

Supplementary Information

Architectures of transition metal(II) polymeric frameworks constructed by 3- fluorophthalic acid and 1,3-bis(4-pyridyl)propane: synthesis, crystal structures and properties

Yu -E Cha^a, Xia Li^{*a}, Xu Ma^a, Chong-Qing Wan^a, Xue-Bin Deng^b, Lin-Pei Jin^b

Table S1 Bond lengths [Å] and angles [°] for complexes **1-5**

| complex 1 | | | |
|-------------------|------------|-------------------|-----------|
| Cu(1)-O(3)#1 | 1.9330(19) | Cu(1)-N(2) | 1.990(2) |
| Cu(1)-O(2) | 1.9915(19) | Cu(1)-N(1) | 2.015(2) |
| Cu(1)-O(1) | 2.418(2) | | |
| O(3)#1-Cu(1)-N(2) | 96.61(9) | O(3)#1-Cu(1)-O(2) | 159.23(9) |
| N(2)-Cu(1)-O(2) | 89.48(9) | O(3)#1-Cu(1)-N(1) | 94.82(9) |
| N(2)-Cu(1)-N(1) | 146.65(10) | O(2)-Cu(1)-N(1) | 90.78(9) |
| O(3)#1-Cu(1)-O(1) | 100.46(8) | N(2)-Cu(1)-O(1) | 108.53(9) |
| O(2)-Cu(1)-O(1) | 58.82(7) | N(1)-Cu(1)-O(1) | 99.98(9) |
| complex 2 | | | |
| Cu(1)-O(3) | 1.946(9) | Cu(1)-O(9) | 1.982(16) |
| Cu(1)-O(5) | 1.997(11) | Cu(1)-N(1) | 2.051(11) |
| Cu(1)-N(2) | 2.115(12) | Cu(1)-O(6) | 2.153(14) |
| Cu(2)-N(3) | 1.998(10) | Cu(2)-O(1) | 2.001(8) |
| Cu(2)-O(10) | 2.010(8) | Cu(2)-O(7) | 2.036(8) |
| Cu(2)-N(4) | 2.181(11) | | |
| O(3)-Cu(1)-O(9) | 95.9(6) | O(3)-Cu(1)-O(5) | 159.6(5) |
| O(9)-Cu(1)-O(5) | 71.9(6) | O(3)-Cu(1)-N(1) | 96.8(4) |
| O(9)-Cu(1)-N(1) | 85.8(6) | O(5)-Cu(1)-N(1) | 98.5(5) |
| O(3)-Cu(1)-N(2) | 93.5(5) | O(9)-Cu(1)-N(2) | 169.0(6) |
| O(5)-Cu(1)-N(2) | 97.4(5) | N(1)-Cu(1)-N(2) | 98.8(5) |
| O(3)-Cu(1)-O(6) | 100.9(4) | O(9)-Cu(1)-O(6) | 77.6(6) |
| O(5)-Cu(1)-O(6) | 61.2(5) | N(1)-Cu(1)-O(6) | 156.8(4) |
| N(2)-Cu(1)-O(6) | 95.1(5) | N(3)-Cu(2)-O(1) | 94.0(4) |
| N(3)-Cu(2)-O(10) | 179.0(5) | O(1)-Cu(2)-O(10) | 85.5(3) |
| N(3)-Cu(2)-O(7) | 91.9(4) | O(1)-Cu(2)-O(7) | 151.3(4) |
| O(10)-Cu(2)-O(7) | 88.9(4) | N(3)-Cu(2)-N(4) | 92.4(4) |
| O(1)-Cu(2)-N(4) | 107.5(4) | O(10)-Cu(2)-N(4) | 87.0(4) |
| O(7)-Cu(2)-N(4) | 100.3(4) | | |

^a Department of Chemistry, Capital Normal University, Beijing 100048, P. R.China Tel.: +86 10 68902320; fax: +86 10 68902320. Email: xiali@mail.cnu.edu.cn (Xia Li).

^b Department of Chemistry, Beijing Normal University, Beijing 100875, P. R. China.

| complex 3 | | | |
|---------------------|------------|--------------------|------------|
| Cd(1)-N(1) | 2.316(3) | Cd(1)-O(1) | 2.321(2) |
| Cd(1)-N(2)#1 | 2.335(3) | Cd(1)-O(4) | 2.419(3) |
| Cd(1)-O(3) | 2.453(3) | Cd(1)-O(5) | 2.517(3) |
| Cd(1)-O(2) | 2.583(3) | Cd(2)-O(8)#2 | 2.184(3) |
| Cd(2)-O(6) | 2.277(2) | Cd(2)-O(10) | 2.349(3) |
| Cd(2)-O(7) | 2.563(2) | Cd(2)-N(3) | 2.347(3) |
| Cd(2)-N(4)#3 | 2.303(3) | | |
| N(1)-Cd(1)-O(1) | 132.37(9) | N(1)-Cd(1)-N(2)#1 | 92.69(10) |
| O(1)-Cd(1)-N(2)#1 | 107.67(10) | N(1)-Cd(1)-O(4) | 86.60(10) |
| O(1)-Cd(1)-O(4) | 125.11(9) | N(2)#1-Cd(1)-O(4) | 106.58(11) |
| N(1)-Cd(1)-O(3) | 138.18(10) | O(1)-Cd(1)-O(3) | 86.21(9) |
| N(2)#1-Cd(1)-O(3) | 88.47(10) | O(4)-Cd(1)-O(3) | 53.39(10) |
| N(1)-Cd(1)-O(5) | 85.26(9) | O(1)-Cd(1)-O(5) | 75.74(9) |
| N(2)#1-Cd(1)-O(5) | 176.53(10) | O(4)-Cd(1)-O(5) | 70.54(10) |
| O(3)-Cd(1)-O(5) | 91.19(9) | N(1)-Cd(1)-O(2) | 84.04(9) |
| O(1)-Cd(1)-O(2) | 52.76(8) | N(2)#1-Cd(1)-O(2) | 93.99(10) |
| O(4)-Cd(1)-O(2) | 157.76(10) | O(3)-Cd(1)-O(2) | 137.61(9) |
| O(5)-Cd(1)-O(2) | 88.59(9) | O(8)#2-Cd(2)-O(6) | 99.79(9) |
| O(8)#2-Cd(2)-N(4)#3 | 99.09(10) | O(6)-Cd(2)-N(4)#3 | 157.36(10) |
| O(8)#2-Cd(2)-N(3) | 110.82(11) | O(6)-Cd(2)-N(3) | 99.70(10) |
| N(4)#3-Cd(2)-N(3) | 85.07(11) | O(8)#2-Cd(2)-O(10) | 90.09(11) |
| O(6)-Cd(2)-O(10) | 85.28(9) | N(4)#3-Cd(2)-O(10) | 82.31(10) |
| N(3)-Cd(2)-O(10) | 157.07(10) | O(8)#2-Cd(2)-O(7) | 152.82(9) |
| O(6)-Cd(2)-O(7) | 53.72(8) | N(4)#3-Cd(2)-O(7) | 105.67(9) |
| N(3)-Cd(2)-O(7) | 82.68(10) | O(10)-Cd(2)-O(7) | 82.41(9) |
| complex 4 | | | |
| Co(1)-O(6) | 2.025(4) | Co(1)-O(2) | 2.111(5) |
| Co(1)-O(1) | 2.157(4) | Co(1)-O(5) | 2.151(4) |
| Co(1)-N(2)#1 | 2.103(5) | Co(1)-N(1) | 2.222(5) |
| Co(2)-O(3)#2 | 2.006(4) | Co(2)-O(8) | 2.106(4) |
| Co(2)-O(10) | 2.189(4) | Co(2)-O(9) | 2.240(5) |
| Co(2)-N(3) | 2.095(5) | Co(2)-N(4)#3 | 2.110(5) |
| O(6)-Co(1)-N(2)#1 | 101.3(2) | O(6)-Co(1)-N(1) | 91.7(2) |
| N(2)#1-Co(1)-N(1) | 90.0(2) | O(6)-Co(1)-O(5) | 89.16(18) |
| N(2)#1-Co(1)-O(5) | 87.1(2) | N(1)-Co(1)-O(5) | 177.0(2) |
| O(6)-Co(1)-O(1) | 159.00(17) | N(2)#1-Co(1)-O(1) | 98.10(19) |
| N(1)-Co(1)-O(1) | 96.27(19) | O(5)-Co(1)-O(1) | 83.87(17) |
| O(6)-Co(1)-O(2) | 99.80(18) | N(2)#1-Co(1)-O(2) | 158.57(19) |
| N(1)-Co(1)-O(2) | 93.0(2) | O(5)-Co(1)-O(2) | 89.63(18) |
| O(1)-Co(1)-O(2) | 60.49(16) | O(6)-Co(1)-C(14) | 128.1(2) |
| N(2)#1-Co(1)-C(14) | 128.4(2) | N(1)-Co(1)-C(14) | 101.1(2) |
| O(5)-Co(1)-C(14) | 80.6(2) | O(1)-Co(1)-C(14) | 31.13(19) |
| O(2)-Co(1)-C(14) | 30.35(18) | O(3)#2-Co(2)-N(3) | 98.80(19) |

| | | | |
|---------------------|------------|---------------------|------------|
| O(3)#2-Co(2)-O(8) | 160.24(18) | N(3)-Co(2)-O(8) | 99.5(2) |
| O(3)#2-Co(2)-N(4)#3 | 90.5(2) | N(3)-Co(2)-N(4)#3 | 94.9(2) |
| O(8)-Co(2)-N(4)#3 | 95.4(2) | O(3)#2-Co(2)-O(10) | 88.79(18) |
| N(3)-Co(2)-O(10) | 85.3(2) | O(8)-Co(2)-O(10) | 85.23(18) |
| N(4)#3-Co(2)-O(10) | 179.3(2) | O(3)#2-Co(2)-O(9) | 99.94(18) |
| N(3)-Co(2)-O(9) | 159.18(19) | O(8)-Co(2)-O(9) | 60.91(17) |
| N(4)#3-Co(2)-O(9) | 93.9(2) | O(10)-Co(2)-O(9) | 86.15(18) |
| complex 5 | | | |
| Ni(1)-O(6) | 2.012(3) | Ni(1)-O(5) | 2.103(4) |
| Ni(1)-O(2) | 2.126(3) | Ni(1)-O(1) | 2.176(4) |
| Ni(1)-N(1) | 2.061(4) | Ni(1)-N(2)#3 | 2.059(4) |
| Ni(2)-O(3)#4 | 1.997(3) | Ni(2)-O(9) | 2.102(4) |
| Ni(2)-O(10) | 2.119(4) | Ni(2)-O(8) | 2.181(4) |
| Ni(2)-N(4)#5 | 2.078(4) | N(3)-Ni(2) | 2.045(4) |
| O(6)-Ni(1)-N(1) | 91.55(15) | N(2)#3-Ni(1)-N(1) | 91.97(17) |
| O(6)-Ni(1)-O(5) | 89.38(14) | N(2)#3-Ni(1)-O(5) | 86.21(18) |
| N(1)-Ni(1)-O(5) | 178.05(18) | O(6)-Ni(1)-O(2) | 160.40(14) |
| N(2)#3-Ni(1)-O(2) | 100.11(15) | N(1)-Ni(1)-O(2) | 94.97(15) |
| O(5)-Ni(1)-O(2) | 84.69(15) | O(6)-Ni(1)-O(1) | 99.84(15) |
| N(2)#3-Ni(1)-O(1) | 161.19(15) | N(1)-Ni(1)-O(1) | 93.15(17) |
| O(5)-Ni(1)-O(1) | 88.37(17) | O(2)-Ni(1)-O(1) | 61.41(13) |
| O(6)-Ni(1)-C(1) | 129.34(17) | N(2)#3-Ni(1)-C(1) | 130.20(17) |
| N(1)-Ni(1)-C(1) | 99.86(16) | O(5)-Ni(1)-C(1) | 80.84(17) |
| O(2)-Ni(1)-C(1) | 31.19(15) | O(1)-Ni(1)-C(1) | 30.99(16) |
| O(3)#4-Ni(2)-N(3) | 96.97(16) | O(3)#4-Ni(2)-N(4)#5 | 90.38(16) |
| N(3)-Ni(2)-N(4)#5 | 95.32(18) | O(3)#4-Ni(2)-O(9) | 161.62(15) |
| N(3)-Ni(2)-O(9) | 100.32(16) | N(4)#5-Ni(2)-O(9) | 94.17(17) |
| O(3)#4-Ni(2)-O(10) | 89.41(15) | N(3)-Ni(2)-O(10) | 85.41(17) |
| N(4)#5-Ni(2)-O(10) | 179.26(18) | O(9)-Ni(2)-O(10) | 85.81(15) |
| O(3)#4-Ni(2)-O(8) | 100.24(14) | N(3)-Ni(2)-O(8) | 160.99(15) |
| N(4)#5-Ni(2)-O(8) | 92.60(17) | O(9)-Ni(2)-O(8) | 61.80(14) |
| O(10)-Ni(2)-O(8) | 86.73(15) | | |

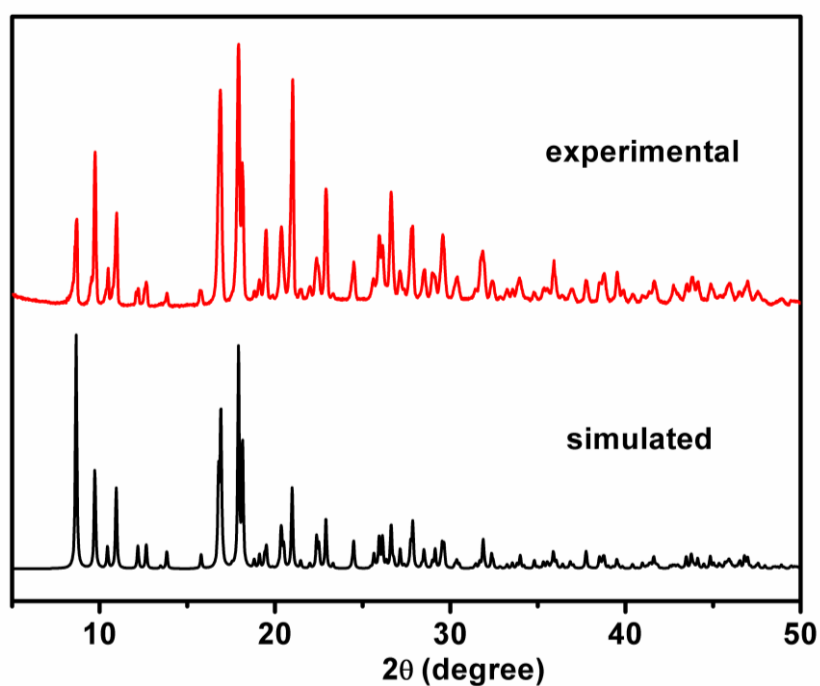
Symmetry transformations used to generate equivalent atoms: For **1**: #1: $-x+3/2, y+1/2, -z+3/2$. For **3**: #1 $-x, -y+2, -z$; #2: $-x, -y+2, -z+1$; #3: $-x+1, -y+1, -z+1$. For **4**: #1 $x, y, z+1$; #2 $-x+1, y+1/2, -z+1$; #3 $x+1, y, z$. For **5**, #1 $x, y, z-1$; #2 $x-1, y, z$; #3 $x, y, z+1$; #4 $-x+1, y-1/2, -z+2$; #5 $x+1, y, z$.

Table S2 Hydrogen bond distance (Å) and angle (°) data for compound **3**

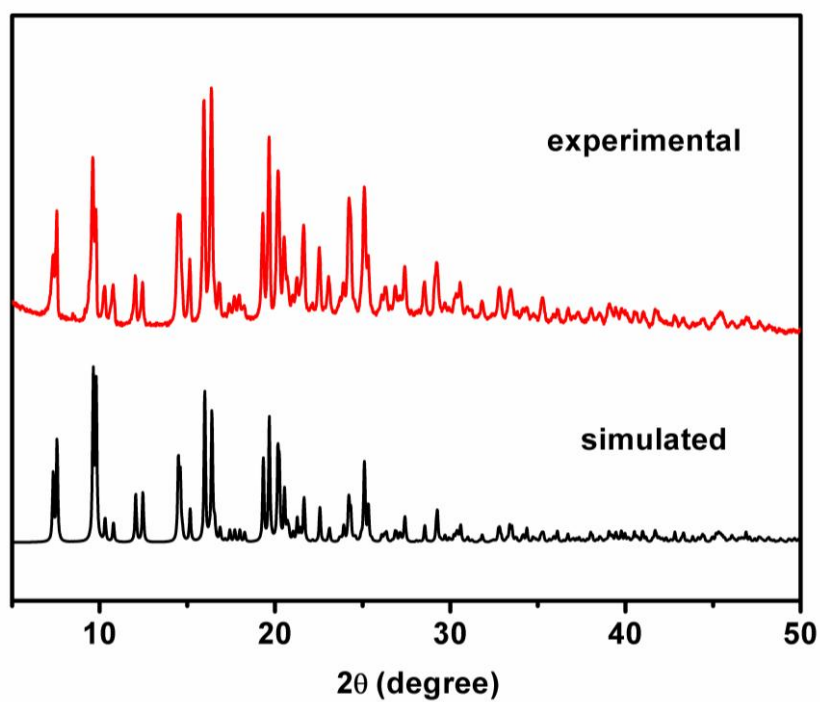
| D-H ...A | d(D-H) | d(H...A) | <DHA | d(D...A) |
|-----------------|--------|----------|--------|----------|
| O10A-H10c...O11 | 0.850 | 1.851 | 176.25 | 2.700 |
| O10A-H10d...O12 | 0.850 | 1.970 | 175.66 | 2.818 |
| O11-H11c...O6B | 0.850 | 2.018 | 163.98 | 2.845 |
| O11-H11d...O9A | 0.850 | 1.988 | 164.03 | 2.815 |
| O12-H12c...O2 | 0.850 | 2.042 | 179.71 | 2.892 |

O12-H12d... O7 0.850 1.968 179.93 2.818

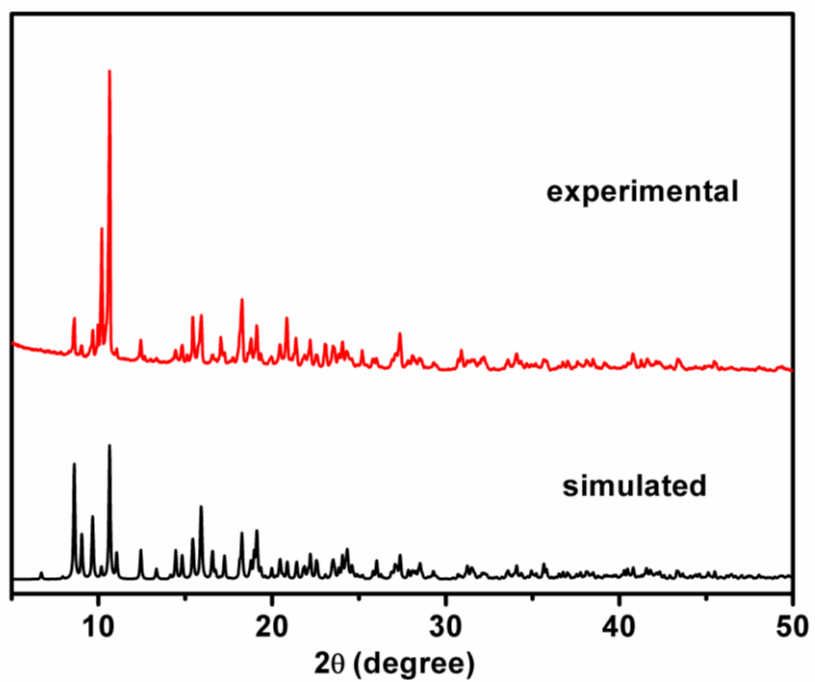
Symmetry transformations used to generate equivalent atoms: A: $-x+1, -y+2, -z+1$ B: $x+1, y, z$



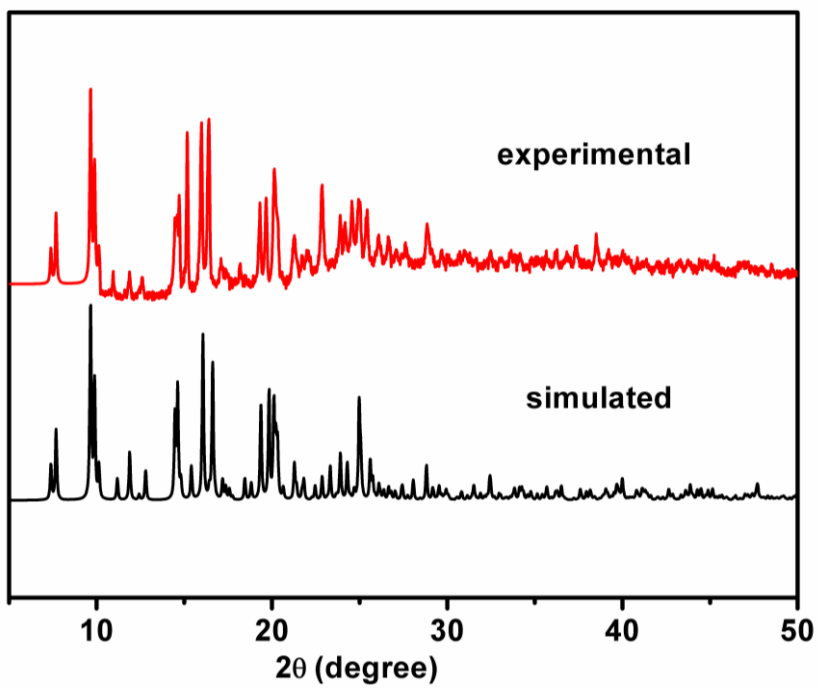
(a)



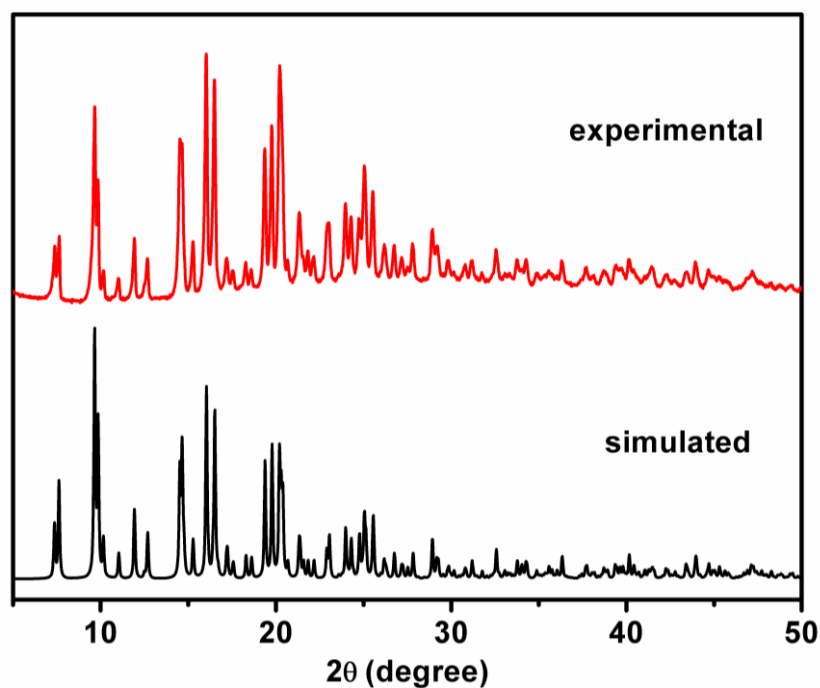
(b)



(c)



(d)



(e)

Fig. S1 The PXR D patterns for complexes 1(a), 2(b), 3(c), 4(d) and 5(e)

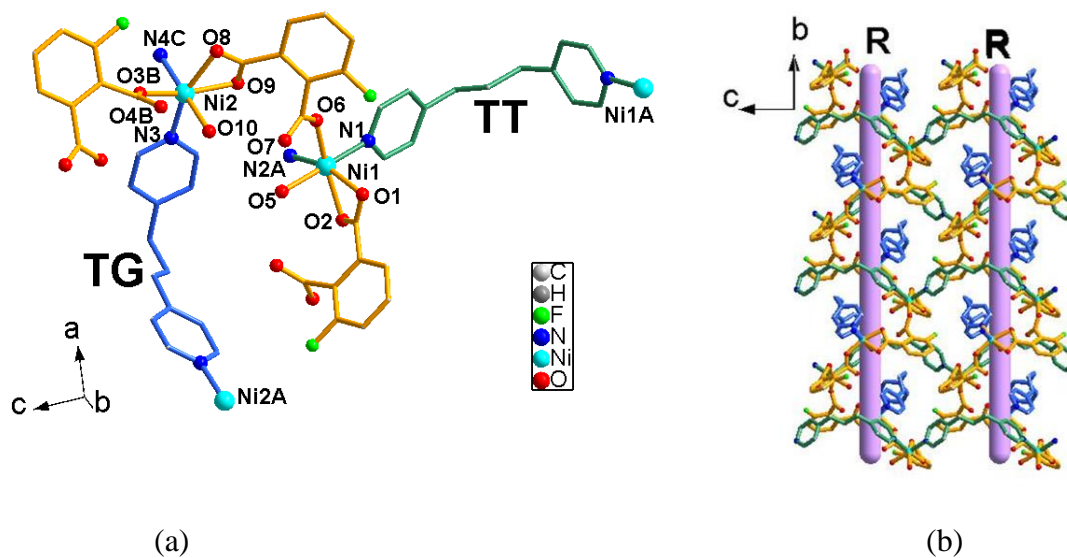


Fig. S2. View of the structure of **5**. (a) The coordination environments of Ni1 and Ni2, showing coordination conformations of ligands between the Ni(II) ions. H atoms are omitted for clarity. Symmetry code: A $x, y, z+1$; B $-x+1, y-1/2, -z+2$; C $x+1, y, z$. (b) Ni-Fpht right-handed helices.