Electronic Supplementary Information

Controllable preparation, network structures and properties of unusual metal-organic frameworks constructed from 4,4'-(hexafluoroisopropylidene)diphthalic acid and 4,4'-bipyridyl

Rui-Qin Zhong,[a,b] Ru-Qiang Zou,[a,b] Miao Du,[a] Tetsuya Yamada,[c] Goro Maruta,[c] Sadamu Takeda [c] and Qiang Xu,[a,b]*

[a] *National Institute of Advanced Industrial Science and Technology (AIST), Ikeda, Osaka 563-8577, Japan*

[b] *Graduate School of Engineering, Kobe University, Nada Ku, Kobe, Hyogo 657-8501, Japan*

[c] Department of Chemistry, Faculty of Science and Graduate School of Science, Hokkaido University, Sapporo 060-0810, Japan

Table S1 Selected bond lengths and angles for **1**

Ni(1)-O(1W)	2.048(3)	Ni(1)-O(4)#1	2.055(2)
Ni(1)-O(3)	2.065(2)	Ni(1)-O(2)	2.068(2)
Ni(1)-N(2)#2	2.103(3)	Ni(1)-N(1)	2.117(3)
O(1W)-Ni(1)-O(4)#1	94.65(10)	O(1W)-Ni(1)-O(3)	175.77(10)
O(4)#1-Ni(1)-O(3)	81.14(9)	O(1W)-Ni(1)-O(2)	91.33(10)
O(4)#1-Ni(1)-O(2)	170.66(10)	O(3)-Ni(1)-O(2)	92.79(9)
O(1W)-Ni(1)-N(2)#2	89.45(12)	O(4)#1-Ni(1)-N(2)#2	95.43(10)
O(3)-Ni(1)-N(2)#2	91.39(12)	O(2)-Ni(1)-N(2)#2	91.79(11)
O(1W)-Ni(1)-N(1)	90.52(12)	O(4)#1-Ni(1)-N(1)	85.87(10)
O(3)-Ni(1)-N(1)	88.73(12)	O(2)-Ni(1)-N(1)	86.91(11)
N(2)#2-Ni(1)-N(1)	178.70(11)		

Symmetry transformations used to generate equivalent atoms: #1: -*x*+0.5, *y*-0.5, -*z*+1; #2: *x*, *y*, *z*-1; #3: -*x*, -*y*+1, *z*; #4: *x*, *y*, *z*+1; #5: -*x*+0.5, *y*+0.5, -*z*+1; #6: -*x*, -*y*+2, *z*.

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

Ni(1)-O(3)	2.062(1)	Ni(1)-N(2)	2.089(2)
Ni(1)-O(4)#1	2.095(1)	Ni(1)-O(1)	2.102(2)
Ni(1)-N(1)	2.127(2)	Ni(1)-N(3)	2.136(2)
Ni(2)-N(4)#2	2.044(2)	Ni(2)-O(6)	2.056(1)
Ni(2)-O(5)	2.148(2)		
O(3)-Ni(1)-N(2)	178.36(8)	O(3)-Ni(1)-O(4)#1	89.14(7)
N(2)-Ni(1)-O(4)#1	89.37(8)	O(3)-Ni(1)-O(1)	85.87(8)
N(2)-Ni(1)-O(1)	95.47(8)	O(4)#1-Ni(1)-O(1)	168.12(8)
O(3)-Ni(1)-N(1)	95.08(8)	N(2)-Ni(1)-N(1)	85.85(9)
O(4)#1-Ni(1)-N(1)	99.88(8)	O(1)-Ni(1)-N(1)	91.31(8)
O(3)-Ni(1)-N(3)	89.07(8)	N(2)-Ni(1)-N(3)	90.08(9)
O(4)#1-Ni(1)-N(3)	83.52(8)	O(1)-Ni(1)-N(3)	85.62(8)
N(1)-Ni(1)-N(3)	174.65(9)	N(4)#2-Ni(2)-N(4)#3	90.68(14)
N(4)#2-Ni(2)-O(6)	99.44(9)	N(4)#3-Ni(2)-O(6)	96.73(9)
O(6)#4-Ni(2)-O(6)	156.92(11)	N(4)#2-Ni(2)-O(5)	93.21(9)
N(4)#3-Ni(2)-O(5)	162.48(9)	O(6)#4-Ni(2)-O(5)	99.47(8)
O(6)-Ni(2)-O(5)	63.14(7)	O(5)-Ni(2)-O(5)#4	88.20(12)

Symmetry transformations used to generate equivalent atoms: #1: $-x+0.5$, $-y+0.5$,$-z+1$; #2: $-x+0.5$, $y+1.5$, $-z+0.5$; #3: $x-0.5$, $y+1.5$, z; #4: $-x$, y, $-z+0.5$.

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

Mn(1)-O(2)#1	2.085(2)	Mn(1)-O(4)#2	2.098(2)
Mn(1)-O(1)	2.121(2)	Mn(1)-O(3)#3	2.180(2)
Mn(1)-O(1W)	2.199(2)		
O(2)#1-Mn(1)-O(4)#2	111.54(5)	O(2)#1-Mn(1)-O(1)	91.49(6)
O(4)#2-Mn(1)-O(1)	89.83(5)	O(2)#1-Mn(1)-O(3)#3	119.39(5)
O(4)#2-Mn(1)-O(3)#3	126.14(5)	O(1)-Mn(1)-O(3)#3	104.68(5)
O(2)#1-Mn(1)-O(1W)	82.03(6)	O(4)#2-Mn(1)-O(1W)	86.17(6)
O(1)-Mn(1)-O(1W)	170.53(5)	O(3)#3-Mn(1)-O(1W)	84.57(6)

Symmetry transformations used to generate equivalent atoms: #1: -*x*+0.5, *y*-0.5, -*z*+1.5; #2: -*x*+0.5, *y*+0.5, -*z*+1.5; #3: x, -*y*+2, *z*-0.5.

Table S4 Hydrogen-bonding geometry (Å, °) for **1-3**

D–H···A	*H···A*	*D···A*	*D–H···A*
	1		
O1W-H1WA···O2W#1	1.861	2.670	168.93
O1W-H1WB···O4#2	2.050	2.835	156.56
O1W-H1WB···O3#3	2.463	3.063	129.61
	2		
O8-H8···O2#1	1.910	2.685	157.15
O1W-H1WA···O2	2.036	2.841	165.57
O1W-H1WB···O7#2	2.221	2.950	147.90
	3		
O1W-H1WA···O3#1	2.115	2.893	164.79
O1W-H1WB···O2#2	2.340	2.993	142.87
O1W-H1WB···O1#3	2.430	3.052	138.37

Symmetry transformations used to generate equivalent atoms: **1**: #1: *x*, *y*-1, *z*; #2: *x*, *y*-1, *z*; #3: -*x*+0.5, *y*-0.5, -*z*+1; **2**: #1: *x*, *y*+1, *z*; #2: *x*, *y*-1, *z*; **3**: #1: -*x*+0.5, *y*-0.5, -*z*+1.5; #2: -*x*+0.5, -*y*+2.5, -*z*+1; #3: *x*, -*y*+2, *z*-0.5.

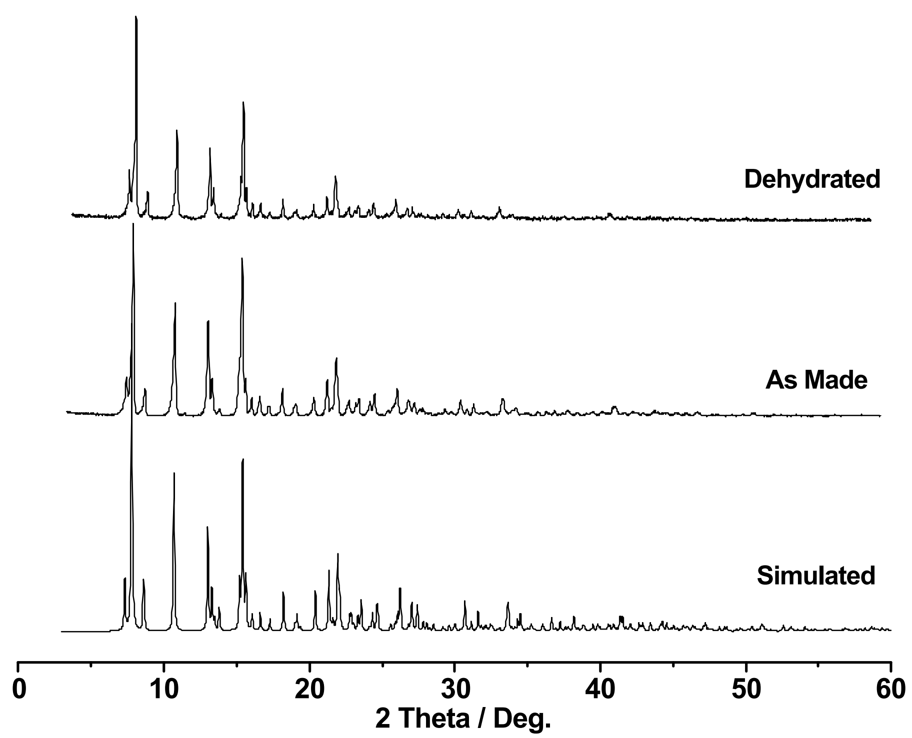

Fig. S1 PXRD patterns of **1**: simulated, as made and dehydrated.

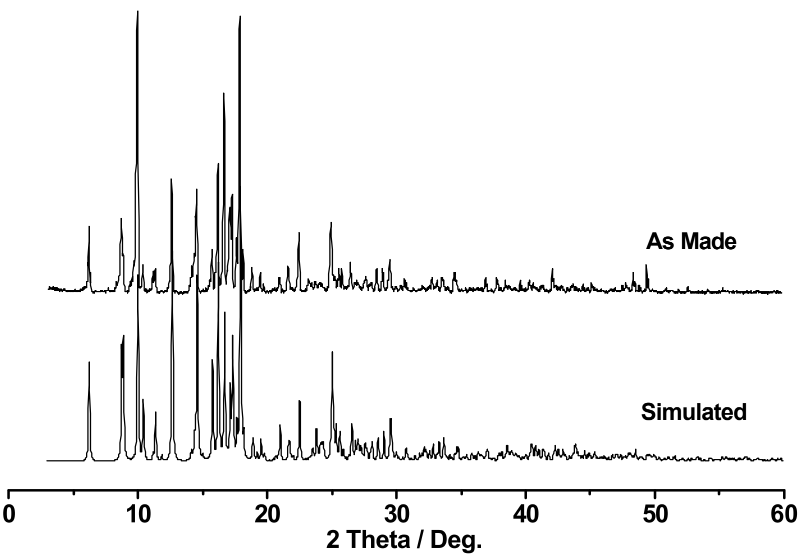

Fig. S2 PXRD patterns of **2**: simulated and as made.

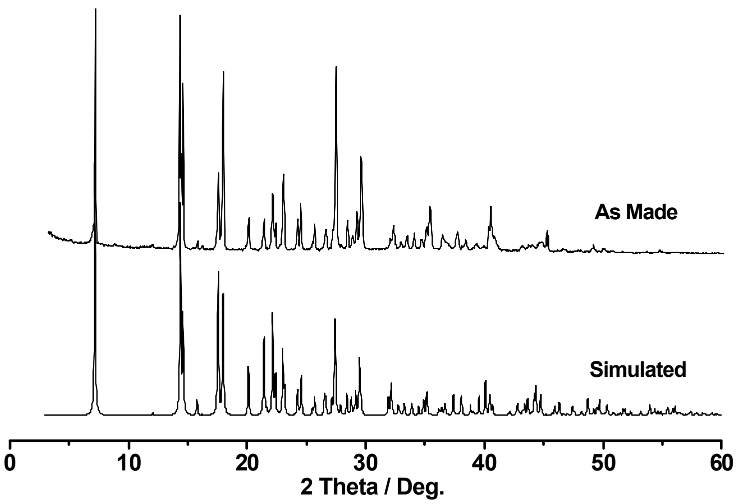

Fig. S3 PXRD patterns of **3**: simulated and as made.

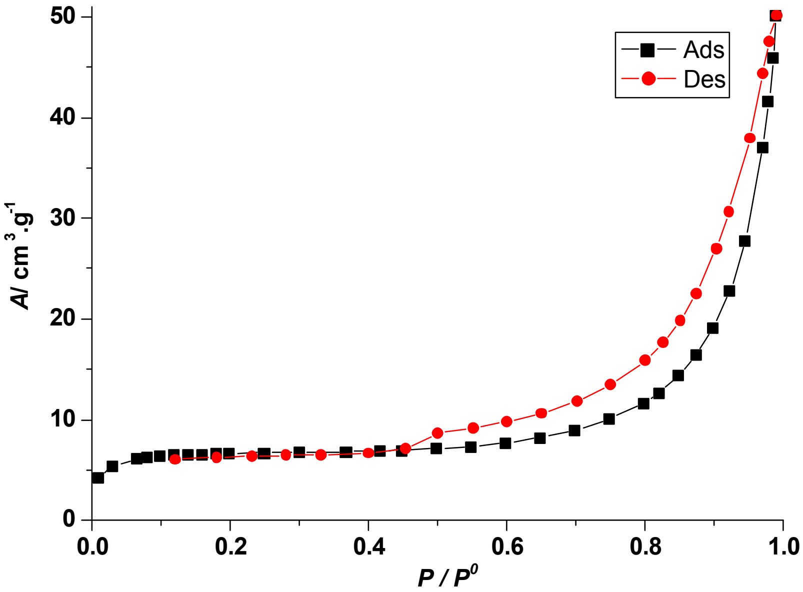

Figure S4 Nitrogen adsorption and desorption curves of **1** in the range of 0 to 1 atm at 77K.