Electronic Supplementary Material for CrystEngComm

[Supporting information]

Entangled Metal-Organic Frameworks Modulated by N-Donor Ligands of Different Conformations

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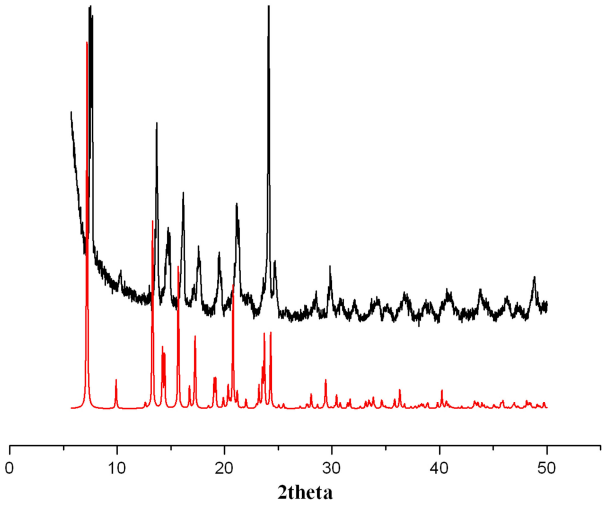

Figure S1. The simulated (red) and experimental (black) XRPD patterns for **1**.

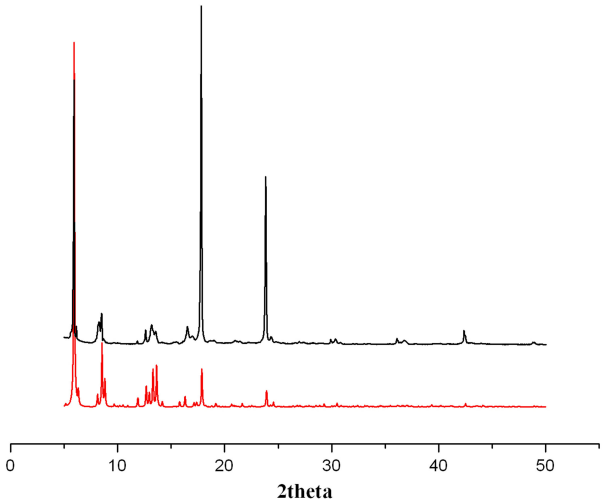

Figure S2. The simulated (red) and experimental (black) XRPD patterns for **2**.

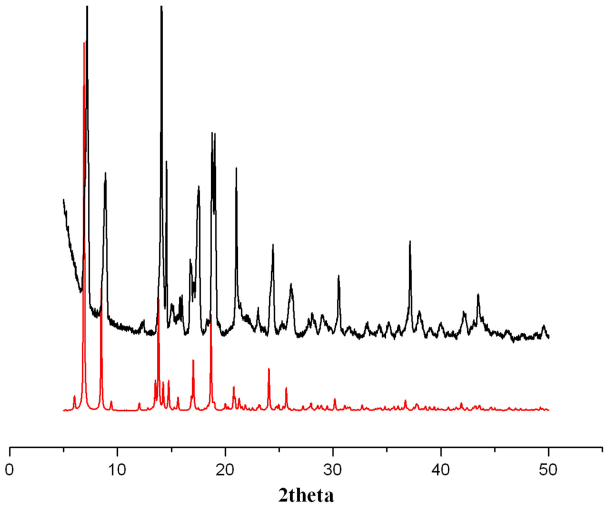

Figure S3. The simulated (red) and experimental (black) XRPD patterns for **3**.

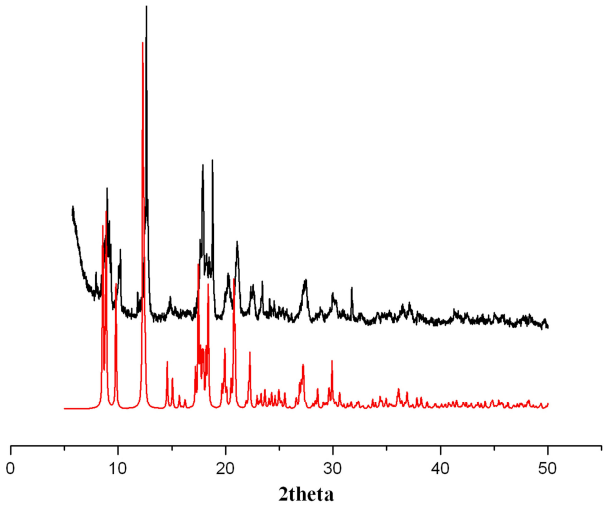

Figure S4. The simulated (red) and experimental (black) XRPD patterns for **4**.

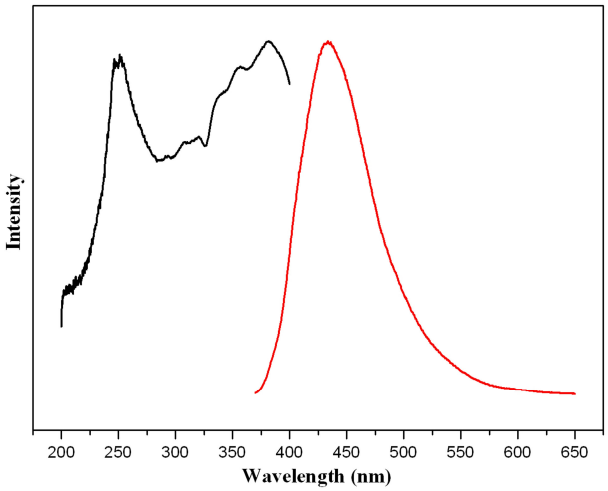

Figure S5. Excitation (black) and emission (red) spectra of **1**.

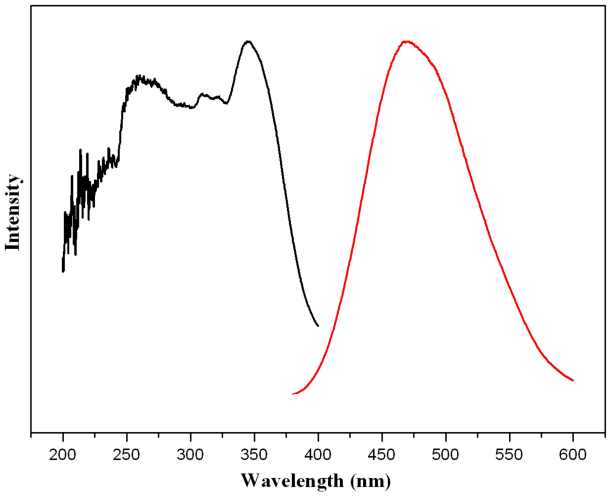

Figure S6. Excitation (black) and emission (red) spectra of **2**.

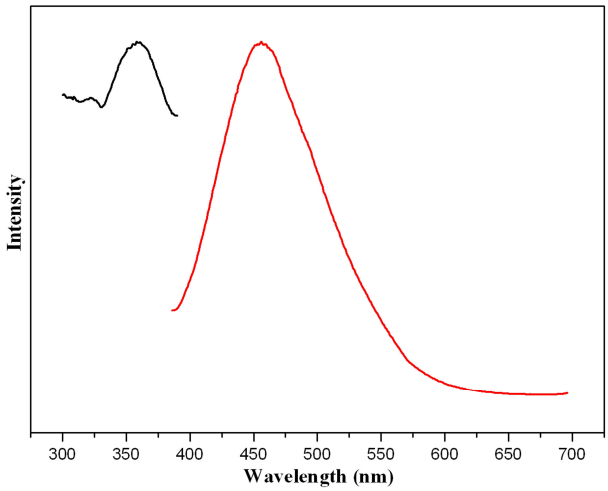

Figure S7. Excitation (black) and emission (red) spectra of **3**.

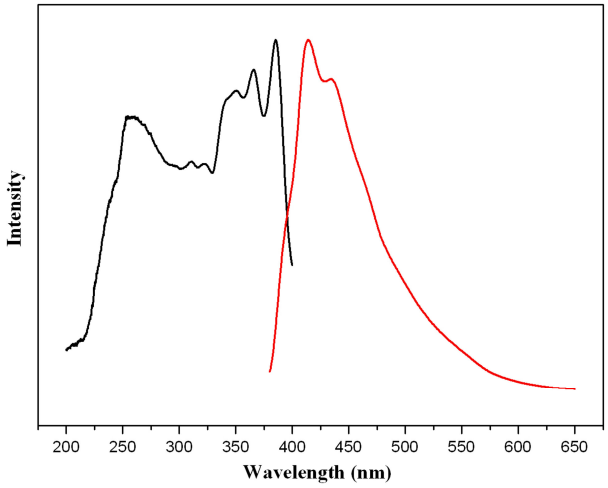

Figure S8. Excitation (black) and emission (red) spectra of **4**.

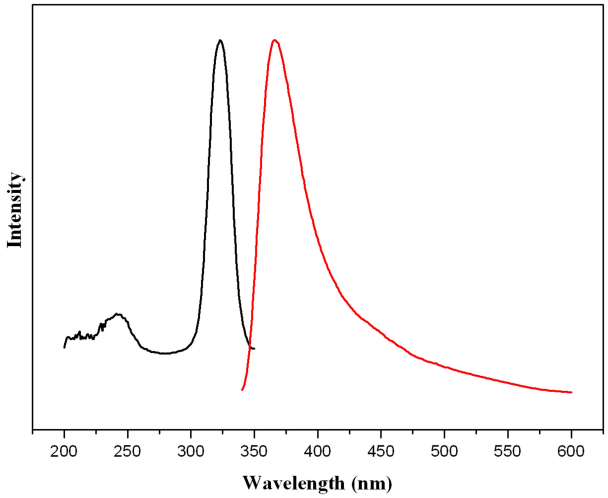

Figure S9. Excitation (black) and emission (red) spectra of $\mathbf{L}^2$.

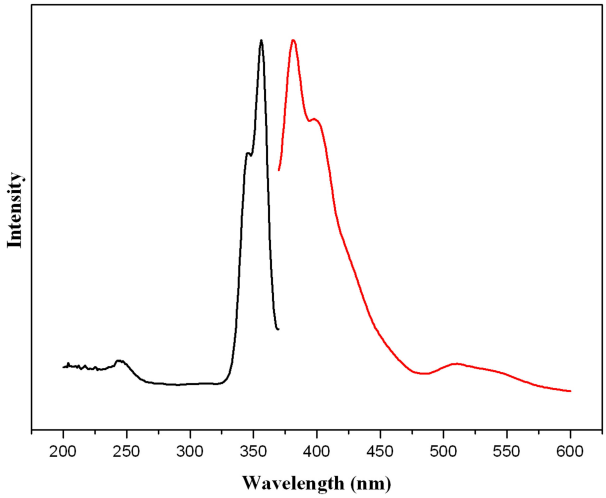

Figure S10. Excitation (black) and emission (red) spectra of $\mathbf{L^3}$.

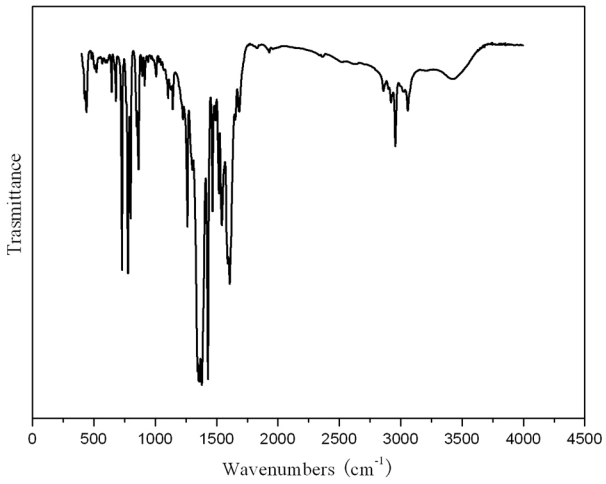

Figure S11. IR (4000-400 cm^{-1}) spectrum of the compound **1**.

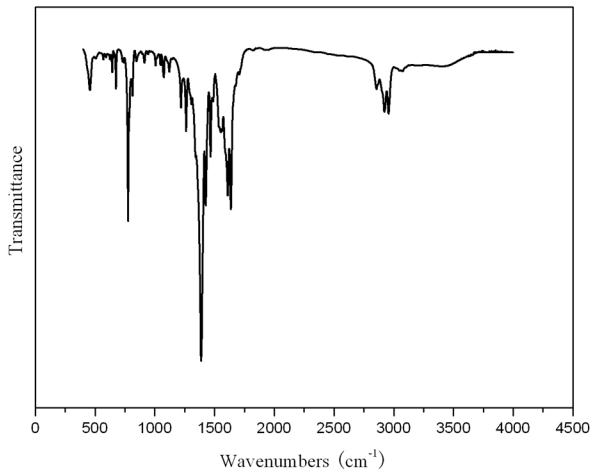

Figure S12. IR (4000-400 cm^{-1}) spectrum of the compound **2**.

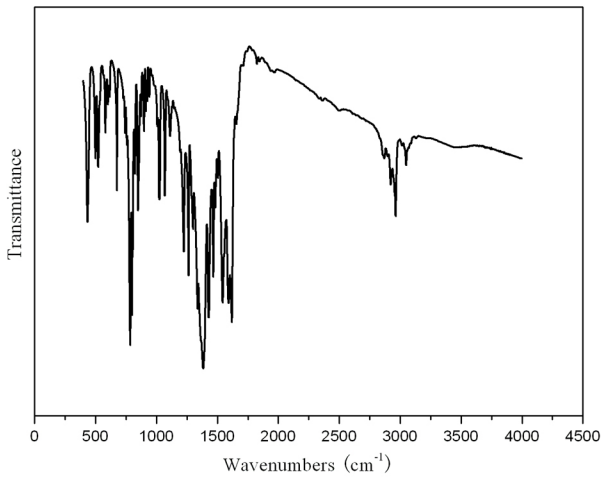

Figure S13. IR (4000-400 cm^{-1}) spectrum of the compound **3**.

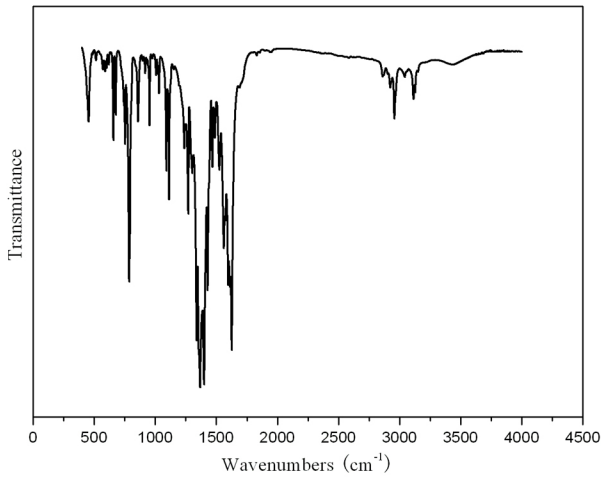

Figure S14. IR (4000-400 cm^{-1}) spectrum of the compound **4**.

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Zn(1)-O(2)	1.930(3)
Zn(1)-O(3)#1	2.073(3)
Zn(1)-N(1)	2.074(4)
Zn(1)-N(2)	2.107(5)
Zn(1)-O(4)#1	2.232(3)
O(3)-Zn(1)#2	2.073(3)
O(4)-Zn(1)#2	2.232(3)
O(2)-Zn(1)-O(3)#1	114.91(16)
O(2)-Zn(1)-N(1)	141.86(18)
O(3)#1-Zn(1)-N(1)	102.86(17)
O(2)-Zn(1)-N(2)	99.12(17)
O(3)#1-Zn(1)-N(2)	98.48(16)
N(1)-Zn(1)-N(2)	79.62(11)
O(2)-Zn(1)-O(4)#1	99.49(11)
O(3)#1-Zn(1)-O(4)#1	59.96(13)
N(1)-Zn(1)-O(4)#1	94.63(15)
N(2)-Zn(1)-O(4)#1	156.16(15)

Symmetry transformations used to generate equivalent atoms:
#1 x+1/2,-y-1/2,z+1/2 #2 x-1/2,-y-1/2,z-1/2

Table S2. Selected bond distances (Å) and angles (°) for **2**.

N(1)-Zn(2)	2.035(5)
N(2)-Zn(1)	2.038(5)
O(1)-Zn(1)	2.019(4)
O(2)-Zn(2)	2.037(4)
O(3)-Zn(2)#3	2.032(4)
O(4)-Zn(1)#3	2.037(4)
O(5)-Zn(2)	2.023(4)
O(6)-Zn(1)	2.026(4)
O(7)-Zn(2)#4	2.027(4)
O(8)-Zn(1)#4	2.052(4)
Zn(1)-O(4)#5	2.037(4)
Zn(1)-O(8)#6	2.052(4)
Zn(1)-Zn(2)	2.9349(9)
Zn(2)-O(7)#6	2.027(4)
Zn(2)-O(3)#5	2.032(4)
O(1)-Zn(1)-O(6)	88.7(2)
O(1)-Zn(1)-O(4)#5	90.7(2)
O(6)-Zn(1)-O(4)#5	156.52(18)
O(1)-Zn(1)-N(2)	100.13(19)
O(6)-Zn(1)-N(2)	101.49(19)
O(4)#5-Zn(1)-N(2)	101.72(19)
O(1)-Zn(1)-O(8)#6	164.32(18)
O(6)-Zn(1)-O(8)#6	87.6(2)
O(4)#5-Zn(1)-O(8)#6	86.7(2)
N(2)-Zn(1)-O(8)#6	95.54(18)
O(1)-Zn(1)-Zn(2)	87.20(14)
O(6)-Zn(1)-Zn(2)	74.73(13)
O(4)#5-Zn(1)-Zn(2)	81.79(12)
N(2)-Zn(1)-Zn(2)	171.77(14)
O(8)#6-Zn(1)-Zn(2)	77.13(12)
O(5)-Zn(2)-O(7)#6	88.89(19)
O(5)-Zn(2)-O(3)#5	162.72(17)
O(7)#6-Zn(2)-O(3)#5	88.01(19)
O(5)-Zn(2)-N(1)	99.53(18)
O(7)#6-Zn(2)-N(1)	106.19(18)
O(3)#5-Zn(2)-N(1)	97.65(18)
O(5)-Zn(2)-O(2)	88.3(2)
O(7)#6-Zn(2)-O(2)	155.09(18)
O(3)#5-Zn(2)-O(2)	87.4(2)
N(1)-Zn(2)-O(2)	98.69(19)
O(5)-Zn(2)-Zn(1)	84.71(13)

O(7)#6-Zn(2)-Zn(1)	82.71(12)
O(3)#5-Zn(2)-Zn(1)	78.04(12)
N(1)-Zn(2)-Zn(1)	170.11(14)
O(2)-Zn(2)-Zn(1)	72.39(13)

Symmetry transformations used to generate equivalent atoms:
#1 x-1/2,-y+1/2,z-1/2 #2 x+1/2,-y+1/2,z+1/2
#3 x,-y,z-1/2 #4 x,-y+1,z-1/2 #5 x,-y,z+1/2
#6 x,-y+1,z+1/2

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O(10)	1.979(3)
Zn(1)-O(1)	2.008(3)
Zn(1)-O(2)#1	2.026(3)
Zn(1)-O(5)	2.034(3)
Zn(1)-O(6)#1	2.034(3)
Zn(1)-Zn(1)#1	2.9499(10)
Zn(2)-N(3)	2.030(4)
Zn(2)-O(7)#2	2.034(3)
Zn(2)-O(8)#3	2.038(3)
Zn(2)-O(3)	2.047(3)
Zn(2)-O(4)#4	2.063(3)
O(2)-Zn(1)#1	2.026(3)
O(6)-Zn(1)#1	2.034(3)
O(7)-Zn(2)#5	2.034(3)
O(8)-Zn(2)#6	2.038(3)
O(10)-Zn(1)-O(1)	100.06(14)
O(10)-Zn(1)-O(2)#1	100.44(14)
O(1)-Zn(1)-O(2)#1	159.42(15)
O(10)-Zn(1)-O(5)	102.39(14)
O(1)-Zn(1)-O(5)	86.74(17)
O(2)#1-Zn(1)-O(5)	90.56(16)
O(10)-Zn(1)-O(6)#1	98.12(14)
O(1)-Zn(1)-O(6)#1	87.92(16)
O(2)#1-Zn(1)-O(6)#1	87.49(17)
O(5)-Zn(1)-O(6)#1	159.40(15)
O(10)-Zn(1)-Zn(1)#1	173.48(10)
O(1)-Zn(1)-Zn(1)#1	81.05(11)
O(2)#1-Zn(1)-Zn(1)#1	78.38(10)
O(5)-Zn(1)-Zn(1)#1	84.06(11)
O(6)#1-Zn(1)-Zn(1)#1	75.46(11)
N(3)-Zn(2)-O(7)#2	98.18(14)
N(3)-Zn(2)-O(8)#3	100.39(14)
O(7)#2-Zn(2)-O(8)#3	88.66(13)
N(3)-Zn(2)-O(3)	103.66(14)
O(7)#2-Zn(2)-O(3)	90.63(13)
O(8)#3-Zn(2)-O(3)	155.79(14)
N(3)-Zn(2)-O(4)#4	101.41(14)
O(7)#2-Zn(2)-O(4)#4	160.28(14)
O(8)#3-Zn(2)-O(4)#4	85.62(12)
O(3)-Zn(2)-O(4)#4	86.97(12)
N(3)-Zn(2)-Zn(2)#4	176.63(11)

O(7)#2-Zn(2)-Zn(2)#4	82.33(9)
O(8)#3-Zn(2)-Zn(2)#4	76.28(9)
O(3)-Zn(2)-Zn(2)#4	79.65(10)
O(4)#4-Zn(2)-Zn(2)#4	77.98(10)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1/2,-y+1/2,-z+1 #2 x,y+1,z
#3 -x+1,y+1,-z+1/2 #4 -x+1,y,-z+1/2
#5 x,y-1,z #6 -x+1,y-1,-z+1/2 #7 x,-y,z+1/2
#8 -x+1,y,-z+3/2 #9 x,-y,z-1/2

Table S4. Selected bond distances (Å) and angles (°) for **4**.

N(1)-Zn(1)	1.981(6)
O(1)-Zn(1)#2	1.938(4)
O(2)-Zn(1)	1.948(4)
O(3)-Zn(1)#3	1.910(4)
Zn(1)-O(3)#4	1.910(4)
Zn(1)-O(1)#2	1.938(4)
O(3)#4-Zn(1)-O(1)#2	108.16(19)
O(3)#4-Zn(1)-O(2)	95.98(19)
O(1)#2-Zn(1)-O(2)	114.2(2)
O(3)#4-Zn(1)-N(1)	121.2(2)
O(1)#2-Zn(1)-N(1)	110.9(2)
O(2)-Zn(1)-N(1)	105.8(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,y,-z-1/2 #2 -x+1,-y,-z #3 x+1/2,y-1/2,-z+1/2
#4 x-1/2,y+1/2,-z+1/2