Electronic Supplementary Information for Dalton Transactions

Supporting Information for

Constructions of 1D helical chains with left-handed/right-handed helicity: a correlation between the helicity of 1D chains and the chirality of building blocks

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Table S1 Selected bond distances (Å) and angles (deg) for **1**~**3**

S-**1**

Ni(1)-N(5)	2.129(5)	Ni(1)-N(8)	2.067(5)	Ni(1)-N(2)	2.147(5)
Ni(1)-N(4)	2.154(4)	Ni(1)-N(1)	2.184(5)	Ni(1)-N(3)	2.199(5)
N(5)-Ni(1)-N(8)	86.89(19)	N(5)-Ni(1)-N(2)	87.07(18)	N(8)-Ni(1)-N(2)	170.3(2)
N(5)-Ni(1)-N(4)	170.85(18)	N(8)-Ni(1)-N(4)	88.06(19)	N(2)-Ni(1)-N(4)	98.90(18)
N(5)-Ni(1)-N(1)	86.57(19)	N(8)-Ni(1)-N(1)	103.58(19)	N(2)-Ni(1)-N(1)	83.62(18)
N(4)-Ni(1)-N(1)	87.22(18)	N(5)-Ni(1)-N(3)	104.21(19)	N(8)-Ni(1)-N(3)	87.38(19)
N(2)-Ni(1)-N(3)	86.75(18)	N(4)-Ni(1)-N(3)	83.16(18)	N(1)-Ni(1)-N(3)	165.18(19)
C(17)-N(6)-C(18)	117.1(5)	C(19)-N(9)-C(20)	117.1(6)		
N(3)…N(7)#1	3.247(8)	N(2)…N(6)#3	3.099(7)	N(1)…N(10)#2	3.172(8)
N(3)-H(3A)…N(7)#1	166.3	N(2)-H(2C)…N(2C)#2	169.2	N(1)-H(1C)…N(10)#2	162.0

R-**1**

Ni(1)-N(5)	2.0561(16)	Ni(1)-N(8)	2.1166(16)	Ni(1)-N(2)	2.1301(16)
Ni(1)-N(4)	2.1480(15)	Ni(1)-N(1)	2.1721(16)	Ni(1)-N(3)	2.1825(16)
N(5)-Ni(1)-N(8)	86.88(6)	N(5)-Ni(1)-N(2)	170.27(7)	N(8)-Ni(1)-N(2)	87.01(6)
N(5)-Ni(1)-N(4)	88.33(6)	N(8)-Ni(1)-N(4)	170.75(6)	N(2)-Ni(1)-N(4)	98.73(6)
N(5)-Ni(1)-N(1)	103.42(6)	N(8)-Ni(1)-N(1)	86.53(6)	N(2)-Ni(1)-N(1)	83.76(6)
N(4)-Ni(1)-N(1)	86.90(6)	N(5)-Ni(1)-N(3)	87.49(6)	N(8)-Ni(1)-N(3)	104.10(6)
N(2)-Ni(1)-N(3)	86.66(6)	N(4)-Ni(1)-N(3)	83.57(6)	N(1)-Ni(1)-N(3)	165.31(6)

C(17)-N(6)-C(18)	119.40(17)	C(19)-N(9)-C(20)	116.88(17)		
N(1)…N(7)#1	3.151(2)	N(2)…N(9)#2	3.093(2)	N(3)…N(10)#3	3.239(3)
N(1)-H(1C)…N(7)#1	161.4	N(2)-H(2C)…N(9)#2	169.0	N(3)-H(3A)…N(10)#3	166.3

Δ-2

N(1)-Ni(1)	2.166(3)	N(2)-Ni(1)	2.117(4)	N(3)-Ni(1)	2.175(3)
N(4)-Ni(1)	2.122(4)	N(5)-Ni(2)	2.169(4)	N(6)-Ni(2)	2.144(4)
N(7)-Ni(2)	2.165(4)	N(8)-Ni(2)	2.120(3)	N(9)-Ni(1)	2.117(4)
N(11)-Ni(2)	2.104(3)	N(12)-Ni(1)	2.095(4)	N(15)-Ni(2)	2.131(4)
C(33)-N(9)-Ni(1)	148.5(4)	N(9)-Ni(1)-N(3)	86.25(14)	N(11)-Ni(2)-N(8)	169.78(16)
C(34)-N(10)-C(33)	122.4(5)	N(2)-Ni(1)-N(3)	88.95(13)	N(6)-Ni(2)-N(8)	98.98(15)
C(34)-N(11)-Ni(2)	158.5(4)	N(12)-Ni(1)-N(3)	100.94(14)	N(15)-Ni(2)-N(5)	103.74(16)
C(35)-N(12)-Ni(1)	163.0(5)	N(4)-Ni(1)-N(3)	83.48(13)	N(11)-Ni(2)-N(5)	86.13(14)
C(36)-N(13)-C(35)	117.4(6)	N(9)-Ni(1)-N(1)	101.67(15)	N(6)-Ni(2)-N(5)	83.72(15)
C(37)-N(15)-Ni(2)	140.8(4)	N(2)-Ni(1)-N(1)	84.20(15)	N(8)-Ni(2)-N(5)	87.34(14)
C(37)-N(16)-C(38)	125.0(6)	N(12)-Ni(1)-N(1)	87.28(14)	N(15)-Ni(2)-N(7)	85.93(16)
N(9)-Ni(1)-N(2)	170.63(14)	N(4)-Ni(1)-N(1)	89.23(13)	N(11)-Ni(2)-N(7)	102.83(15)
N(9)-Ni(1)-N(12)	84.47(17)	N(3)-Ni(1)-N(1)	169.18(15)	N(6)-Ni(2)-N(7)	87.92(15)
N(2)-Ni(1)-N(12)	88.55(16)	N(15)-Ni(2)-N(11)	84.24(15)	N(8)-Ni(2)-N(7)	84.88(14)
N(9)-Ni(1)-N(4)	89.08(16)	N(15)-Ni(2)-N(6)	168.88(15)	N(5)-Ni(2)-N(7)	167.56(14)
N(2)-Ni(1)-N(4)	98.37(15)	N(11)-Ni(2)-N(6)	88.11(14)	N(15)-Ni(2)-N(8)	89.70(15)
N(12)-Ni(1)-N(4)	171.90(16)				
N(1)…N(17)#1	3.170(6)	N(2)…O(5)	2.972(5)	N(4)…O(5)	2.956(6)
N(7)…N(14)#2	3.150(7)	N(6)…O(2)	3.187(6)	N(8)…O(3)	3.109(7)
N(1)-H(1C)…N(17)#1	162.7	N(2)-H(2C)…O(5)	159.3	N(4)-H(4D)…O(5)	166.1
N(7)-H(7D)…N(14)#2	154.0	N(6)-H(6A)…O(2)	159.7	N(8)-H(8D)…O(3)	164.4

Λ-2

N(1)-Ni(1)	2.169(3)	N(2)-Ni(1)	2.111(3)	N(3)-Ni(1)	2.166(3)
N(4)-Ni(1)	2.148(3)	N(5)-Ni(2)	2.166(3)	N(6)-Ni(2)	2.119(3)

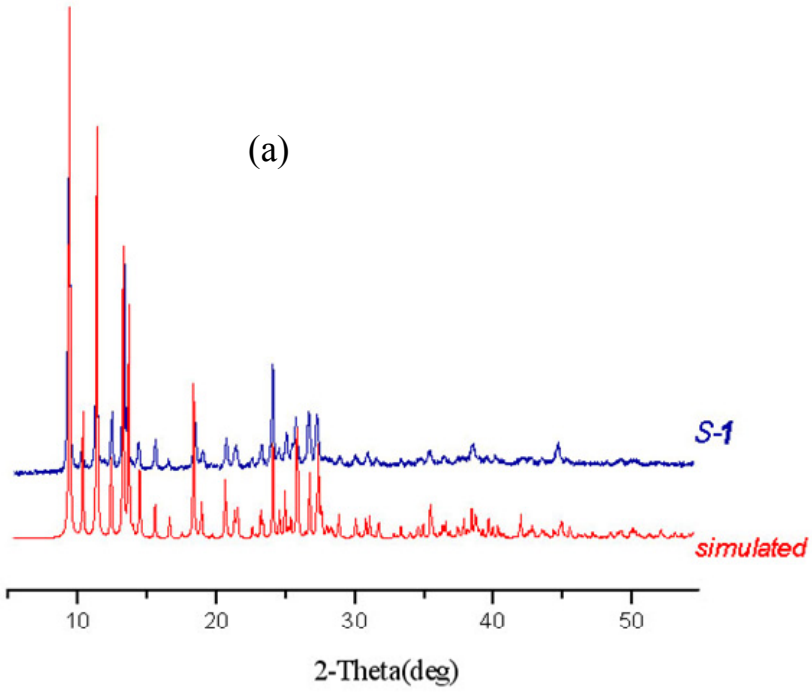
N(7)-Ni(2)	2.172(3)	N(8)-Ni(2)	2.121(3)	N(9)-Ni(1)	2.109(3)
N(11)-Ni(2)	2.119(3)	N(12)-Ni(1)	2.132(4)	N(15)-Ni(2)	2.102(3)
C(33)-N(9)-Ni(1)	158.2(3)	N(2)-Ni(1)-N(4)	98.72(12)	N(8)-Ni(2)-N(15)	171.96(13)
C(33)-N(10)-C(34)	122.2(4)	N(12)-Ni(1)-N(1)	85.95(13)	N(11)-Ni(2)-N(6)	170.80(12)
C(34)-N(11)-Ni(2)	148.6(3)	N(9)-Ni(1)-N(1)	84.11(13)	N(8)-Ni(2)-N(6)	98.04(12)
C(35)-N(12)-Ni(1)	141.1(3)	N(2)-Ni(1)-N(1)	84.59(11)	N(15)-Ni(2)-N(6)	88.64(13)
C(35)-N(13)-C(36)	125.2(4)	N(4)-Ni(1)-N(1)	87.80(12)	N(11)-Ni(2)-N(7)	85.97(12)
C(37)-N(15)-Ni(2)	163.1(4)	N(12)-Ni(1)-N(3)	103.77(13)	N(8)-Ni(2)-N(7)	83.85(12)
C(38)-N(16)-C(37)	117.5(5)	N(9)-Ni(1)-N(3)	85.90(12)	N(15)-Ni(2)-N(7)	100.80(12)
N(12)-Ni(1)-N(9)	84.11(13)	N(2)-Ni(1)-N(3)	87.67(11)	N(6)-Ni(2)-N(7)	89.21(11)
N(12)-Ni(1)-N(2)	90.02(13)	N(4)-Ni(1)-N(3)	83.80(12)	N(11)-Ni(2)-N(5)	101.82(13)
N(9)-Ni(1)-N(2)	170.01(13)	N(1)-Ni(1)-N(3)	167.59(12)	N(8)-Ni(2)-N(5)	89.32(12)
N(12)-Ni(1)-N(4)	168.73(12)	N(11)-Ni(2)-N(8)	89.23(13)	N(15)-Ni(2)-N(5)	86.93(12)
N(9)-Ni(1)-N(4)	88.18(12)	N(11)-Ni(2)-N(15)	84.59(14)	N(6)-Ni(2)-N(5)	83.98(12)
N(7)-Ni(2)-N(5)	169.60(12)				
N(1)…N(17)#1	3.158(6)	N(2)…O(3)	3.097(5)	N(4)…O(1)	3.187(5)
N(6)…O(5)	2.967(4)	N(5)…N(14)#2	3.173(5)	N(8)…O(5)	2.943(5)
N(1)-H(1C)…N(17)#1	154.0	N(2)-H(2C)…O(3)	164.1	N(4)-H(4D)…O(1)	159.2
N(6)-H(6A)…O(5)	159.6	N(5)-H(5C)…N(14)#2	162.6	N(8)-H(8D)…O(5)	165.8

3

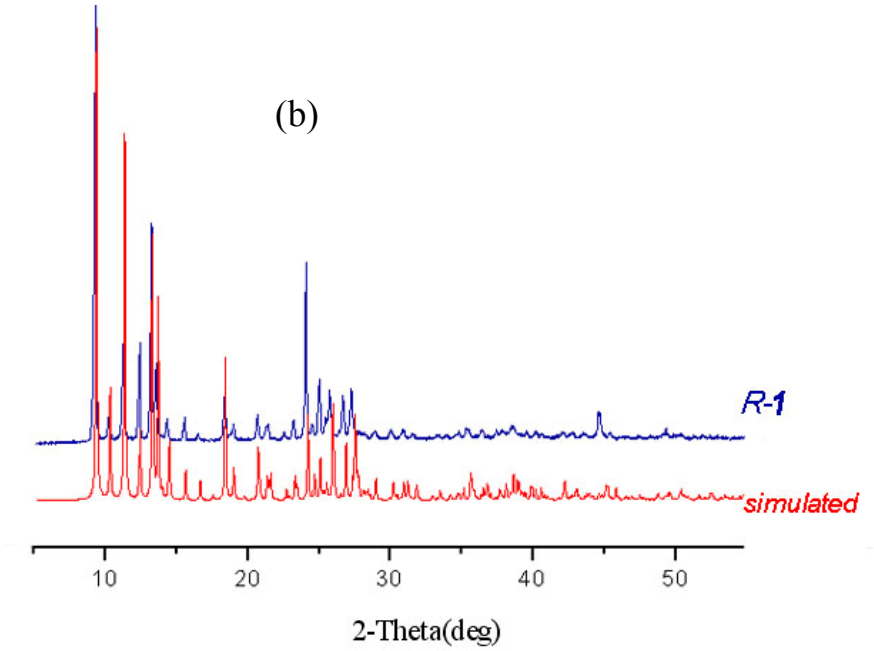
N(1)-Ni(1)	2.170(7)	N(2)-Ni(1)	2.123(8)	N(3)-Ni(1)	2.193(8)
N(4)-Ni(1)	2.125(8)	N(5)-Ni(2)	2.152(6)	N(6)-Ni(2)	2.128(6)
N(7)-Ni(1)	2.114(8)	N(9)-Ni(2)	2.106(7)	Ni(2)-N(9)#1	2.106(7)
Ni(2)-N(6)#1	2.128(6)	Ni(2)-N(5)#1	2.152(6)		
C(27)-N(10)-Ni(1)	149.8(10)	C(27)#1-N(11)-C(27)	119(2)	C(27')-N(11')-C(27)	27.2(19)
C(27')-N(11')-C(27)#1	113(3)	C(27)-N(11')-C(27)#1	90(2)	C(25)-N(7)-Ni(1)	169.0(7)
C(25)-N(8)-C(26)	126.3(9)	C(26)-N(9)-Ni(2)	175.5(7)	N(10)-Ni(1)-N(7)	85.5(3)
N(10)-Ni(1)-N(2)	168.5(3)	N(7)-Ni(1)-N(2)	87.0(3)	N(10)-Ni(1)-N(4)	88.9(3)
N(7)-Ni(1)-N(4)	170.5(3)	N(2)-Ni(1)-N(4)	99.6(3)	N(10)-Ni(1)-N(1)	103.8(3)
N(7)-Ni(1)-N(1)	85.9(3)	N(2)-Ni(1)-N(1)	84.3(3)	N(4)-Ni(1)-N(1)	88.0(3)
N(10)-Ni(1)-N(3)	86.0(3)	N(7)-Ni(1)-N(3)	102.8(3)	N(2)-Ni(1)-N(3)	87.2(3)
N(4)-Ni(1)-N(3)	84.4(3)	N(1)-Ni(1)-N(3)	167.5(3)	N(9)-Ni(2)-N(9)#1	88.0(3)

N(9)-Ni(2)-N(6)#1	170.4(2)	N(9)#1-Ni(2)-N(6)#1	87.5(2)	N(9)-Ni(2)-N(6)	87.5(2)
N(9)#1-Ni(2)-N(6)	170.4(2)	N(6)#1-Ni(2)-N(6)	98.1(4)	N(9)-Ni(2)-N(5)#1	104.3(2)
N(9)#1-Ni(2)-N(5)#1	85.7(2)	N(6)#1-Ni(2)-N(5)#1	83.9(2)	N(6)-Ni(2)-N(5)#1	87.1(2)
N(9)-Ni(2)-N(5)	85.7(2)	N(9)#1-Ni(2)-N(5)	104.3(2)	N(6)#1-Ni(2)-N(5)	87.1(2)
N(6)-Ni(2)-N(5)	83.9(2)	N(5)#1-Ni(2)-N(5)	166.2(3)		

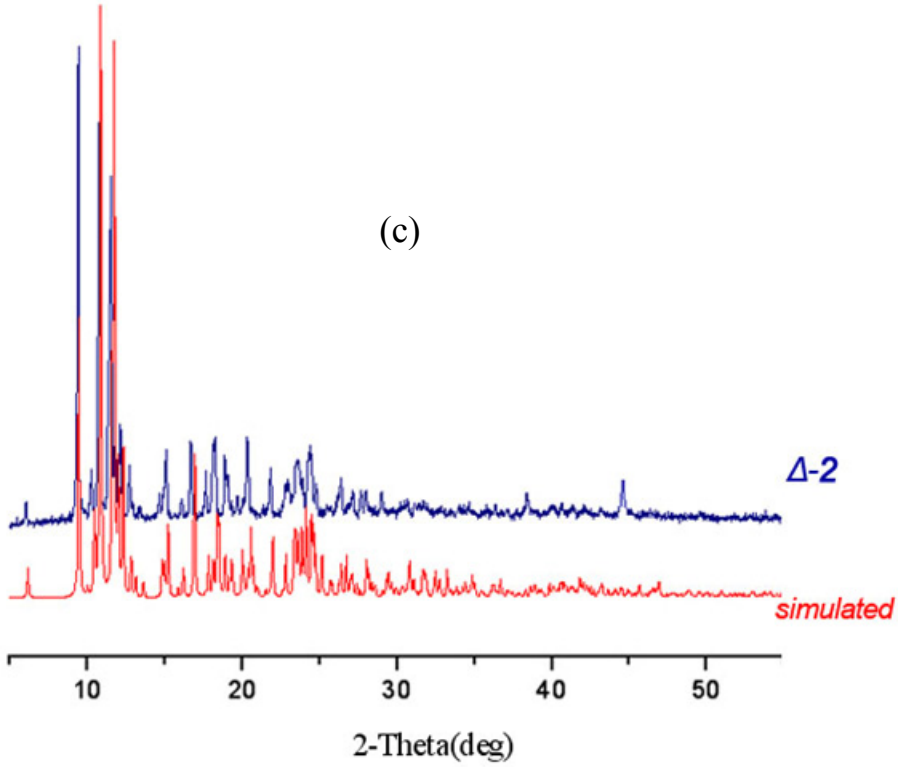
Symmetry transformations used to generate equivalent atoms: *S*-**1**: #1 x, y, z+1; #2 x, y, z-1; #3 x-1, y, z; *R*-**1**: x, y, z+1; #2 x+1, y, z; #3 x, y, z-1; Λ-**2**: # x-1, y, z; #2 x+1, y, z; Δ-**2**: # x-1, y, z; #2 x+1, y, z; **3**: #1 -x+2, y, -z+1/2.



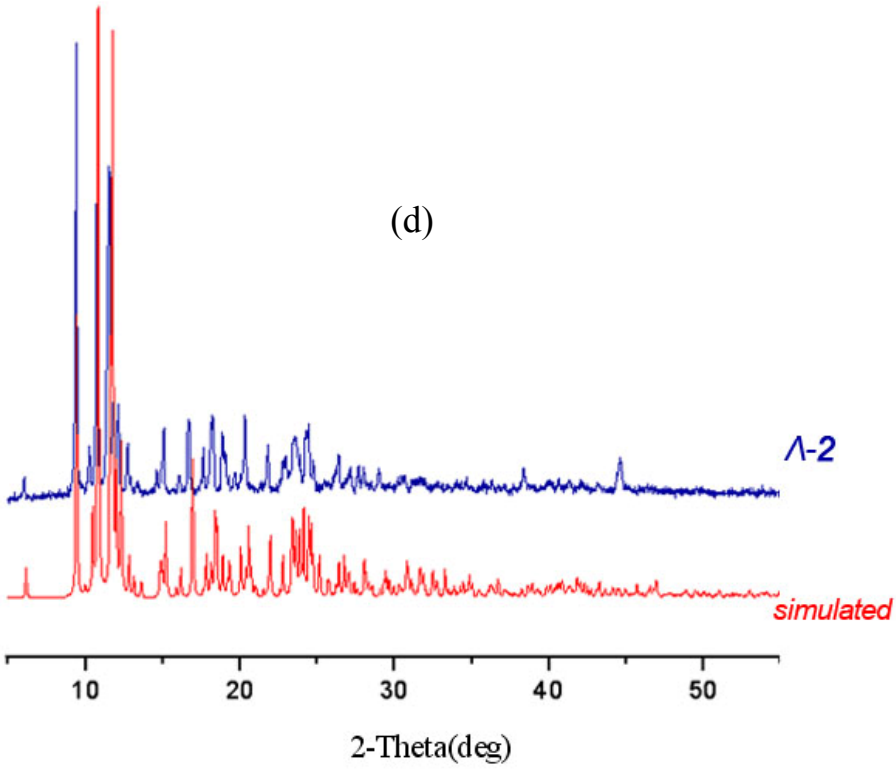
(b)


R-1
simulated
10
20
30
40
50
2-Theta(deg)

(c)


Δ-2
simulated
10
20
30
40
50
2-Theta(deg)

(d)



(e)

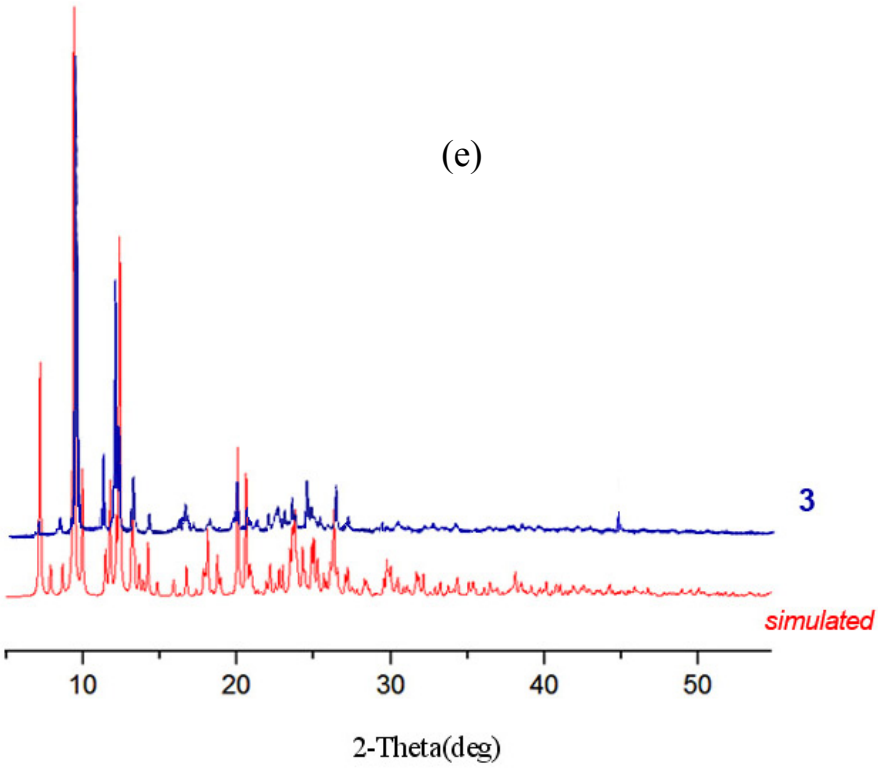


Figure S1. The XRD patterns of the simulated from the single-crystal diffraction data and as-synthesized for (a) *S*-**1**, (b) *R*-**2**, (c) Δ-**2**, (d) Λ-**2**, and (e) **3**.