Supporting Information

Construction of Three *p*H-dependent Metal-Organic Frameworks with 3-(4-carboxyphenyl)-1, 3-benzoimidazole

Teng Li,[a] Xu-Jia Hong,[a,b] Xiang Liu,[a] Rong Chen,[a] Qing-Guang Zhan,*[a] Xuan Xu,[a] and Yue-Peng Cai*[a,b]

[a]*School of Chemistry and Environment, South China Normal University;* Guangzhou Key Laboratory of Materials for Energy Conversion and Storage*, Guangzhou 510006, P.R. China.*

[b]*State Key Laboratory of Structure Chemistry, Fujian, Fuzhou 350002, P.R. China*

Contents

Table S1 The crystal data and structure refinements for **1–3.**

	1	**2**	**3**
Chemical formula	$C_{42}H_{27}N_6O_6Er$	$C_{28}H_{18}N_4O_4Zn$	$C_{56}H_{72}C_{l6}N_8O_{44}Er_4Zn$
M	878.96	539.83	2508.33
Crystal system	Monoclinic	Monoclinic	Tetragonal
Space group	*P*2(1)/*c*	*P*2(1)/*c*	*I*4(1)/*a*
a /Å	15.355(5)	11.359(3)	18.8840(17)
b /Å	6.908(2)	14.308(6)	18.8840(17)
c /Å	32.838(11)	18.162(7)	22.448(3)
α/°	90	90	90
β/°	99.157(5)	127.87(2)	90
γ/°	90	90	90
V/Å^3	3439(2)	2330.1(15)	8005.1(15)
Z	4	4	4
T /*K*	298(2)	298(2)	298(2)
F(000)	1748	1104	4880
D_{calcd} / Mg m^{-3}	1.698	1.539	2.081
μ /mm^{-1}	2.502	1.099	4.747
λ /Å	0.71073	0.71073	0.71073
R_{int}	0.0866	0.1174	0.1124
data/restraint/parm	5901/3/484	3403/0/334	3625/21/301
GOF	1.053	1.050	1.030
R_1 [$I = 2\sigma(I)$]^a	0.0660	0.0573	0.0553
wR_2 [$I = 2\sigma(I)$]^b	0.1498	0.0963	0.1241
Largest diff. peak and hole(e Å^{-3})	1.691 / -1.574	0.322 / -0.379	1.674 / -1.149

$^a R_1 = \Sigma||F_o| - |F_c||/|F_o|$, $^b wR_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$, where $w = 1/[\sigma^2(F_o^2) + (aP)_2 + bP]$. $P = (F_o^2 + 2F_c^2)/3$.

Table S**2** Selected Bond Distances (Å) and Angles (°) for complex **1-3**

		1	
Er(1)-O(6)#1	2.323(4)	O(1)#2-Er(1)-O(3)	116.21(12)
Er(1)-O(3)#2	2.349(4)	O(5)-Er(1)-O(3)	83.89(13)
Er(1)-O(1)#2	2.353(4)	O(1)-Er(1)-O(3)	63.90(12)
Er(1)-O(5)	2.380(4)	O(4)-Er(1)-O(3)	52.91(12)
Er(1)-O(1)	2.415(3)	O(6)-Er(1)-O(3)	135.63(13)
Er(1)-O(4)	2.421(4)	O(6)#1-Er(1)-O(2)	109.77(13)
Er(1)-O(6)	2.454(4)	O(3)#2-Er(1)-O(2)	73.01(13)
Er(1)-O(3)	2.486(4)	O(1)#2-Er(1)-O(2)	133.74(12)
Er(1)-Er(1)#1	3.5672(11)	O(5)-Er(1)-O(2)	72.73(14)
Er(1)-Er(1)#2	3.5672(11)	O(1)-Er(1)-O(2)	52.53(12)
O(6)#1-Er(1)-O(3)#2	79.19(13)	O(4)-Er(1)-O(2)	144.44(15)
O(6)#1-Er(1)-O(1)#2	84.34(13)	O(6)-Er(1)-O(2)	75.08(12)
O(3)#2-Er(1)-O(1)#2	66.66(13)	O(3)-Er(1)-O(2)	110.05(12)
O(6)#1-Er(1)-O(5)	156.35(13)	O(6)#1-Er(1)-Er(1)#1	43.12(9)
O(3)#2-Er(1)-O(5)	122.72(13)	O(3)#2-Er(1)-Er(1)#1	111.82(9)
O(1)#2-Er(1)-O(5)	111.38(13)	O(1)#2-Er(1)-Er(1)#1	122.45(9)
O(6)#1-Er(1)-O(1)	73.50(13)	O(5)-Er(1)-Er(1)#1	114.28(8)
O(3)#2-Er(1)-O(1)	101.96(13)	O(1)-Er(1)-Er(1)#1	40.91(8)
O(1)#2-Er(1)-O(1)	156.88(6)	O(4)-Er(1)-Er(1)#1	88.76(9)
O(5)-Er(1)-O(1)	91.74(13)	O(6)-Er(1)-Er(1)#1	165.27(9)
O(6)#1-Er(1)-O(4)	95.30(14)	O(3)-Er(1)-Er(1)#1	40.96(9)
O(3)#2-Er(1)-O(4)	138.35(13)	O(2)-Er(1)-Er(1)#	92.68(9)
O(1)#2-Er(1)-O(4)	71.73(13)	O(6)#1-Er(1)-Er(1)#2	108.80(9)
O(5)-Er(1)-O(4)	74.35(15)	O(3)#2-Er(1)-Er(1)#2	43.51(9)
O(1)-Er(1)-O(4)	116.10(12)	O(1)#2-Er(1)-Er(1)#2	42.23(8)
O(6)#1-Er(1)-O(6)	148.89(12)	O(5)-Er(1)-Er(1)#2	94.40(8)
O(3)#2-Er(1)-O(6)	72.90(13)	O(1)-Er(1)-Er(1)#2	140.36(9)
O(1)#2-Er(1)-O(6)	72.27(12)	O(4)-Er(1)-Er(1)#2	103.24(8)
O(5)-Er(1)-O(6)	54.69(12)	O(6)-Er(1)-Er(1)#2	40.32(9)
O(1)-Er(1)-O(6)	125.29(12)	O(3)-Er(1)-Er(1)#2	155.72(8)
O(4)-Er(1)-O(6)	96.45(13)	O(2)-Er(1)-Er(1)#2	92.36(9)
O(6)#1-Er(1)-O(3)	73.10(13)	Er(1)#1-Er(1)-Er(1)#2	151.08(2)
O(3)#2-Er(1)-O(3)	151.47(11)		
		2	
Zn(1)-O(3)	1.945(5)	O(3)-Zn(1)-N(4)#4	103.1(2)

Zn(1)-N(2)#3	2.044(5)	N(2)#3-Zn(1)-N(4)#3	107.7(2)
Zn(1)-O(1)	2.059(8)	O(1)-Zn(1)-N(4)#4	86.8(3)
Zn(1)-N(4)#4	2.071(6)	O(3)-Zn(1)-O(2)	101.0(2)
Zn(1)-O(2)	2.417(8)	N(2)#3-Zn(1)-O(2)	113.8(2)
O(3)-Zn(1)-N(2)#3	95.6(2)	O(1)-Zn(1)-O(2)	57.6(3)
O(3)-Zn(1)-O(1)	156.9(3)	N(4)#4-Zn(1)-O(2)	128.9(2)
N(2)#3-Zn(1)-O(1)	101.2(3)		
		3	
Er(1)-O(2)#5	2.239(12)	O(2)#5-Er(1)-O(3)	57.4(8)
Er(1)-O(1)	2.245(11)	O(1)-Er(1)-O(3)	60.7(8)
Er(1)-O(5)	2.310(16)	O(5)-Er(1)-O(3)	64.5(9)
Er(1)-O(4)#5	2.318(8)	O(4)#5-Er(1)-O(3)	137.1(7)
Er(1)-O(4)#6	2.332(9)	O(4)#6-Er(1)-O(3)	134.9(7)
Er(1)-O(7)	2.359(19)	O(7)-Er(1)-O(3)	114.9(8)
Er(1)-O(4)	2.361(10)	O(4)-Er(1)-O(3)	84.9(6)
Er(1)-O(6)	2.49(2)	O(6)-Er(1)-O(3)	117.2(8)
Er(1)-O(3)	2.54(3)	O(2)#1-Er(1)-Er(1)#7	119.8(4)
Er(1)-Er(1)#7	3.7298(12)	O(1)-Er(1)-Er(1)#7	116.2(3)
Er(1)-Er(1)#5	3.7325(11)	O(5)-Er(1)-Er(1)#7	133.3(7)
Er(1)-Er(1)#6	3.7326(11)	O(4)#1-Er(1)-Er(1)#7	36.8(2)
Zn(1)-N(2)#8	2.006(10)	O(4)#2-Er(1)-Er(1)#7	36.6(2)
Zn(1)-N(2)#9	2.006(10)	O(7)-Er(1)-Er(1)#7	81.2(5)
Zn(1)-N(2)#10	2.006(10)	O(4)-Er(1)-Er(1)#7	77.3(2)
Zn(1)-N(2)	2.006(10)	O(6)-Er(1)-Er(1)#7	77.6(5)
O(2)#5-Er(1)-O(1)	117.5(5)	O(3)-Er(1)-Er(1)#7	162.2(6)
O(2)#5-Er(1)-O(5)	81.7(6)	O(2)#1-Er(1)-Er(1)#7	68.8(4)
O(1)-Er(1)-O(5)	79.7(6)	O(1)-Er(1)-Er(1)#5	123.5(3)
O(2)#5-Er(1)-O(4)#5	83.1(4)	O(5)-Er(1)-Er(1)#5	148.5(5)
O(1)-Er(1)-O(4)#5	147.6(4)	O(4)#5-Er(1)-Er(1)#5	37.5(2)
O(5)-Er(1)-O(4)#5	130.4(7)	O(4)#6-Er(1)-Er(1)#5	77.6(2)
O(2)#5-Er(1)-O(4)#6	146.4(4)	O(7)-Er(1)-Er(1)#5	107.3(5)
O(1)-Er(1)-O(4)#6	79.7(4)	O(4)-Er(1)-Er(1)#5	37.1(2)
O(5)-Er(1)-O(4)#6	131.5(6)	O(6)-Er(1)-Er(1)#5	137.0(5)
O(4)#5-Er(1)-O(4)#6	70.8(4)	O(3)-Er(1)-Er(1)#5	105.8(6)
O(2)#5-Er(1)-O(7)	85.8(7)	Er(1)#7-Er(1)-Er(1)#5	60.025(11)
O(1)-Er(1)-O(7)	128.6(6)	O(2)#5-Er(1)-Er(1)#6	117.3(3)
O(5)-Er(1)-O(7)	57.9(8)	O(1)-Er(1)-Er(1)#7	70.6(3)
O(4)#5-Er(1)-O(7)	74.1(5)	O(5)-Er(1)-Er(1)#6	149.7(5)

O(4)#6-Er(1)-O(7)	106.2(7)	O(4)#5-Er(1)-Er(1)#6	77.7(2)
O(2)#5-Er(1)-O(4)	80.6(4)	O(4)#6-Er(1)-Er(1)#6	37.6(2)
O(1)-Er(1)-O(4)	86.6(4)	O(7)-Er(1)-Er(1)#6	140.8(6)
O(5)-Er(1)-O(4)	149.4(7)	O(4)-Er(1)-Er(1)#6	36.7(2)
O(4)#5-Er(1)-O(4)	71.6(4)	O(6)-Er(1)-Er(1)#6	106.3(5)
O(4)#6-Er(1)-O(4)	71.4(4)	O(3)-Er(1)-Er(1)#6	104.3(6)
O(7)-Er(1)-O(4)	144.3(5)	Er(1)#7-Er(1)-Er(1)#6	60.025(11)
O(2)#5-Er(1)-O(6)	136.1(6)	Er(1)#5-Er(1)-Er(1)#6	59.95(2)
O(1)-Er(1)-O(6)	80.3(6)	N(2)#8-Zn(1)-N(2)#9	105.8(3)
O(5)-Er(1)-O(6)	61.4(8)	N(2)#8-Zn(1)-N(2)#10	105.8(3)
O(4)#5-Er(1)-O(6)	102.5(6)	N(2)#9-Zn(1)-N(2)#10	117.1(7)
O(4)#6-Er(1)-O(6)	72.1(6)	N(2)#8-Zn(1)-N(2)	117.1(7)
O(7)-Er(1)-O(6)	55.5(8)	N(2)#9-Zn(1)-N(2)	105.8(3)
O(4)-Er(1)-O(6)	142.8(6)	N(2)#10-Zn(1)-N(2)	105.8(3)

*Symmetry transformations used to generate equivalent atoms: #**1** -x,y+1/2,-z+1/2; #**2** -x,y-1/2,-z+1/2; #**3** x+1,y,z ; #**4** x-1,-y+1/2,z-1/2; #**5** y-1/4,-x+1/4,-z+1/4; #**6** -y+1/4,x+1/4,-z+1/4; #**7** -x+0,-y+1/2,z+0; #**8** -x+1,-y+3/2,z+0; #**9** -y+5/4,x+1/4,-z+1/4; #**10** y-1/4,-x+5/4,-z+1/4.

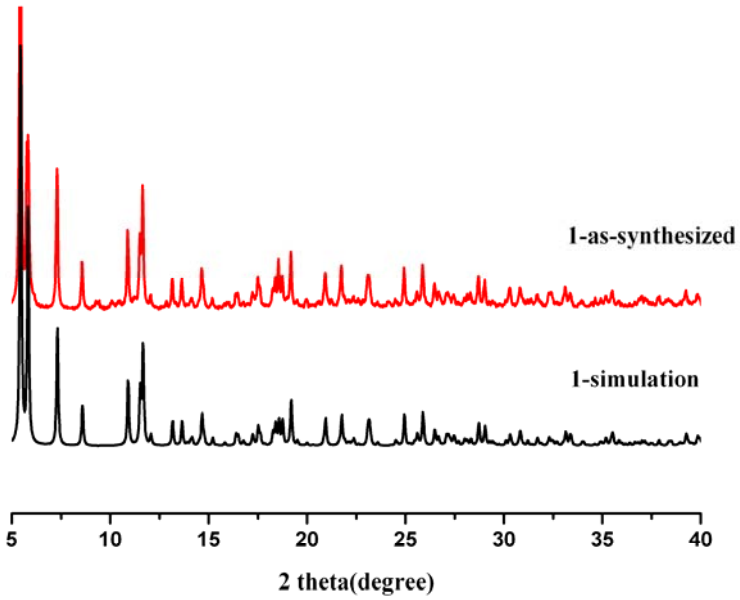
Table S3 Hydrogen bond parameters of complex **3**.

D-H···A	d (D-H) (Å)	d (H···A) (Å)	d (D···A) (Å)	∠DHA (°)
		3		
O(6)-H(6B)...O(5)	0.852(11)	1.98(5)	2.46(3)	115(5)
O(6)-H(6A)...O(8)	0.851(11)	2.05(3)	2.87(3)	162(3)
O(3)-H(3A)...Cl(2)	0.851(10)	2.56(17)	2.91(4)	106(14)
O(6)-H(6B)...Cl(2)#1	0.852(11)	2.2(3)	2.85(4)	128(30)
O(7)-H(7A)...O(6)#2	0.851(11)	2.03(8)	2.84(3)	158(22)
O(4)-H(4A)...O(1)#3	0.819(11)	2.46(14)	2.934(14)	118(13)

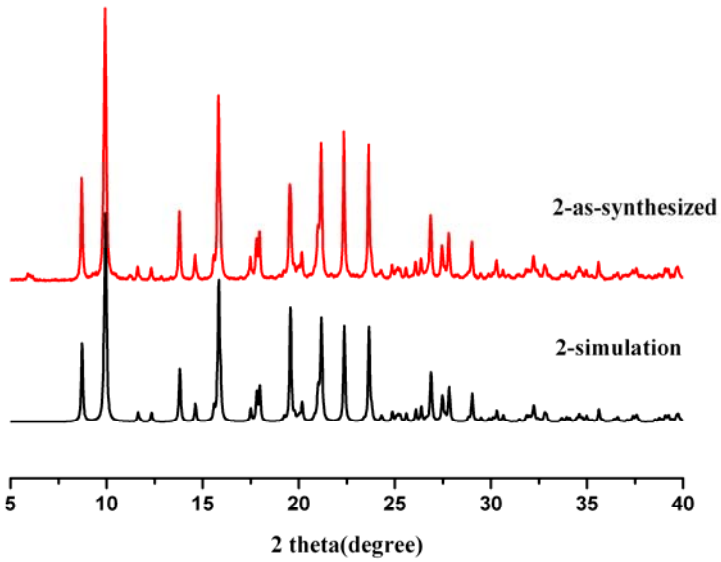
*Symmetry codes: #1 –x,2-y,-0.5+z; #2 -0.5+x,0.5-y,-0.5+z; #3 1+x,y,1+z.

Figure S1

(**a**) for **1**



(**b**) for **2**



(**c**) for **3**

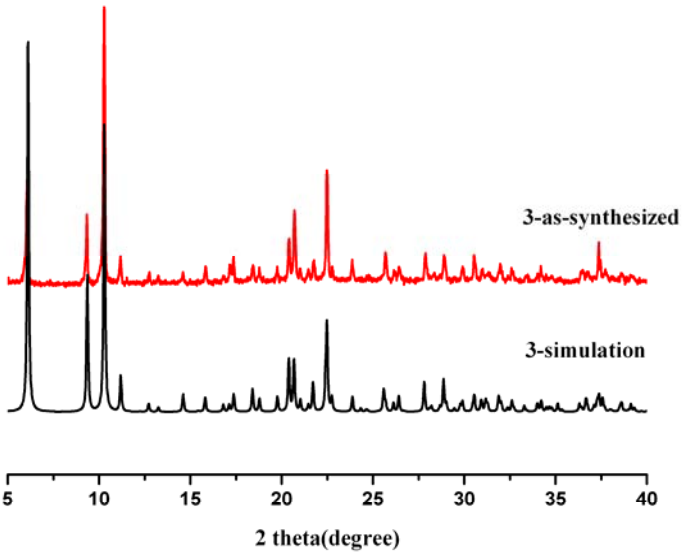

3-as-synthesized
3-simulation
5
10
15
20
25
30
35
40
2 theta(degree)

Figure S2

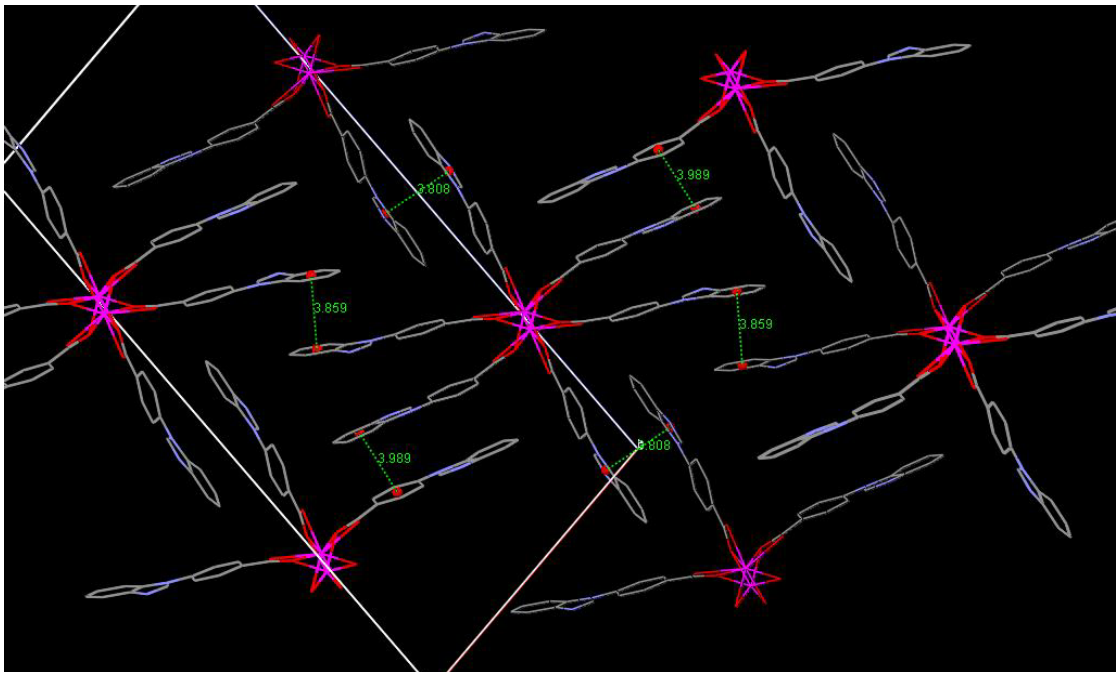


Figure S3