Supplementary Material (ESI) for CrystEngComm

SUPPORTING INFORMATION

to the paper entitled

Synthesis and structures of helical and meso-helical coordination polymers directed by the conformation restriction of flexible / angular pyridine-containing ligands

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Table of contents

1. Fig. S1 π-π Interactions between chains in **1**. (a) viewing along the *c* axis; (b) showing π-π interactions between metallacycles from neighboring chains.
2. Fig. S2 The O-H···O helical chains along the *b* axis in **1**.
3. Fig. S3 Packing diagram of **5** along the *a* and *b* axes.
4. Fig. S4 The arrangement in an ···ABAB··· fashion of 1D zigzag chains in **6**.
5. Table S1 Selected bond Lengths (Å) for complexes **1**, **2**, **3**, **4, 5 and 6**.

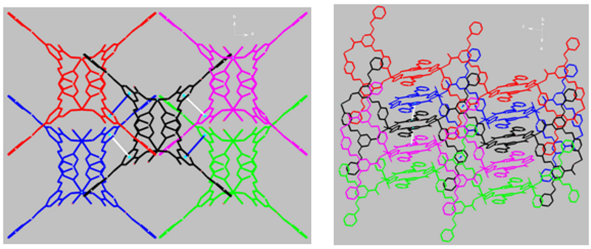

Fig. S1 π-π Interactions between chains in **1**. (a) viewing along the *c* axis; (b) showing π-π interactions between metallacycles from neighboring chains.

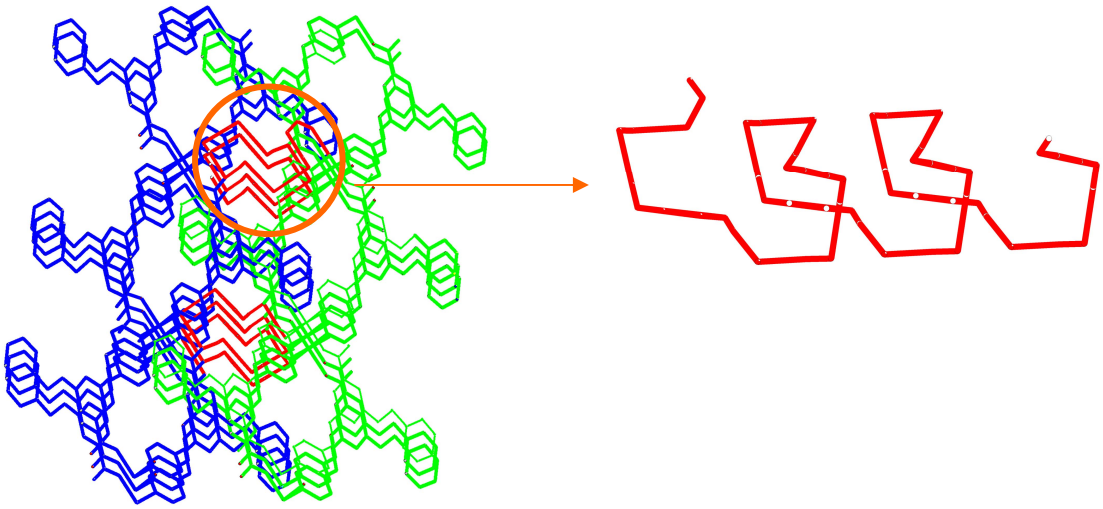

Fig. S2 The O-H···O helical chains along the *b* axis in **1**.

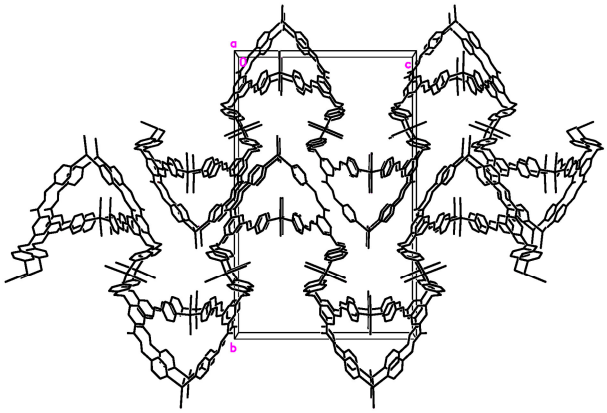

Fig. S3 Packing diagram of **5** along the *a* and *b* axes.

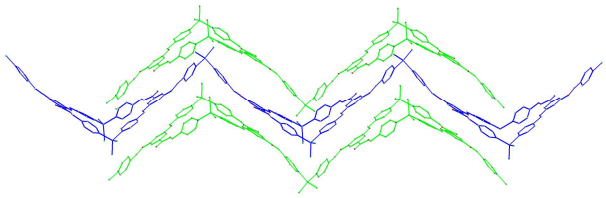

Fig. S4 The arrangement in an ···ABAB··· fashion of 1D zigzag chains in **6**.

Table S1. Selected bond Lengths (Å) and angles (°) for complexes 1, 2, 3,4,5 and 6

1

Ni(1)-O(1)	2.049(2)	O(1)-Ni(1)-N(2)^{ii}	91.09(9)
Ni(1)-O(5)	2.091(2)	O(5)-Ni(1)-N(2)^{ii}	174.03(10)
Ni(1)-N(2)^{i}	2.108(3)	O(5)^{i}-Ni(1)-N(2)^{ii}	88.96(10)
O(1)^{i}-Ni(1)-O(1)	174.79(12)	O(1)-Ni(1)-N(2)^{iii}	92.75(10)
O(1)-Ni(1)-O(5)	89.00(9)	O(5)-Ni(1)-N(2)^{iii}	88.96(10)
O(1)-Ni(1)-O(5)^{i}	87.55(9)	O(5)^{i}-Ni(1)-N(2)^{iii}	174.03(10)
O(5)-Ni(1)-O(5)^{i}	97.01(13)	N(2)^{ii}-Ni(1)-N(2)^{iii}	85.08(15)

i -x,y,-z-1/2 ii -x,-y+1,-z iii x,-y+1,z-1/2

2

Co(1)-O(2)	2.069(2)	O(2)-Co(1)-N(1)^{ii}	91.82(11)
Co(1)-O(5)	2.137(3)	O(5)-Co(1)-N(1)^{ii}	173.47(13)
Co(1)-N(1)^{iii}	2.158(3)	O(5)^{i} -Co(1)-N(1)^{ii}	89.03(12)
O(2)^{i} -Co(1)-O(2)	174.85(16)	O(2)-Co(1)-N(1)^{iii}	91.99(11)
O(2)-Co(1)-O(5)	88.62(10)	O(5)-Co(1)-N(1)^{iii}	89.03(12)
O(2)-Co(1)-O(5)^{i}	87.99(10)	O(5)^{i} -Co(1)-N(1)^{iii}	173.47(13)
O(5)-Co(1)-O(5)^{i}	97.50(17)	N(1)^{ii} -Co(1)-N(1)^{iii}	84.45(19)

i -x,y,-z+3/2 ii -x,-y,-z+2 iii x,-y,z-1/2

3

Co(1)-O(1)	2.0699(19)	O(1)-Co(1)-O(2)^{i}	99.60(8)
Co(1)-N(1)^{ii}	2.083(2)	N(1)^{ii} -Co(1)-O(2)^{i}	160.04(8)
Co(1)-O(2)	2.235(2)	O(1)-Co(1)-O(2)	61.17(7)
O(1)^{i} -Co(1)-O(1)	153.20(12)	N(1)^{ii} -Co(1)-O(2)	89.51(8)
O(1)-Co(1)-N(1)^{ii}	99.37(9)	N(1)^{iii} -Co(1)-O(2)	160.04(8)
O(1)-Co(1)-N(1)^{iii}	98.88(8)	O(2)^{i} -Co(1)-O(2)	94.26(11)
N(1)^{ii} -Co(1)-N(1)^{iii}	93.61(13)		

i -x,y,-z-1/2 ii x-1/2,y+1/2,z iii -x+1/2,y+1/2,-z-1/2

4

Hg(1)-Cl(1)	2.356(8)	Cl(1)-Hg(1)-N(2)	99.1(6)
Hg(1)-N(2)	2.42(3)	N(2)^{i} -Hg(1)-N(2)	98.5(11)
Hg(2)-Cl(2)	2.389(6)	Cl(2)-Hg(2)-Cl(3)	148.2(3)
Hg(2)-Cl(3)	2.402(7)	Cl(2)-Hg(2)-N(1)	97.6(6)
Hg(2)-N(1)	2.407(19)	Cl(3)-Hg(2)-N(1)	102.5(6)
Hg(2)-N(3)^{ii}	2.43(2)	Cl(2)-Hg(2)-N(3)^{ii}	97.2(5)
Cl(1)^{i} -Hg(1)-Cl(1)	154.8(4)	Cl(3)-Hg(2)-N(3)^{ii}	102.4(6)
Cl(1)-Hg(1)-N(2)^{i}	97.4(6)	N(1)-Hg(2)-N(3)^{ii}	101.9(6)

i -x,y,-z+1/2 ii x,-y,z+1/2

5

Hg(1)-N(1)	2.360(11)	N(1)-Hg(1)-I(2)	101.4(4)
Hg(1)-I(1)	2.6453(18)	I(1)-Hg(1)-I(2)	136.74(6)
Hg(1)-I(2)	2.6721(19)	N(2)-Hg(2)-N(2)^{ii}	79.9(5)
Hg(2)-N(2)	2.450(12)	N(2)-Hg(2)-I(4)	109.0(3)
Hg(2)-I(4)	2.630(2)	N(2)-Hg(2)-I(3)	102.5(3)
Hg(2)-I(3)	2.6447(19)	I(4)-Hg(2)-I(3)	138.51(7)
Hg(3)-N(3)	2.458(10)	N(3)-Hg(3)-N(3)^{ii}	80.7(5)
Hg(3)-I(5)	2.6377(10)	N(3)-Hg(3)-I(5)	98.6(3)
N(1)-Hg(1)-N(1)^{i}	90.4(6)	N(3)-Hg(3)-I(5)^{ii}	104.2(3)
N(1)-Hg(1)-I(1)	108.7(4)	I(5)-Hg(3)-I(5)^{ii}	149.92(7)

i x,y,-z+1/2 ii x,-y+1/2,-z

6

Zn(1)-N(1)	2.027(4)	N(2)^{i}-Zn(1)-Cl(1)	105.25(13)
Zn(1)-N(2)^{i}	2.040(4)	N(1)-Zn(1)-Cl(2)	104.82(12)
Zn(1)-Cl(1)	2.2017(15)	N(2)^{i}-Zn(1)-Cl(2)	108.18(13)
Zn(1)-Cl(2)	2.2215(16)	Cl(1)-Zn(1)-Cl(2)	118.86(7)
Zn(2)-N(3)	2.034(4)	N(3)^{ii}-Zn(2)-N(3)	103.5(2)
Zn(2)-Cl(3)	2.2268(16)	N(3)-Zn(2)-Cl(3)^{ii}	109.01(13)
N(1)-Zn(1)-N(2)^{i}	105.87(16)	N(3)-Zn(2)-Cl(3)	106.89(12)
N(1)-Zn(1)-Cl(1)	113.14(12)	Cl(3)^{ii}-Zn(2)-Cl(3)	120.31(11)

i -x+1,y,-z+1/2 ii -x,y,-z-1/2