The Structure and Property of Two Different Metal-Organic Frameworks based on N/O-Donor Mixed Ligands

Table S1. Bond lengths [Å] and bond angles [º] for MOFs **1** and **2.**

1			
Cd(1)-N(1)	2.2955(17)	Cd(1)-O(7)	2.2994(15)
Cd(1)-O(1)	2.3079(17)	Cd(1)-O(13)	2.3271(18)
Cd(1)-O(8)	2.5657(15)	Cd(2)-O(3)#1	2.2232(14)
Cd(2)-N(6)	2.2464(16)	Cd(2)-O(11)	2.3448(15)
Cd(2)-O(15)	2.3947(19)	Cd(2)-O(16)	2.408(2)
Cd(2)-O(12)	2.4469(15)		
N(1)-Cd(1)-O(7)	141.65(6)	N(1)-Cd(1)-O(1)	130.42(6)
O(7)-Cd(1)-O(1)	87.38(6)	N(1)-Cd(1)-O(13)	97.26(7)
O(7)-Cd(1)-O(13)	87.54(7)	O(1)-Cd(1)-O(13)	90.12(7)
N(1)-Cd(1)-O(8)	88.82(5)	O(7)-Cd(1)-O(8)	52.85(5)
O(1)-Cd(1)-O(8)	139.75(5)	O(13)-Cd(1)-O(8)	93.61(6)
O(3)#1-Cd(2)-N(6)	129.30(6)	O(3)#1-Cd(2)-O(11)	87.08(5)
N(6)-Cd(2)-O(11)	143.30(6)	O(3)#1-Cd(2)-O(15)	89.95(6)
N(6)-Cd(2)-O(15)	82.57(6)	O(11)-Cd(2)-O(15)	94.28(6)
O(3)#1-Cd(2)-O(16)	90.87(6)	N(6)-Cd(2)-O(16)	91.49(6)
O(15)-Cd(2)-O(16)	172.93(6)	O(3)#1-Cd(2)-O(12)	140.31(5)
N(6)-Cd(2)-O(12)	89.02(6)	O(11)-Cd(2)-O(12)	54.32(5)
O(15)-Cd(2)-O(12)	84.77(6)	O(16)-Cd(2)-O(12)	99.02(6)
2			
Zn(1)-O(1)	1.9074(19)	Zn(1)-N(1)	2.003(2)
Zn(2)-O(6)	1.9940(17)	Zn(2)-N(3)#3	2.057(2)
Zn(2)-O(3)#4	2.150(2)	Zn(2)-O(7)	2.175(3)
Zn(2)-O(4)#4	2.185(2)	Zn(2)-O(8)	2.198(3)
O(1)-Zn(1)-O(1)#2	116.56(16)	O(1)-Zn(1)-N(1)	118.56(10)
O(1)#2-Zn(1)-N(1)	98.60(9)	O(1)-Zn(1)-N(1)#2	98.60(9)
O(1)#2-Zn(1)-N(1)#2	118.56(10)	N(1)-Zn(1)-N(1)#2	106.70(13)
O(6)-Zn(2)-N(3)#3	102.63(8)	O(6)-Zn(2)-O(3)#4	94.27(8)
N(3)#3-Zn(2)-O(3)#4	162.48(8)	O(6)-Zn(2)-O(7)	90.42(8)
N(3)#3-Zn(2)-O(7)	89.26(10)	O(3)#4-Zn(2)-O(7)	95.26(11)
O(6)-Zn(2)-O(4)#4	154.80(8)	N(3)#3-Zn(2)-O(4)#4	102.36(8)
O(3)#4-Zn(2)-O(4)#4	60.56(8)	O(7)-Zn(2)-O(4)#4	93.08(9)
O(6)-Zn(2)-O(8)	85.42(9)	N(3)#3-Zn(2)-O(8)	87.87(9)
O(3)#4-Zn(2)-O(8)	88.93(10)	O(7)-Zn(2)-O(8)	174.31(9)
O(4)#4-Zn(2)-O(8)	92.34(9)	O(6)-Zn(2)-C(18)#4	124.48(9)

symmetry codes: #1 *x-1,y+1,z*, #2 *-x,y,-z*+1/2, #3 *-x*+1/2,*-y*+3/2,*-z*+1, #4 *x,-y+3,z+1/2*.

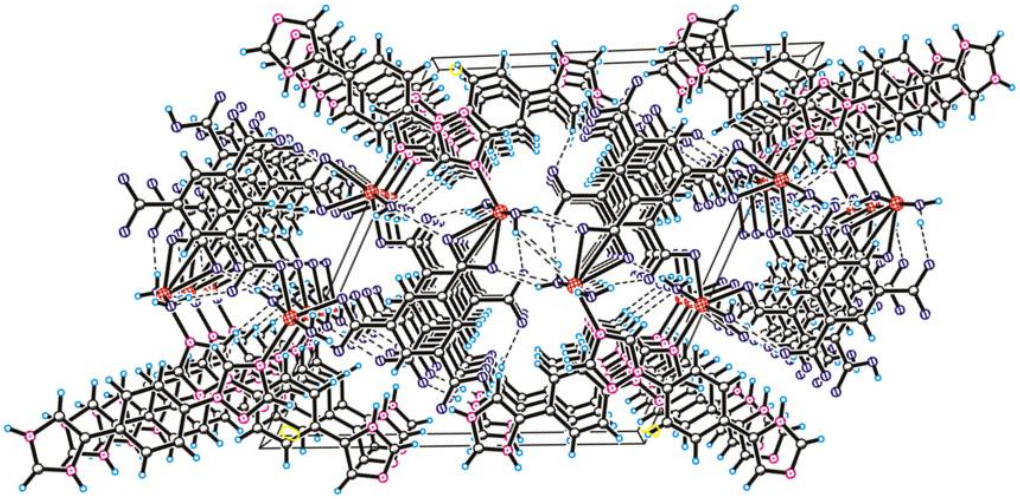

Figure S1. The 3D supramolecular structure of **1**.

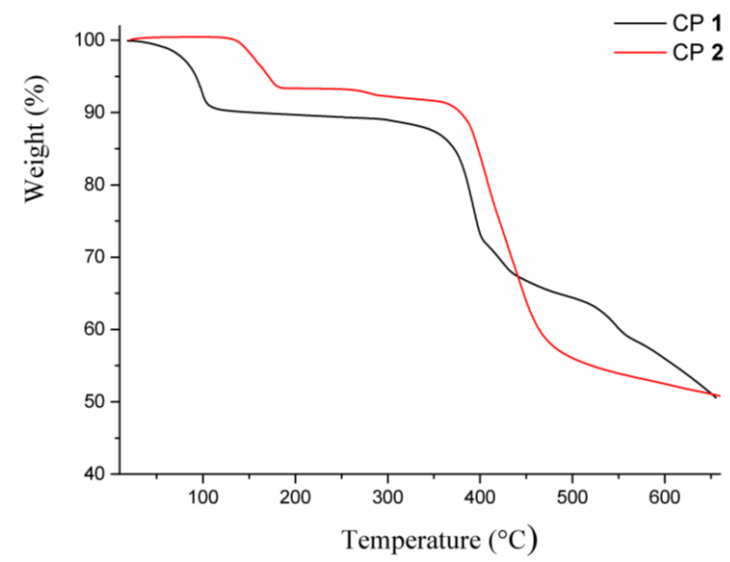

Figure S2. TG curves of MOFs **1** and **2**.

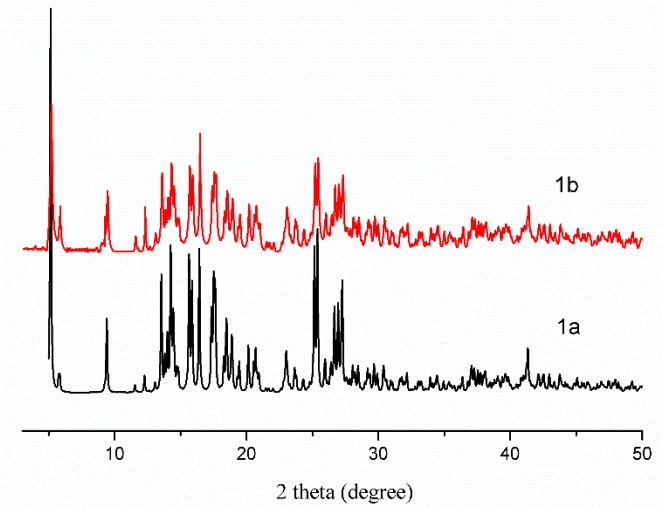

Figure S3. PXRD of MOF **1**: a, simulated; b, experimental.

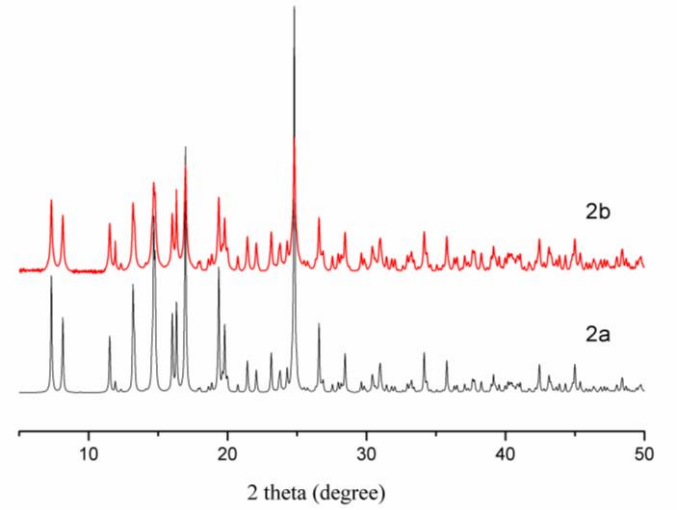

Figure S4. PXRD of MOF **2**: a, simulated; b, experimental.