

Tuning the formation of dicarboxylate linker-assisted supramolecular 1D chains and squares of Ni(II) using coordination and hydrogen bonds

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Electronic Supplementary Information

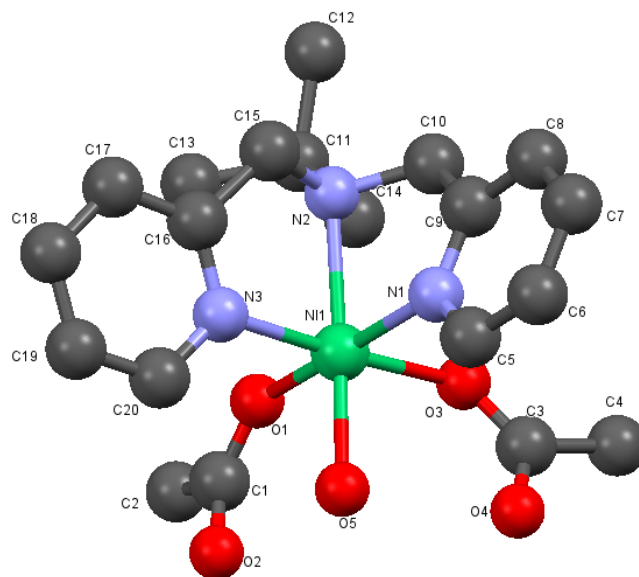


Fig S1. A schematic view of **1** with an atom labeling scheme; hydrogen atoms are omitted for clarity.

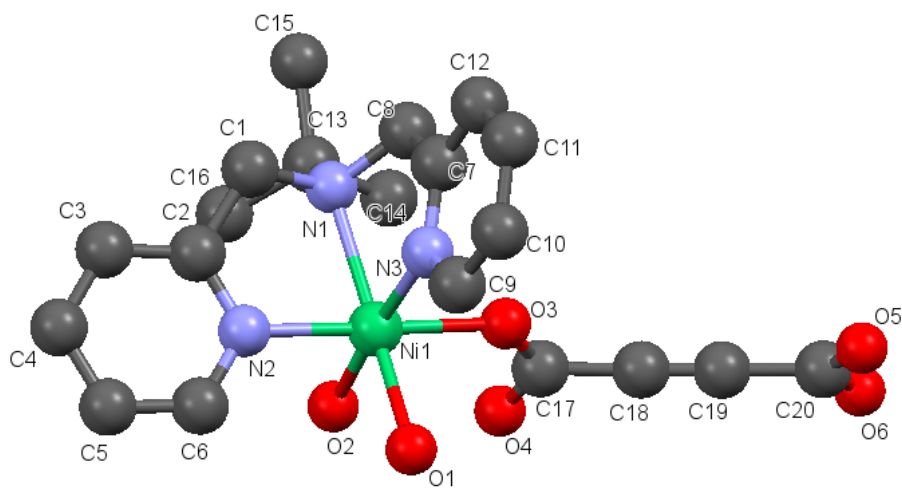


Fig S2. A schematic view of **2** with an atom labeling scheme; hydrogen atoms are omitted for clarity.

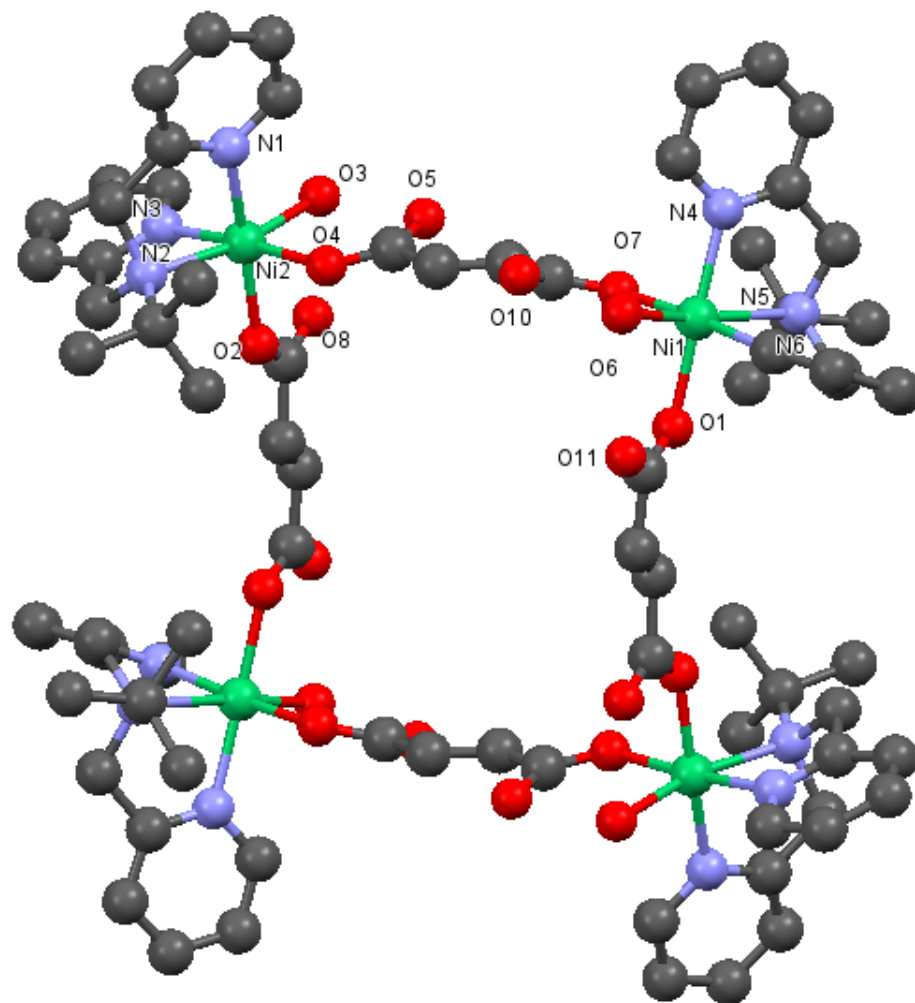


Fig. S3 A schematic view of **3** with an atom labeling scheme; hydrogen atoms are omitted for clarity.

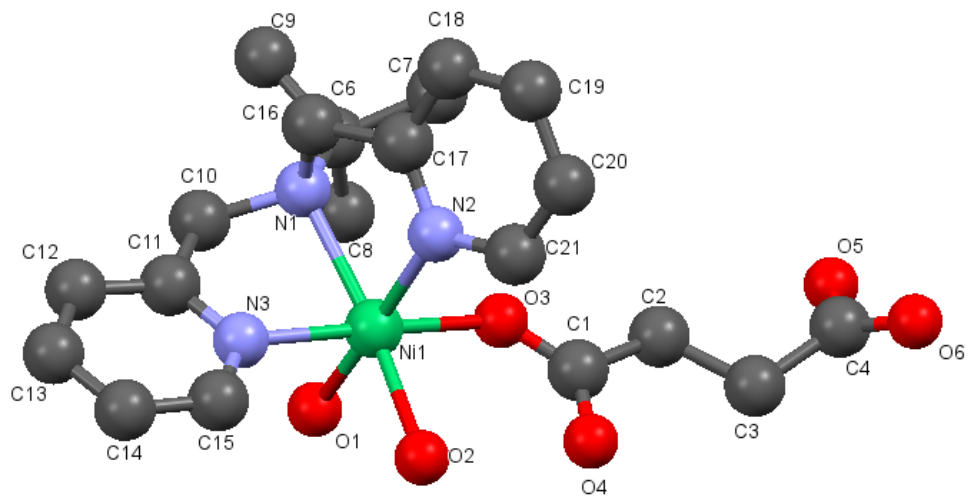


Fig. S4 A schematic view of **4** with an atom labeling scheme; hydrogen atoms are omitted for clarity.

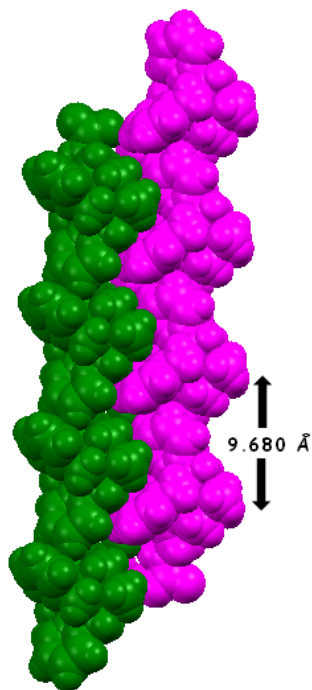


Fig. S5 A helical view of the two adjacent 1D chains in **4**.

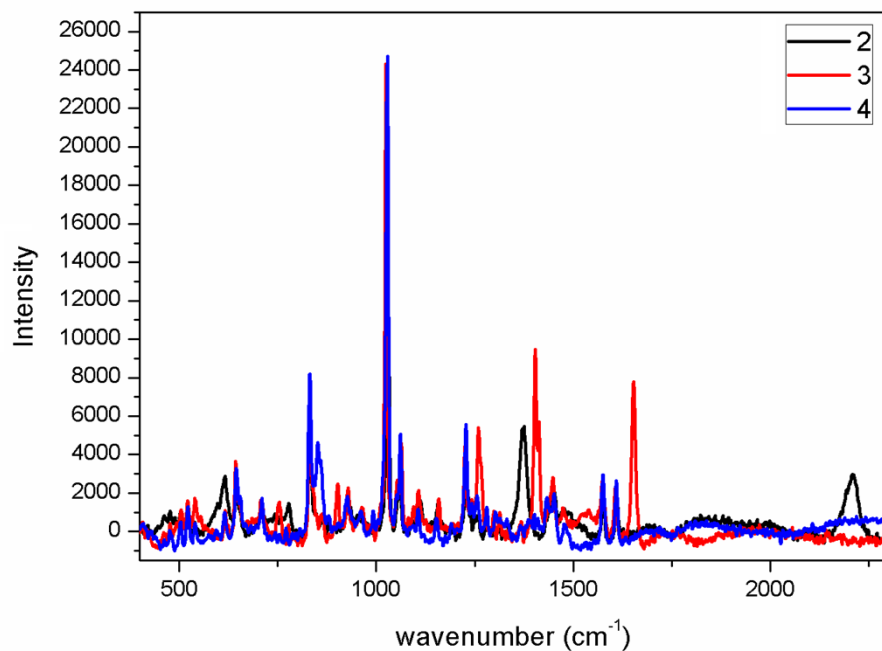


Fig. S6 Raman spectra of **2-4**.

Table S1. Selected Bond distances and bond angles for **1, 2, 3** and **4**.

1

Bond distances (Å)

Ni1-N1	2.063(3)	Ni1-O1	2.021(2)
Ni1-N2	2.255(2)	Ni1-O3	2.092(2)
Ni1-N3	2.061(2)	Ni1-O5	2.079(2)

Bond angles (°)

O1-Ni1-N3	91.97(10)	O1-Ni1-N1	172.32(9)
N3-Ni1-N1	93.66(10)	O1-Ni1-O5	91.05(9)
N3-Ni1-O5	91.07(9)	N1-Ni1-O5	94.05(9)
O1-Ni1-O3	89.49(9)	N3-Ni1-O3	176.74(9)
N1-Ni1-O3	84.62(9)	O5-Ni1-O3	91.82(8)
O1-Ni1-N2	96.99(9)	N3-Ni1-N2	80.63(9)
N1-Ni1-N2	78.82(9)	O5-Ni1-N2	168.60(8)
O3-Ni1-N2	96.30(8)		

2

Bond distances (Å)

Ni1-N1	2.257(2)	Ni1-O1	2.082(2)
Ni1-N2	2.062(2)	Ni1-O3	2.0779(18)
Ni1-N3	2.055(2)	Ni1-O2	2.083(2)

Bond angles (°)

N3-Ni1-N2	95.22(9)	N3-Ni1-O3	85.43(8)
N2-Ni1-O3	177.96(8)	N3-Ni1-O1	175.13(8)
N2-Ni1-O1	89.65(8)	O3-Ni1-O1	89.71(8)
N3-Ni1-O2	91.65(8)	N2-Ni1-O2	93.50(9)
O3-Ni1-O2	88.41(8)	O1-Ni1-O2	87.99(8)
N3-Ni1-N1	78.20(8)	N2-Ni1-N1	80.85(8)
O3-Ni1-N1	97.41(8)	O1-Ni1-N1	102.70(8)
O2-Ni1-N1	167.79(8)		

3

Bond distances (Å)

Ni1-N4	2.056(3)	Ni1-O1	2.072(3)
Ni1-N5	2.272(4)	Ni2-O2	2.051(3)
Ni1-N6	2.084(4)	Ni2-O3	2.080(3)
Ni2-N1	2.061(3)	Ni2-O4	2.050(3)
Ni2-N2	2.212(4)	Ni1-O6	2.037(3)
Ni2-N3	2.084(4)	Ni1-O7	2.086(3)

Bond angles (°)

O6-Ni1-N4	89.29(12)	O6-Ni1-O1	88.78(12)
N4-Ni1-O1	175.69(13)	O6-Ni1-N6	176.01(12)
N4-Ni1-N6	94.35(14)	O1-Ni1-N6	87.48(13)
O6-Ni1-O7	91.99(11)	N4-Ni1-O7	92.78(12)
O1-Ni1-O7	91.14(11)	N6-Ni1-O7	89.46(13)
O6-Ni1-N5	100.68(12)	N4-Ni1-N5	79.43(13)
O1-Ni1-N5	97.15(12)	N6-Ni1-N5	78.44(14)
O7-Ni1-N5	164.96(12)	O4-Ni2-O2	88.77(11)
O4-Ni2-N1	86.04(12)	O2-Ni2-N1	171.59(13)

O4-Ni2-O3	90.22(12)	O2-Ni2-O3	92.10(11)
N1-Ni2-O3	94.52(13)	O4-Ni2-N3	175.15(12)
O2-Ni2-N3	86.39(12)	N1-Ni2-N3	98.78(13)
O3-Ni2-N3	89.93(14)	O4-Ni2-N2	101.20(13)
O2-Ni2-N2	94.00(12)	N1-Ni2-N2	80.55(14)
O3-Ni2-N2	167.15(12)	N3-Ni2-N2	79.20(14)

4

Bond distances (Å)

Ni1-N1	2.230(4)	Ni1-O1	2.055(4)
Ni1-N2	2.112(3)	Ni1-O2	2.112(3)
Ni1-N3	2.072(4)	Ni1-O3	2.054(3)

Bond angles (°)

O3-Ni1-O1	88.75(16)	O3-Ni1-N2	87.75(14)
O1-Ni1-N2	173.32(16)	O3-Ni1-N3	175.84(15)
O1-Ni1-N3	87.16(16)	N2-Ni1-N3	96.24(15)
O3-Ni1-O2	90.38(14)	O1-Ni1-O2	89.90(15)
N2-Ni1-O2	95.81(15)	N3-Ni1-O2	90.39(15)
O3-Ni1-N1	100.58(13)	O1-Ni1-N1	94.74(14)
N2-Ni1-N1	80.32(14)	N3-Ni1-N1	79.00(14)
O2-Ni1-N1	168.17(14)		