A series of coordination polymers exhibiting dual chiral features and diverse interhelical interactions

Zilu Chen,[†] Suni Qin,[†,‡] Dongcheng Liu,[†] Yanling Shen[†] and Fupei Liang[†]*

[†]Key Laboratory for the Chemistry and Molecular Engineering of Medicinal Resources (Ministry of Education of China), School of Chemistry & Chemical Engineering of Guangxi Normal University, Guilin 541004, P. R. China.

[‡]Institute of Karst Geology, Chinese Academy of Geological Science, Guilin 541004, Guangxi, P. R. China.

Electronic Supplementary Information

Table S1. Selected bond lengths (Å) and angles (deg) for complex **1–3**

1							
Co1-O1	1.979(4)	O1-Co1-N1	87.57(16)	N3-Co1-O3A	91.42(16)	O1-Co1-N4	87.37(16)
Co1-N1	2.081(5)	O1-Co1-N3	102.82(17)	O1-Co1-O4A	104.81(16)	N1-Co1-N4	174.69(17)
Co1-N3	2.117(5)	N1-Co1-N3	90.92(18)	N1-Co1-O4A	93.71(17)	N3-Co1-N4	88.64(16)
Co1-O3A	2.172(4)	O1-Co1-O3A	165.48(16)	N3-Co1-O4A	152.14(16)	O3A-Co1-N4	90.18(16)
Co1-O4A	2.177(4)	N1-Co1-O3A	95.12(17)	O3A-Co1-O4A	60.82(15)	O4A-Co1-N4	89.15(16)
Co1-N4	2.193(4)						
Symmetry codes: A) $-x + 1, y - 1/2, -z + 1/2$.							
2							
Ni1-O1	1.994(3)	O1-Ni1-N1	87.32(13)	N3-Ni1-O3A	97.54(12)	O1-Ni1-O4A	100.85(12)
Ni1-N1	2.048(3)	O1-Ni1-N3	99.72(13)	O1-Ni1-N4	88.82(13)	N1-Ni1-O4A	88.68(13)
Ni1-N3	2.066(4)	N1-Ni1-N3	92.29(14)	N1-Ni1-N4	175.29(15)	N3-Ni1-O4A	159.43(12)
Ni1-O3A	2.093(3)	O1-Ni1-O3A	162.69(12)	N3-Ni1-N4	91.02(14)	O3A-Ni1-O4A	61.89(11)
Ni1-N4	2.120(4)	N1-Ni1-O3A	93.34(13)	O3A-Ni1-N4	89.54(13)	N4-Ni1-O4A	89.39(13)
Ni1-O4A	2.148(3)						
Symmetry codes: A) $-x + 1, y - 1/2, -z + 1/2$.							
3							
Cu1-O1	1.891(7)	Cu2-N6	2.039(9)	O1-Cu1-O4A	113.4(3)	O5-Cu2-N6	88.6(3)
Cu1-O3A	1.979(7)	Cu2-O8B	2.409(9)	O3A-Cu1-O4A	57.1(3)	N3-Cu2-N6	167.0(4)
Cu1-N1	1.980(9)	O1-Cu1-O3A	170.5(4)	N1-Cu1-O4A	98.2(3)	O7B-Cu2-N6	91.3(3)
Cu1-N5	2.032(9)	O1-Cu1-N1	89.4(3)	N5-Cu1-O4A	94.4(3)	O5-Cu2-O8B	110.4(3)
Cu1-O4A	2.537(9)	O3A-Cu1-N1	92.5(3)	O5-Cu2-N3	89.6(3)	N3-Cu2-O8B	99.8(3)
Cu2-O5	1.909(7)	O1-Cu1-N5	89.4(3)	O5-Cu2-O7B	169.2(4)	O7B-Cu2-O8B	58.9(3)
Cu2-N3	1.959(9)	O3A-Cu1-N5	90.8(3)	N3-Cu2-O7B	92.9(3)	N6-Cu2-O8B	92.9(3)
Cu2-O7B	1.996(7)	N1-Cu1-N5	166.7(4)				
Symmetry codes: A) $-x + 1, y - 1/2, -z + 2$; B) $-x, y + 1/2, -z + 1$.							

Table S2. Selected bond lengths (Å) and angles (deg) for complex **4** and **5**

4							
Zn1-O5	2.034(4)	O5-Zn1-N4	112.47(18)	N4-Zn1-O7A	90.79(18)	N3-Zn2-O3B	97.56(18)
Zn1-N4	2.055(5)	O5-Zn1-O8A	103.6(2)	O8A-Zn1-O7A	53.14(19)	N1-Zn2-O3B	92.25(18)
Zn1-O8A	2.064(5)	N4-Zn1-O8A	143.9(2)	N5-Zn1-O7A	91.44(18)	O5-Zn2-O3B	99.49(16)
Zn1-N5	2.141(5)	O5-Zn1-N5	85.50(18)	O1-Zn1-O7A	101.81(16)	O1-Zn2-O4B	94.88(17)
Zn1-O1	2.145(4)	N4-Zn1-N5	91.9(2)	O1-Zn2-N3	109.17(17)	N3-Zn2-O4B	155.87(18)
Zn1-O7A	2.602(7)	O8A-Zn1-N5	90.1(2)	O1-Zn2-N1	86.06(18)	N1-Zn2-O4B	85.5(2)
Zn2-O1	2.030(4)	O5-Zn1-O1	80.08(15)	N3-Zn2-N1	94.0(2)	O5-Zn2-O4B	94.4(2)
Zn2-N3	2.093(5)	N4-Zn1-O1	93.55(19)	O1-Zn2-O5	80.16(15)	O3B-Zn2-O4B	58.41(17)
Zn2-N1	2.139(5)	O8A-Zn1-O1	93.3(2)	N3-Zn2-O5	91.74(19)	Zn2-O1-Zn1	99.95(16)
Zn2-O5	2.146(4)	N5-Zn1-O1	165.58(17)	N1-Zn2-O5	166.16(16)	Zn1-O5-Zn2	99.79(17)
Zn2-O3B	2.186(5)	O5-Zn1-O7A	156.60(18)	O1-Zn2-O3B	153.27(18)		
Zn2-O4B	2.235(5)						
Symmetry codes: A) -*x*, *y* + 1/2, -*z*; B) –*x* + 1, *y* - 1/2, -*z* + 1.							
5							
Cd1-O5	2.250(5)	O5-Cd1-N4	107.4(2)	O1-Cd2-N1	79.3(2)	N1-Cd2-O3B	97.4(2)
Cd1-N4	2.279(7)	O5-Cd1-O1	80.54(19)	O1-Cd2-O5	80.92(18)	O5-Cd2-O3B	100.01(19)
Cd1-O1	2.321(5)	N4-Cd1-O1	91.8(2)	N1-Cd2-O5	160.2(2)	N3-Cd2-O3B	101.8(2)
Cd1-N5	2.328(6)	O5-Cd1-N5	78.7(2)	O1-Cd2-N3	105.3(2)	O1-Cd2-O4B	96.61(19)
Cd1-O8A	2.338(5)	N4-Cd1-N5	95.0(3)	N1-Cd2-N3	92.8(2)	N1-Cd2-O4B	86.4(2)
Cd1-O7A	2.374(5)	O1-Cd1-N5	159.2(2)	O5-Cd2-N3	92.9(2)	O5-Cd2-O4B	95.4(2)
Cd2-O1	2.263(5)	O5-Cd1-O8A	99.17(19)	O1-Cd2-O3B	152.83(18)	N3-Cd2-O4B	157.5(2)
Cd2-N1	2.288(7)	N4-Cd1-O8A	153.3(2)	N4-Cd1-O7A	98.2(2)	O3B-Cd2-O4B	56.21(16)
Cd2-O5	2.291(6)	O1-Cd1-O8A	95.0(3)	O1-Cd1-O7A	99.5(2)	Cd2-O1-Cd1	98.62(19)
Cd2-N3	2.292(6)	N5-Cd1-O8A	87.8(3)	N5-Cd1-O7A	99.0(2)	Cd1-O5-Cd2	99.8(2)
Cd2-O3B	2.326(5)	O5-Cd1-O7A	154.40(19)	O8A-Cd1-O7A	55.24(17)		
Cd2-O4B	2.357(5)						
Symmetry codes: A) -*x*, *y* + 1/2, -*z*; B) –*x* + 1, *y* - 1/2, -*z* + 1.							

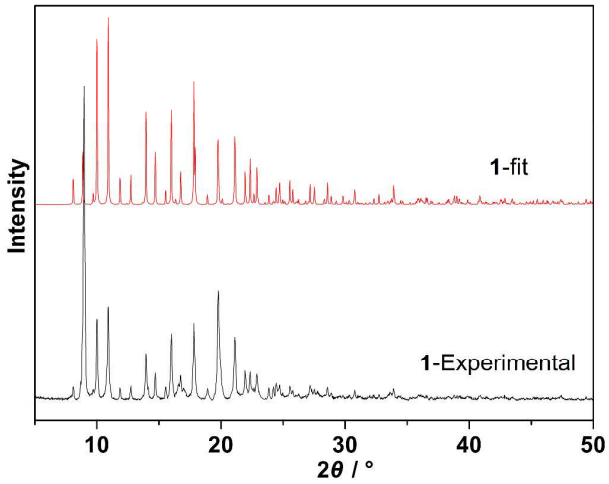

Figure S1. PXRD patterns of **1**.

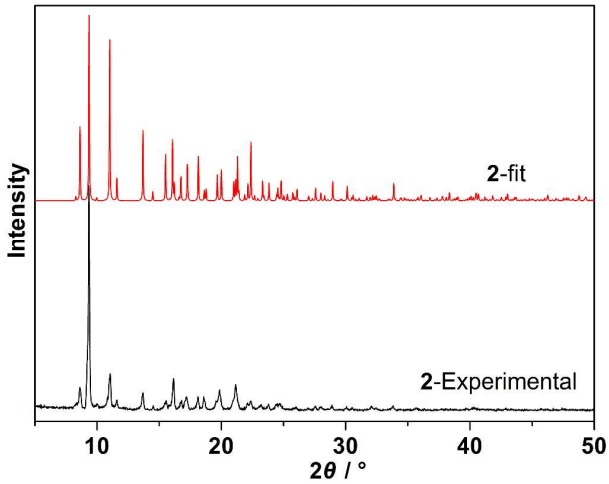

Figure S1. PXRD patterns of **2**.

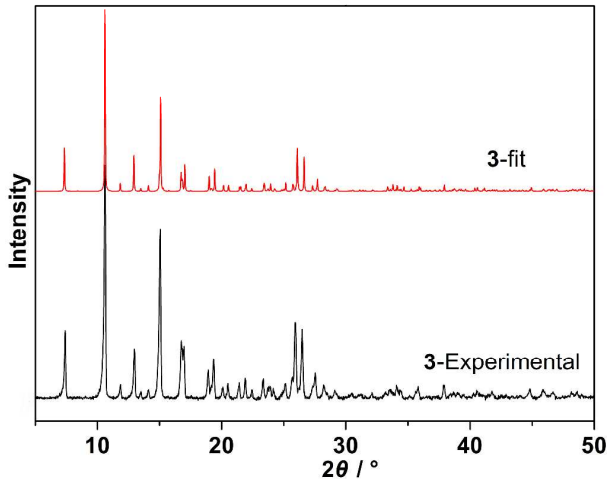

Figure S3. PXRD patterns of **3**.

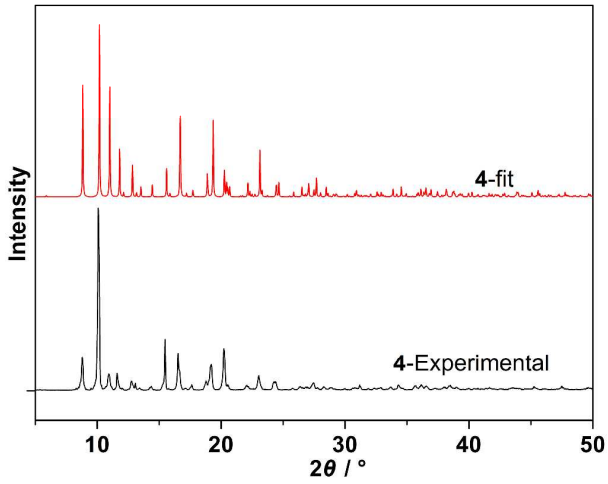

Figure S4. PXRD patterns of **4**.

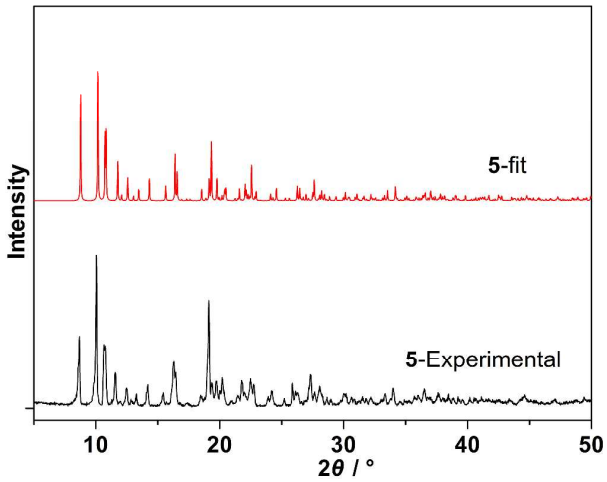

Figure S5. PXRD patterns of **5**.

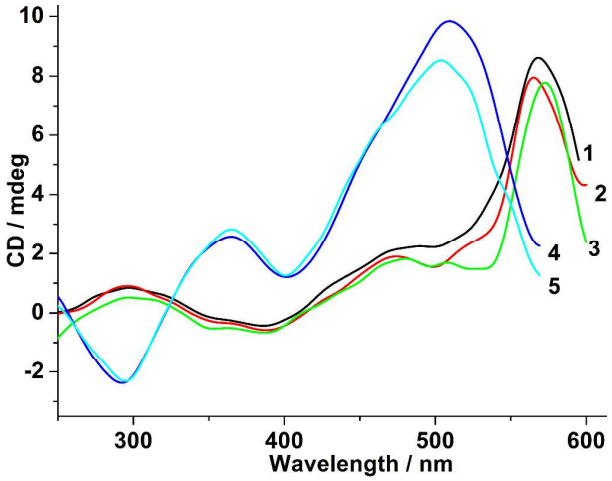

Figure S6. Circular dichroism spectra of **1**-**5** in the solid state.

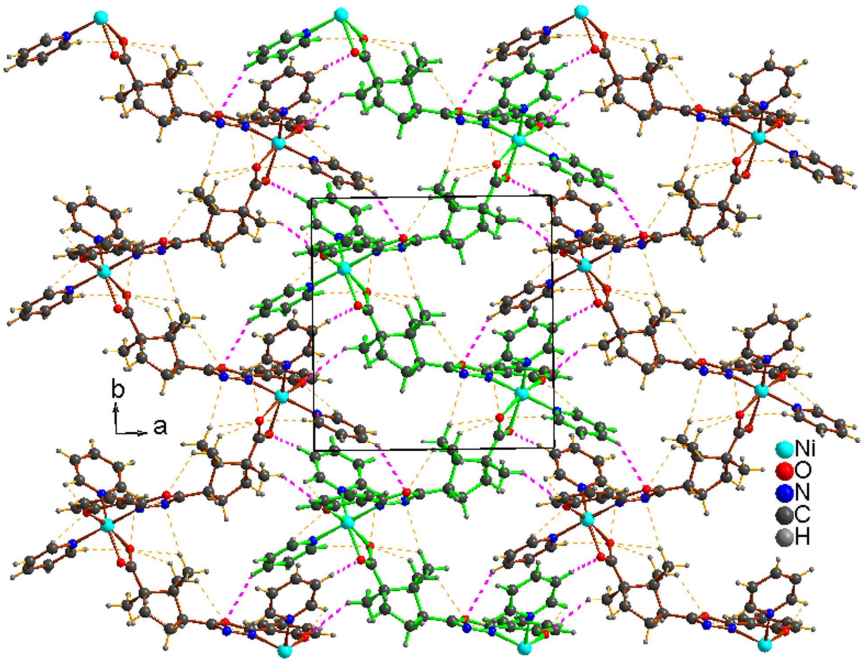

Figure S7. A view of the two-dimensional supramolecular structure of **2**. Purple and yellow dashed lines represent interhelical and intrahelical hydrogen bonds, respectively.

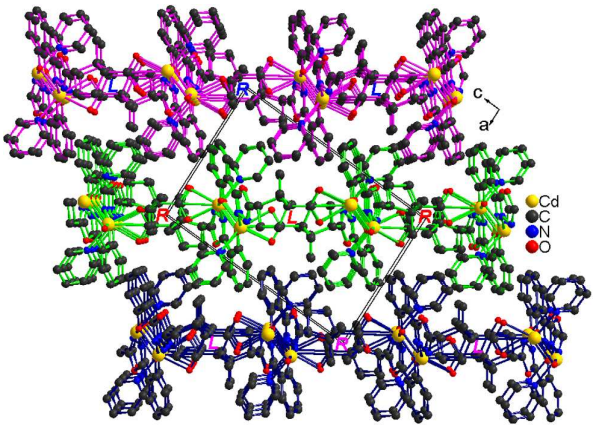

Figure S8. A packing diagram of **5**.

Table S3. Hydrogen bonds in **2**

Hydrogen bonds (symmetry code)	D−H, Å	D···A, Å	D−H···A, º
Intrahelical hydrogen bonds			
C27−H27···O1	0.950(5)	2.936(5)	117.4(3)
C23−H23···O3 (-*x* + 1, +*y* - 1/2, -*z* + 1/2)	0.950(5)	3.076(6)	111.5(3)
C22−H22···O1	0.950(5)	3.370(6)	110.5(3)
C18−H18···O3 (-*x* + 1, +*y* - 1/2, -*z* + 1/2)	0.950(5)	3.272(6)	112.5(3)
C18−H18···N2	0.950(5)	3.377(6)	122.1(3)
C15−H15A···O2	0.980(5)	3.198(6)	117.5(3)
C15−H15B···O3	0.980(7)	3.181(6)	121.2(3)
C14−H14C···O3	0.980(4)	3.382(5)	118.4(3)
C14−H14C···N2 (-*x* + 1, +*y* + 1/2, -*z* + 1/2)	0.980(4)	3.679(6)	167.5(3)
Intralayer hydrogen bonds			
C16−H16A···O1 (*x* + 1, +*y*, +*z*)	0.980(5)	3.662(6)	141.7(3)
C21−H21···O4 (*x* -1, +*y*, +*z*)	0.950(5)	3.197(6)	132.1(3)
C25−H25···O2 (-*x*, +*y* - 1/2, -*z* + 1/2)	0.950(5)	3.634(6)	145.5(3)
Interlayer hydrogen bonds			
C3−H3···O2 (*x* - 1/2, -*y* + 1/2 + 1, -*z* + 1)	0.950(5)	3.395(6)	138.1(3)