

Support Information

Diverse Ni(II) MOFs Constructed from Asymmetric Semi-Rigid V-Shaped Multicarboxylate Ligands: Structures and Magnetic Properties

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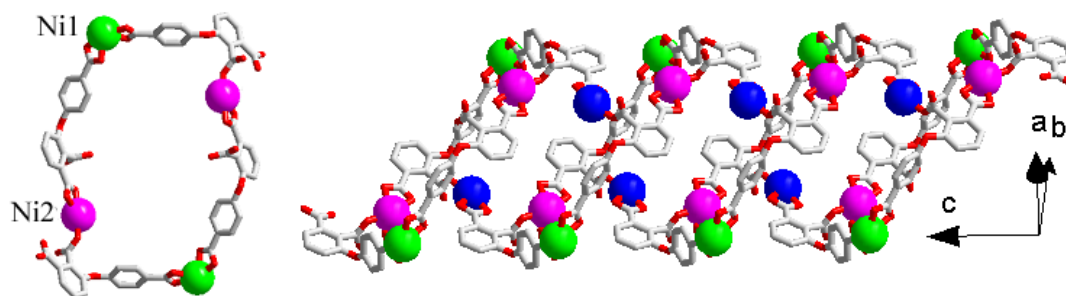


Figure S1. The drawing of 50-membered ring (left) and the tube-like unit, with Ni1 atoms colored green and Ni2 atoms colored pink and blue (right).

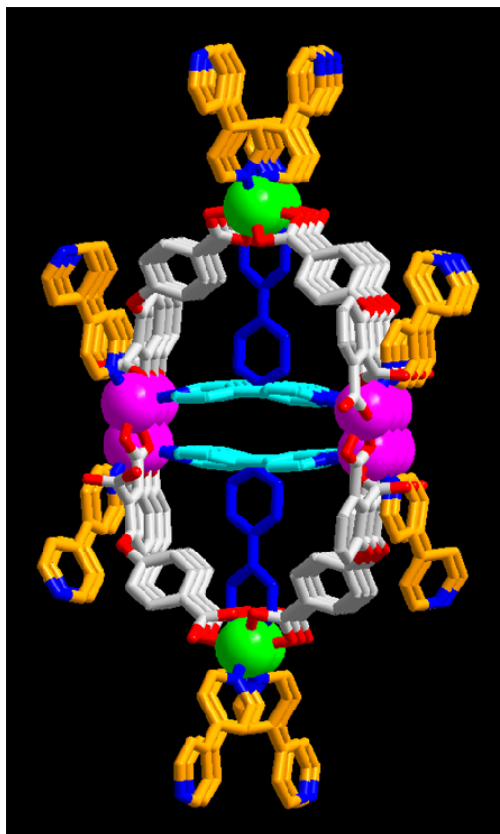


Figure S2. The unit of the isolated tube filled with coordinated and uncoordinated 4,4'-bpy ligand for complex **1**.

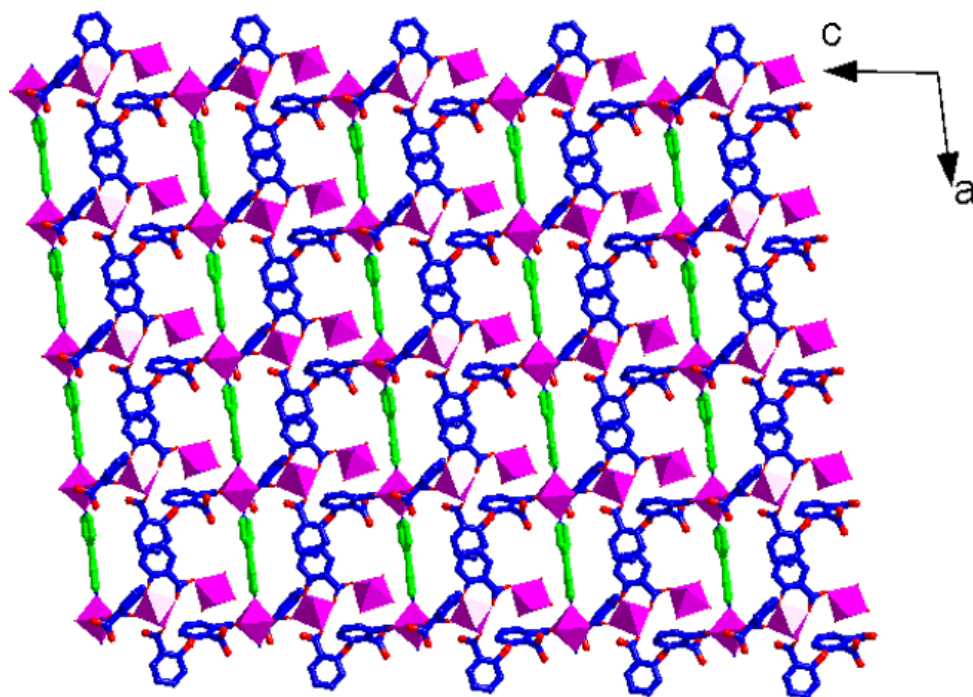


Figure S3. 2D layered network of complex 2.

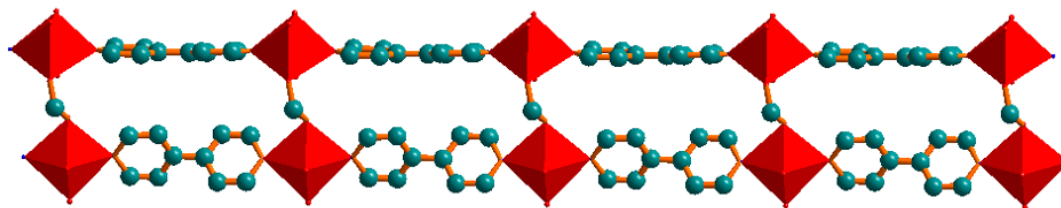


Figure S4. 1D infinite ladder-like unit of complex 2.

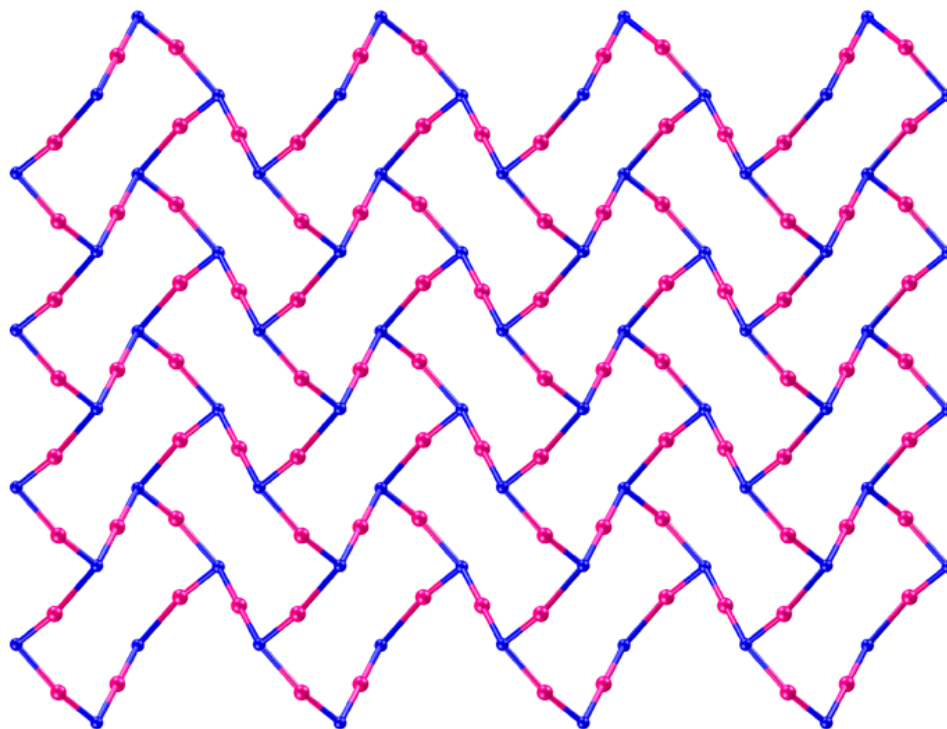


Figure S5. The topology drawing of herringbone motif for **3**.

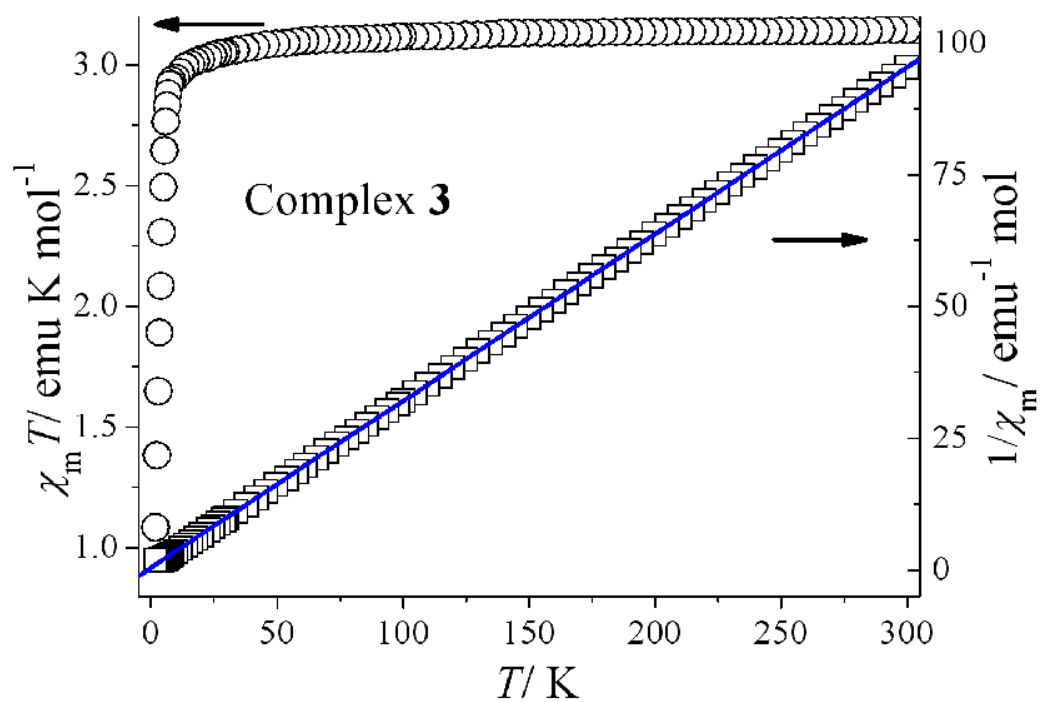


Figure S6. Temperature dependence of $\chi_m T$ for **3**. The blue solid lines represent the best fitting in the temperature range of 2-300 K.

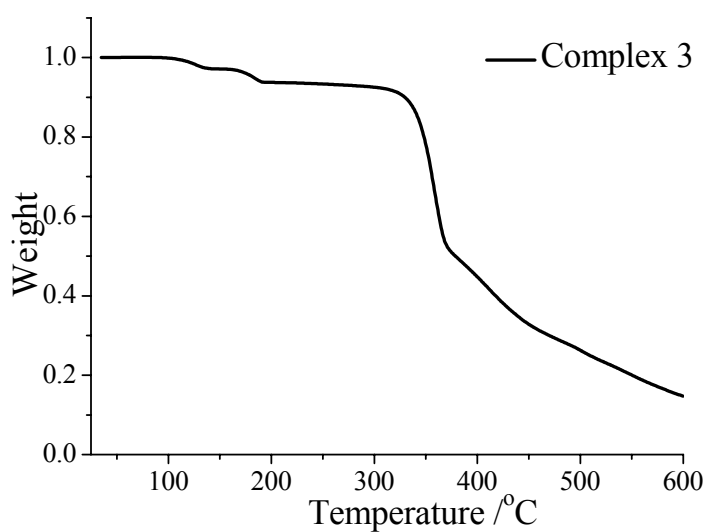
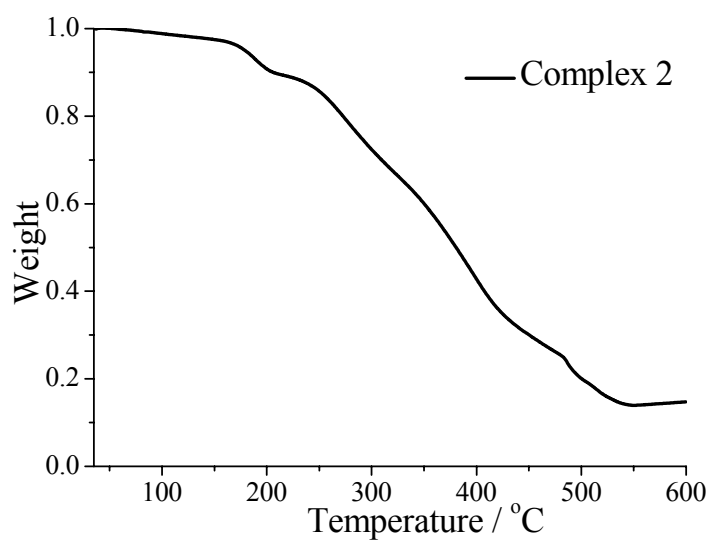
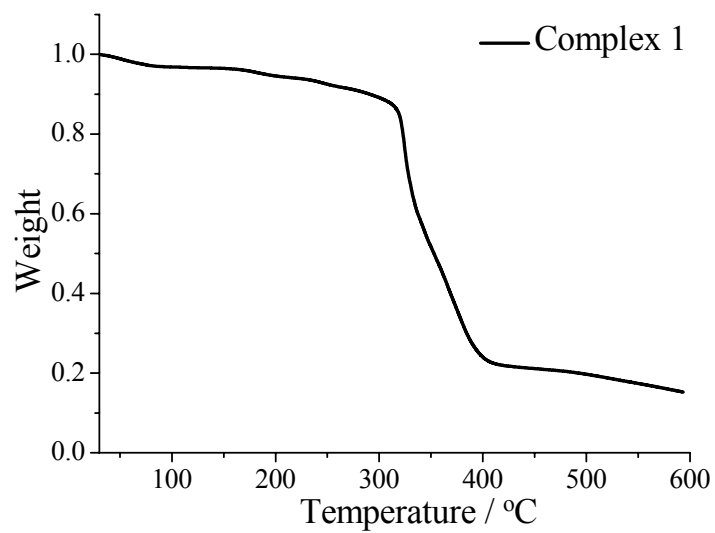


Figure S7. The TGA curves of complex 1-3 in the range of 30-600 °C.

Table S1. Selected bond distances (Å) and bond angles (°).

Complex 1			
N(1)-Ni(1)	2.050(3)	N(2)-Ni(2)	2.062(3)
N(3)-Ni(2)	2.086(3)	O(1)-Ni(2)#1	2.085(3)
O(2)-Ni(2)#1	2.160(3)	O(4)-Ni(2)#4	2.029(3)
O(6)-Ni(1)	2.120(3)	O(7)-Ni(1)	2.094(3)
O(8)-Ni(2)	2.089(3)	Ni(1)-N(1)#5	2.050(3)
Ni(1)-O(7)#5	2.094(3)	Ni(1)-O(6)#5	2.120(3)
Ni(2)-O(1)#7	2.085(3)	Ni(2)-O(4)#6	2.029(3)
Ni(2)-O(2)#7	2.160(3)		
N(1)-Ni(1)-N(1)#5	94.4(2)	N(1)-Ni(1)-O(7)#5	98.45(13)
N(1)#5-Ni(1)-O(7)#5	95.95(13)	N(1)-Ni(1)-O(7)	95.95(13)
N(1)#5-Ni(1)-O(7)	98.45(13)	O(7)#5-Ni(1)-O(7)	158.75(17)
N(1)-Ni(1)-O(6)#5	160.69(13)	N(1)#5-Ni(1)-O(6)#5	91.51(14)
O(7)#5-Ni(1)-O(6)#5	62.60(12)	O(7)-Ni(1)-O(6)#5	101.36(12)
N(1)-Ni(1)-O(6)	91.51(14)	N(1)#5-Ni(1)-O(6)	160.69(13)
O(7)#5-Ni(1)-O(6)	101.36(12)	O(7)-Ni(1)-O(6)	62.60(12)
O(6)#5-Ni(1)-O(6)	88.93(19)	O(4)#6-Ni(2)-N(2)	97.25(12)
O(4)#6-Ni(2)-O(1)#7	164.91(11)	N(2)-Ni(2)-O(1)#7	97.75(12)
O(4)#6-Ni(2)-N(3)	91.05(12)	N(2)-Ni(2)-N(3)	91.27(14)
O(1)#7-Ni(2)-N(3)	90.22(13)	O(4)#6-Ni(2)-O(8)	93.07(11)
N(2)-Ni(2)-O(8)	92.08(12)	O(1)#7-Ni(2)-O(8)	84.79(11)
N(3)-Ni(2)-O(8)	174.32(14)	O(4)#6-Ni(2)-O(2)#7	102.71(11)
N(2)-Ni(2)-O(2)#7	160.04(12)	O(1)#7-Ni(2)-O(2)#7	62.31(10)
N(3)-Ni(2)-O(2)#7	88.18(14)	O(8)-Ni(2)-O(2)#7	87.10(12)
Complex 2			
N(1)-Ni(1)	2.111(10)	N(2)-Ni(1)#3	2.137(10)
N(3)-Ni(3)	2.089(10)	N(4)-Ni(3)	2.101(10)
N(5)-Ni(2)	2.137(10)	N(6)-Ni(2)#1	2.132(10)
O(1)-Ni(1)	2.144(9)	O(2)-Ni(1)	2.092(8)
O(6)-Ni(2)	1.986(8)	O(10)-Ni(1)#4	2.004(8)
O(11)-Ni(2)	2.010(8)	O(12)-Ni(2)	2.120(8)
O(13)-Ni(2)	2.002(8)	O(14)-Ni(3)	2.027(9)
O(15)-Ni(1)	2.047(9)	O(16)-Ni(3)	2.068(11)
O(17)-Ni(3)	2.072(12)	O(18)-Ni(3)	2.060(9)
Ni(1)-O(10)#5	2.004(8)	Ni(1)-N(2)#6	2.137(10)
Ni(2)-N(6)#2	2.132(10)		
O(10)#5-Ni(1)-O(15)	107.1(4)	O(10)#5-Ni(1)-O(2)	158.1(3)
O(15)-Ni(1)-O(2)	94.5(3)	O(10)#5-Ni(1)-N(1)	93.3(4)
O(15)-Ni(1)-N(1)	88.4(4)	O(2)-Ni(1)-N(1)	90.8(4)

O(10)#5-Ni(1)-N(2)#6	87.0(4)	O(15)-Ni(1)-N(2)#6	90.6(4)
O(2)-Ni(1)-N(2)#6	89.3(4)	N(1)-Ni(1)-N(2)#6	179.0(5)
O(10)#5-Ni(1)-O(1)	96.6(3)	O(15)-Ni(1)-O(1)	156.2(4)
O(2)-Ni(1)-O(1)	61.8(3)	N(1)-Ni(1)-O(1)	91.5(4)
N(2)#6-Ni(1)-O(1)	89.5(4)	O(6)-Ni(2)-O(13)	96.3(4)
O(6)-Ni(2)-O(11)	99.8(3)	O(13)-Ni(2)-O(11)	163.8(3)
O(6)-Ni(2)-O(12)	176.9(4)	O(13)-Ni(2)-O(12)	83.6(3)
O(11)-Ni(2)-O(12)	80.2(3)	O(6)-Ni(2)-N(6)#2	90.6(4)
O(13)-Ni(2)-N(6)#2	88.6(4)	O(11)-Ni(2)-N(6)#2	92.3(4)
O(12)-Ni(2)-N(6)#2	92.5(4)	O(6)-Ni(2)-N(5)	84.8(4)
O(13)-Ni(2)-N(5)	88.1(4)	O(11)-Ni(2)-N(5)	92.3(4)
O(12)-Ni(2)-N(5)	92.1(4)	N(6)#2-Ni(2)-N(5)	173.9(4)
O(14)-Ni(3)-O(18)	96.6(4)	O(14)-Ni(3)-O(16)	84.2(4)
O(18)-Ni(3)-O(16)	178.3(4)	O(14)-Ni(3)-O(17)	168.1(6)
O(18)-Ni(3)-O(17)	95.1(6)	O(16)-Ni(3)-O(17)	84.1(6)
O(14)-Ni(3)-N(3)	92.0(4)	O(18)-Ni(3)-N(3)	88.7(4)
O(16)-Ni(3)-N(3)	92.8(4)	O(17)-Ni(3)-N(3)	90.5(5)
O(14)-Ni(3)-N(4)	89.2(4)	O(18)-Ni(3)-N(4)	87.6(4)
O(16)-Ni(3)-N(4)	90.9(4)	O(17)-Ni(3)-N(4)	89.1(4)
N(3)-Ni(3)-N(4)	176.2(4)		
Complex 3			
N(1)-Ni(1)	2.111(2)	N(2)-Ni(2)	2.107(2)
N(3)-Ni(2)	2.111(2)	N(4)-Ni(2)	2.134(2)
O(1)-Ni(1)	2.075(2)	O(4)-Ni(2)#3	2.068(2)
O(6)-Ni(2)#4	2.049(2)	O(8)-Ni(2)	2.086(2)
O(9)-Ni(1)	2.075(2)	Ni(1)-O(1)#5	2.075(2)
Ni(1)-O(9)#5	2.075(2)	Ni(1)-N(1)#5	2.111(2)
Ni(2)-O(6)#4	2.049(2)	Ni(2)-O(4)#6	2.068(2)
O(1)#5-Ni(1)-O(1)	180.0	O(1)#5-Ni(1)-O(9)#5	89.15(9)
O(1)-Ni(1)-O(9)#5	90.85(9)	O(1)#5-Ni(1)-O(9)	90.85(9)
O(1)-Ni(1)-O(9)	89.15(9)	O(9)#5-Ni(1)-O(9)	180.0
O(1)#5-Ni(1)-N(1)#5	89.04(9)	O(1)-Ni(1)-N(1)#5	90.96(9)
O(9)#5-Ni(1)-N(1)#5	90.90(10)	O(9)-Ni(1)-N(1)#5	89.10(10)
O(1)#5-Ni(1)-N(1)	90.96(9)	O(1)-Ni(1)-N(1)	89.04(9)
O(9)#5-Ni(1)-N(1)	89.10(10)	O(9)-Ni(1)-N(1)	90.90(10)
N(1)#5-Ni(1)-N(1)	180.000(1)	O(6)#4-Ni(2)-O(4)#6	175.38(8)
O(6)#4-Ni(2)-O(8)	89.96(9)	O(4)#6-Ni(2)-O(8)	91.35(9)
O(6)#4-Ni(2)-N(2)	91.71(10)	O(4)#6-Ni(2)-N(2)	87.28(9)
O(8)-Ni(2)-N(2)	175.88(9)	O(6)#4-Ni(2)-N(3)	90.69(9)
O(4)#6-Ni(2)-N(3)	93.78(9)	O(8)-Ni(2)-N(3)	88.36(9)
N(2)-Ni(2)-N(3)	87.86(9)	O(6)#4-Ni(2)-N(4)	86.39(9)
O(4)#6-Ni(2)-N(4)	89.13(9)	O(8)-Ni(2)-N(4)	92.42(9)

N(2)-Ni(2)-N(4)	91.44(9)	N(3)-Ni(2)-N(4)	176.97(10)
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Symmetry codes for complexes **1-3**. For complex **1**, #1 $x+1/2, y+1/2, z$; #2 $-x+1, y, -z+1/2$; #3 $-x+2, y, -z+1/2$; #4 $x+1/2, -y+1/2, z+1/2$; #5 $-x+2, y, -z+3/2$; #6 $x-1/2, -y+1/2, z-1/2$; #7 $x-1/2, y-1/2, z$. For **2**, #1 $x+1/2, y+1/2, z$; #2 $x-1/2, y-1/2, z$; #3 $x+1, y, z$; #4 $x, -y, z+1/2$; #5 $x, -y, z-1/2$; #6 $x-1, y, z$. For **3**, #1 $x-1, -y+1/2, z-1/2$; #2 $x+1, -y+1/2, z+1/2$; #3 $-x, y+1/2, -z+3/2$; #4 $-x, -y+1, -z+2$; #5 $-x, -y+1, -z+1$; #6 $-x, y-1/2, -z+3/2$.