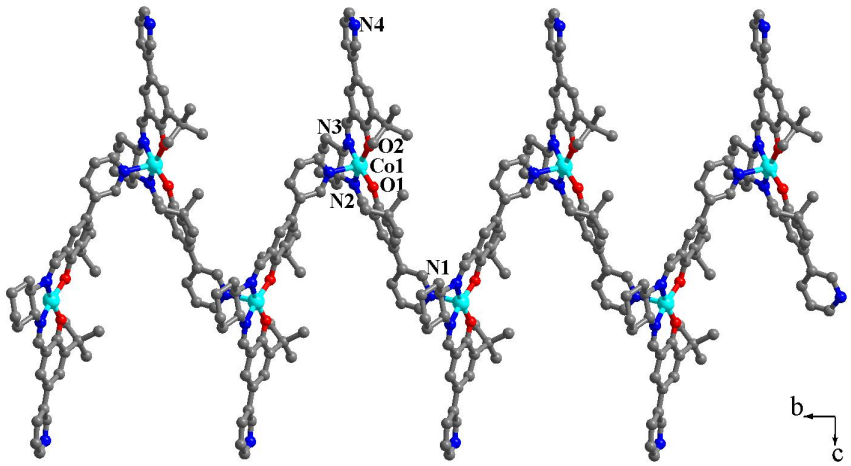

Figure S3. Ball-and-stick representations of a 1D zigzag chain of **3**.

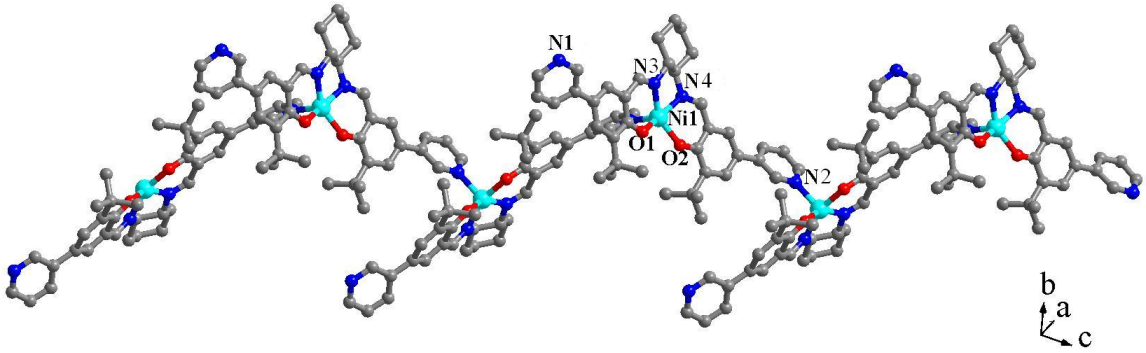

Figure S4. Ball-and-stick representations of a 1D zigzag chain of **4**.

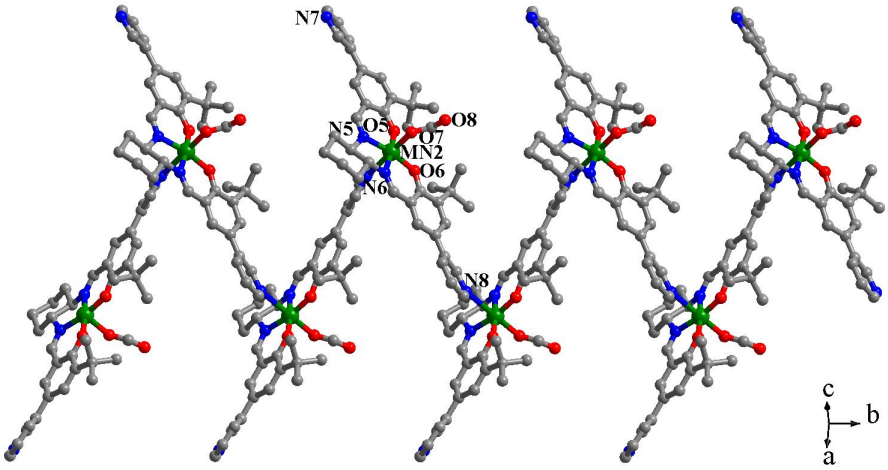

Figure S5. Intermolecular π-π interaction between **1.**

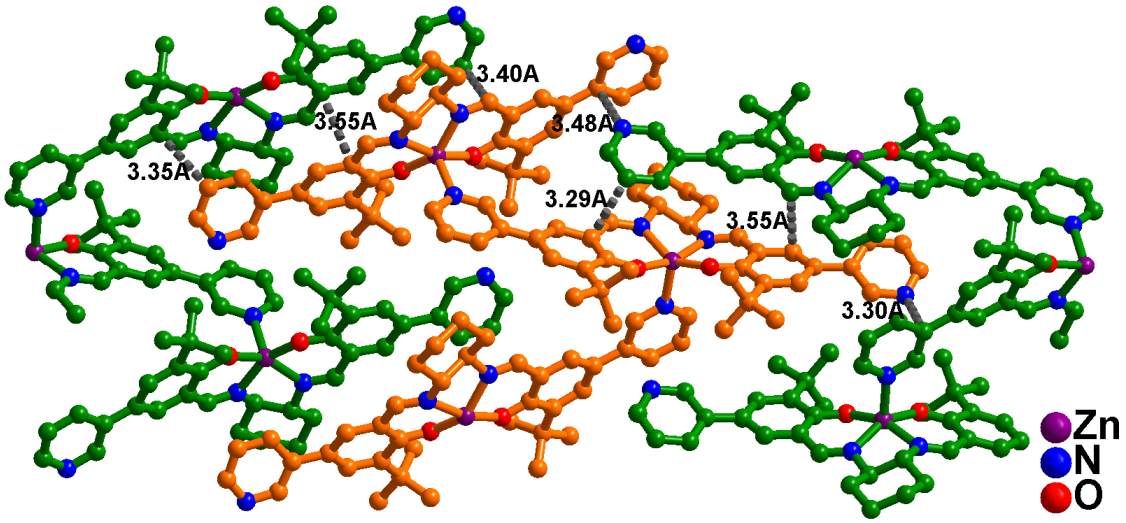

Figure S6. Intermolecular π-π interaction between **2.**

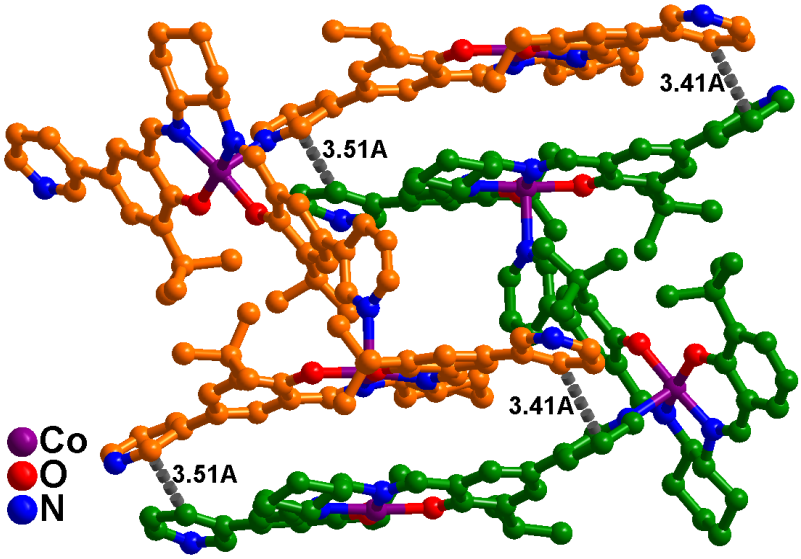

Figure S7. Intermolecular π-π interaction between **3.**

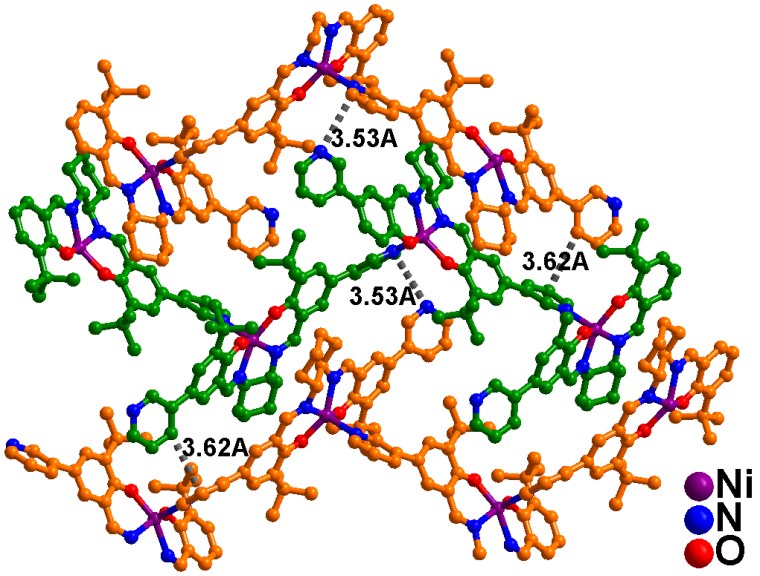

Figure S8. Intermolecular π-π interaction between **4**.

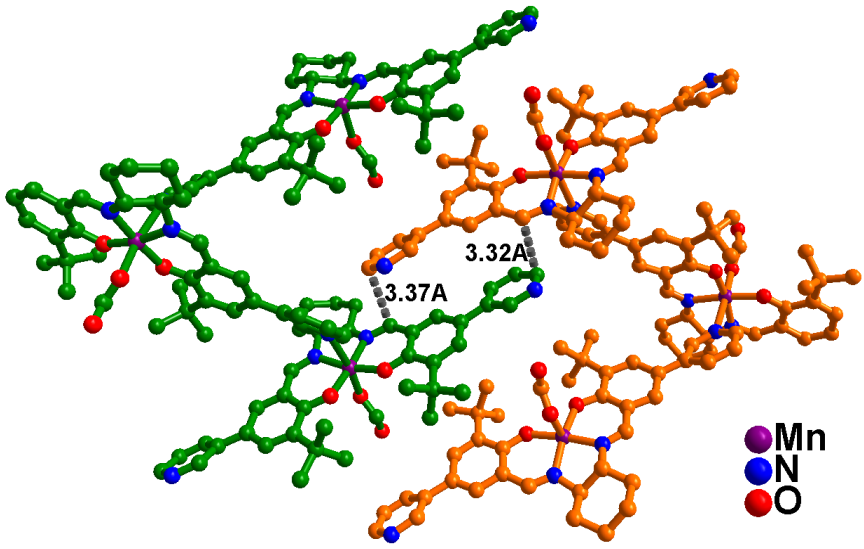

Figure S9. The left-handed helical structure in **1** and **2**.

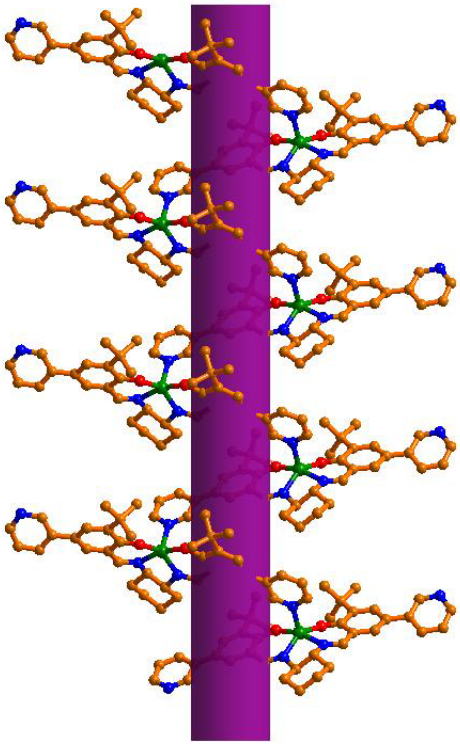

Figure S10. The right-handed helical structure in **4**.

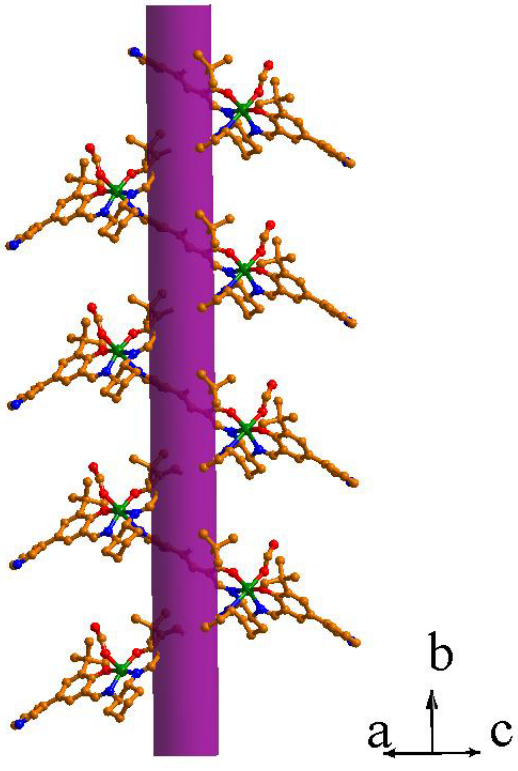

Figure S11. The PXRD pattern and the simulated PXRD pattern of **1**.

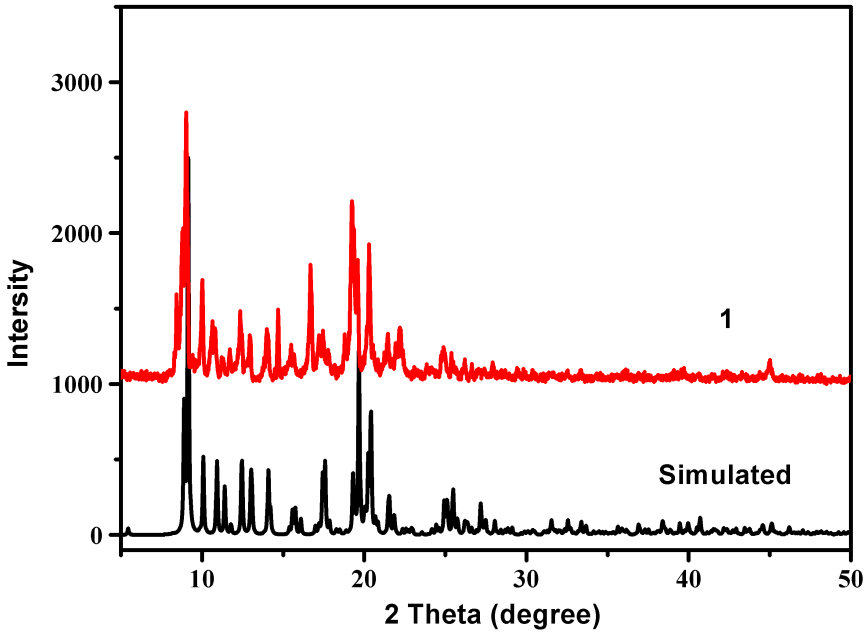

Figure S12. The PXRD pattern and the simulated PXRD pattern of **2**.

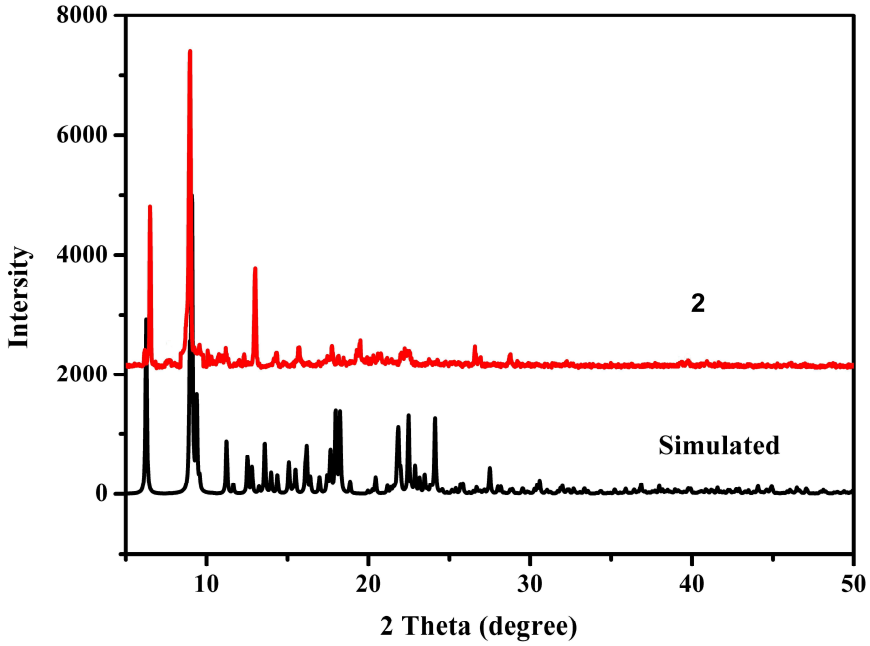

Figure S13. The PXRD pattern and the simulated PXRD pattern of **3**.

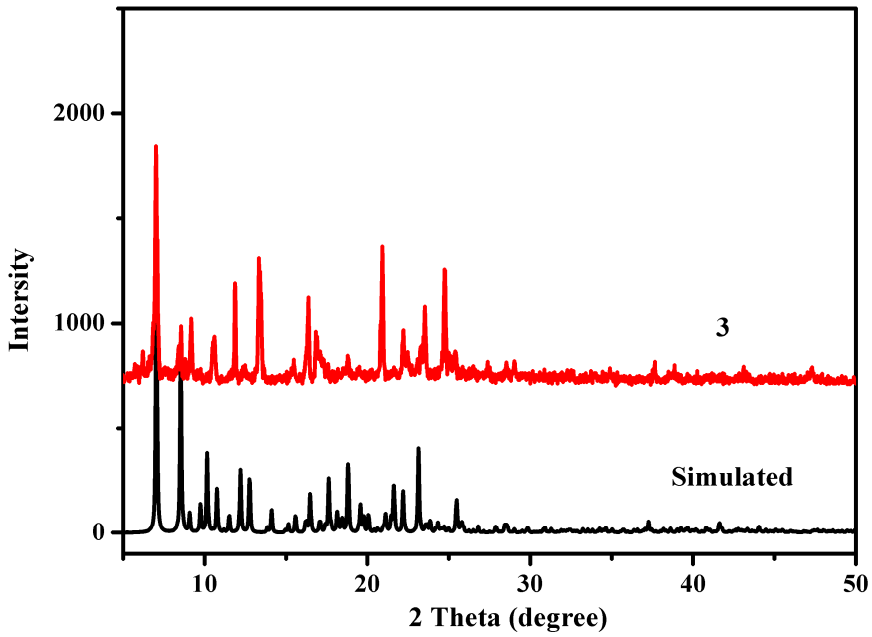

Figure S14. The PXRD pattern and the simulated PXRD pattern of **4**.

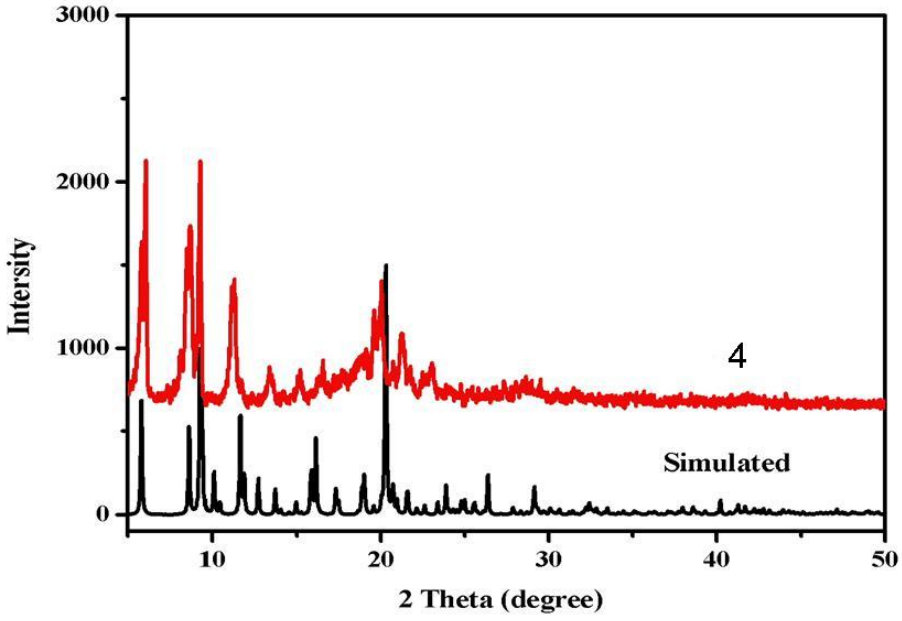

Figure S15. UV-vis spectra for H_2**L**.

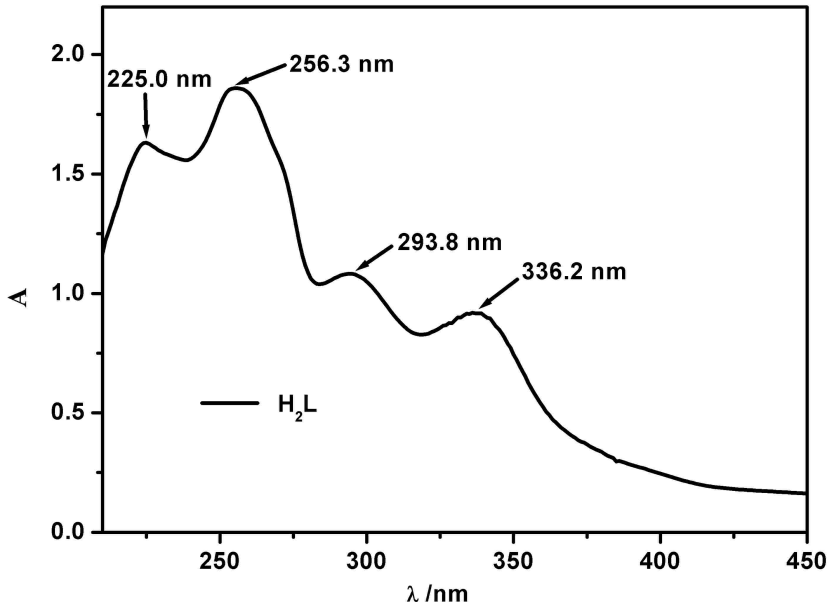

Figure S16. Solid UV-vis spectra for **1**, **3** and **4**.