Effect of pH/metal ion on the structure of metal-organic frameworks based on novel bifunctionalized ligand 4'-carboxy-4,2′:6′,4"-terpyridine

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Table 1S Selected bond distances and bond angles (Å, °)

Compound 1			
Cd(1)-O(3)	2.226(3)	N(4)-C(17)	1.325(5)
Cd(1)-N(3)#1	2.301(3)	N(4)-C(21)	1.341(5)
Cd(1)-N(1)	2.377(3)	N(4)-Cd(1)#5	2.390(3)
Cd(1)-O(1)#2	2.384(3)	N(5)-C(26)	1.330(4)
Cd(1)-N(4)#3	2.390(3)	N(5)-C(22)	1.338(4)
Cd(1)-O(2)#2	2.490(2)	N(6)-C(31)	1.318(7)
Cd(1)-C(16)#2	2.751(4)	N(6)-C(27)	1.322(7)
N(1)-C(5)	1.331(4)	O(1)-C(16)	1.245(4)
N(1)-C(1)	1.346(4)	O(1)-Cd(1)#6	2.384(3)
N(2)-C(10)	1.337(4)	O(2)-C(16)	1.243(4)
N(2)-C(6)	1.344(4)	O(2)-Cd(1)#6	2.490(2)
N(3)-C(11)	1.332(4)	O(3)-C(32)	1.262(5)
N(3)-C(15)	1.336(4)	O(4)-C(32)	1.215(5)
O(3)-Cd(1)-N(3)#1	128.93(11)	N(1)-Cd(1)-N(4)#3	157.00(10)
O(3)-Cd(1)-N(1)	84.90(11)	O(1)#2-Cd(1)-N(4)#3	81.85(12)
N(3)#1-Cd(1)-N(1)	98.61(10)	O(3)-Cd(1)-O(2)#2	96.14(10)
O(3)-Cd(1)-O(1)#2	146.24(10)	N(3)#1-Cd(1)-O(2)#2	134.67(10)
N(3)#1-Cd(1)-O(1)#2	83.49(9)	N(1)-Cd(1)-O(2)#2	78.59(9)
N(1)-Cd(1)-O(1)#2	100.84(11)	O(1)#2-Cd(1)-O(2)#2	53.57(8)
O(3)-Cd(1)-N(4)#3	80.83(11)	N(4)#3-Cd(1)-O(2)#2	85.08(10)
N(3)#1-Cd(1)-N(4)#3	104.39(10)		
Compound 2			
Cd(1)-O(1)	2.2614(18)	N(2)-C(10)	1.342(3)
Cd(1)-O(4)#1	2.2720(18)	N(3)-C(11)	1.340(3)
Cd(1)-O(3)	2.2790(18)	N(3)-C(15)	1.343(3)
Cd(1)-N(3)#2	2.308(2)	N(3)-Cd(1)#5	2.308(2)
Cd(1)-O(2)#3	2.350(2)	O(1)-C(16)	1.255(3)

Cd(1)-N(1)#4	2.399(2)	O(2)-C(16)	1.237(3)
N(1)-C(1)	1.338(3)	O(2)-Cd(1)#3	2.350(2)
N(1)-C(5)	1.338(4)	O(3)-C(17)	1.249(3)
N(1)-Cd(1)#4	2.399(2)	O(4)-C(17)	1.250(3)
N(2)-C(6)	1.337(3)	O(4)-Cd(1)#1	2.2720(18)
O(1)-Cd(1)-O(4)#1	157.44(7)	O(3)-Cd(1)-O(2)#3	85.35(8)
O(1)-Cd(1)-O(3)	83.98(7)	N(3)#2-Cd(1)-O(2)#3	94.42(8)
O(4)#1-Cd(1)-O(3)	73.78(6)	O(1)-Cd(1)-N(1)#4	87.64(7)
O(1)-Cd(1)-N(3)#2	86.91(8)	O(4)#1-Cd(1)-N(1)#4	87.23(7)
O(4)#1-Cd(1)-N(3)#2	115.47(7)	O(3)-Cd(1)-N(1)#4	86.47(8)
O(3)-Cd(1)-N(3)#2	170.48(7)	N(3)#2-Cd(1)-N(1)#4	95.93(8)
O(1)-Cd(1)-O(2)#3	105.32(7)	O(2)#3-Cd(1)-N(1)#4	163.83(8)
O(4)#1-Cd(1)-O(2)#3	77.10(7)		

Compound 3

Zn(1)-N(1)#1	2.073(3)	N(3)-C(11)	1.340(5)
Zn(1)-O(4)	2.096(3)	N(3)-C(15)	1.344(5)
Zn(1)-N(3)#2	2.120(3)	N(3)-Zn(1)#4	2.120(3)
Zn(1)-O(2)	2.154(3)	O(1)-C(16)	1.241(6)
Zn(1)-O(1)	2.260(4)	O(2)-C(16)	1.253(5)
N(1)-Zn(1)#3	2.073(3)	O(3)-C(17)	1.241(4)
N(2)-C(6)	1.334(5)	O(4)-C(18)	1.254(4)
N(2)-C(10)	1.348(5)		
N(1)#1-Zn(1)-O(4)	103.12(13)	O(3)-Zn(1)-O(2)	88.33(12)
N(1)#1-Zn(1)-O(3)	92.16(13)	N(3)#2-Zn(1)-O(2)	101.12(13)
N(1)#1-Zn(1)-N(3)#2	96.28(13)	N(1)#1-Zn(1)-O(1)	158.15(13)
O(4)-Zn(1)-N(3)#2	88.11(12)	O(4)-Zn(1)-O(1)	98.33(12)
O(3)-Zn(1)-N(3)#2	166.21(12)	O(3)-Zn(1)-O(1)	87.73(13)
N(1)#1-Zn(1)-O(2)	98.52(12)	N(3)#2-Zn(1)-O(1)	88.45(13)
O(4)-Zn(1)-O(2)	155.38(12)	O(2)-Zn(1)-O(1)	59.63(11)

Compound 4			
Cu(1)-O(1)#1	1.941(2)	N(3)-C(15)	1.330(4)
Cu(1)-O(4)#2	1.989(2)	N(3)-C(11)	1.341(4)
Cu(1)-O(3)	2.000(2)	N(3)-Cu(1)#4	2.011(3)
Cu(1)-N(3)#3	2.011(3)	O(1)-C(16)	1.280(4)
Cu(1)-N(1)	2.307(3)	O(1)-Cu(1)#1	1.941(2)
N(1)-C(1)	1.329(4)	O(2)-C(16)	1.221(4)
N(1)-C(5)	1.338(4)	O(3)-C(17)	1.252(4)
N(2)-C(6)	1.338(4)	O(4)-C(17)	1.255(4)
N(2)-C(10)	1.346(4)	O(4)-Cu(1)#2	1.989(2)
O(1)#1-Cu(1)-O(4)#2	171.03(10)	O(3)-Cu(1)-N(3)#3	165.21(11)
O(1)#1-Cu(1)-O(3)	88.41(10)	O(1)#1-Cu(1)-N(1)	90.53(10)
O(4)#2-Cu(1)-O(3)	83.67(9)	O(4)#2-Cu(1)-N(1)	94.44(10)
O(1)#1-Cu(1)-N(3)#3	92.06(10)	O(3)-Cu(1)-N(1)	95.75(10)
O(4)#2-Cu(1)-N(3)#3	94.52(10)	N(3)#3-Cu(1)-N(1)	99.03(11)

Symmetry codes

for **1**: #1 (x, -y+1, z-1/2) ;   #2 (-x+5/2, y+1/2, z) ;   #3 (-x+3/2, y+1/2, z) ;

#4 (x, -y+1, z+1/2) ;   #5 (-x+3/2, y-1/2, z) ;   #6 (-x+5/2, y-1/2, z).

for **2**: #1 (-x, -y+2, -z+1) ;   #2 (-x+2, y+1/2, -z+3/2) ;   #3 (-x+1, -y+2, -z+1);

#4 (-x+1, -y+2, -z+2) ;   #5 (-x+2, y-1/2, -z+3/2).

for **3**: #1 (x, y, z-1) ;   #2 (x+1/2, -y+1/2, z) ;   #3 (x, y, z+1) ;

#4 (x-1/2, -y+1/2, z) ;   #5 (x, -y, z).

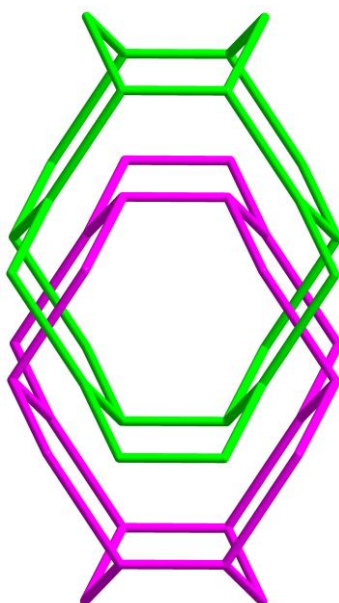for **4**: #1 (-x,y-1/2,-z+3/2) ;   #2 (-x+1,-y,-z+1) ;   #3 (-x+2,-y,-z+2) ;
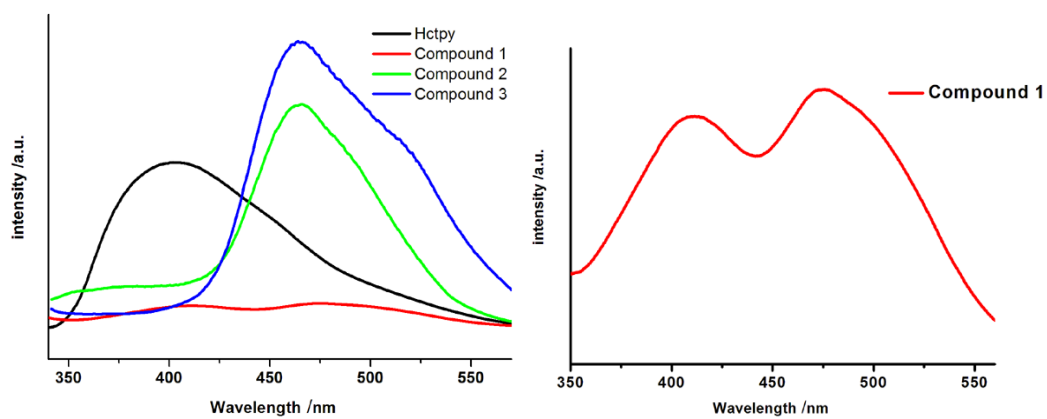
#4 (-x,y+1/2,-z+3/2).
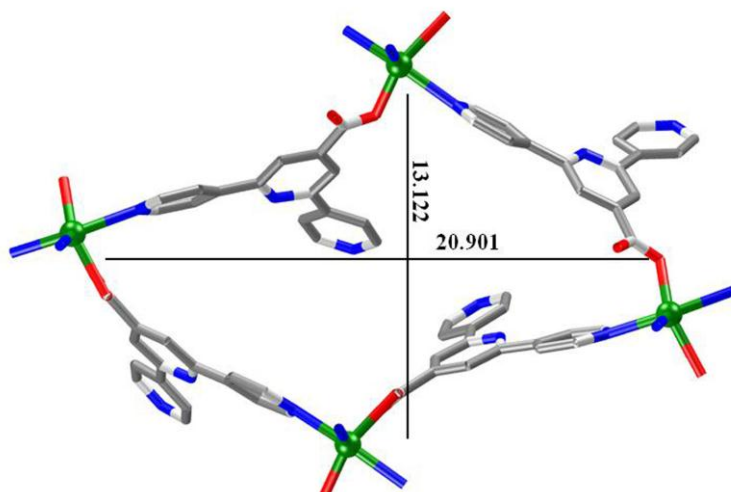
Fig. S1. a single unit square grid of **1.**
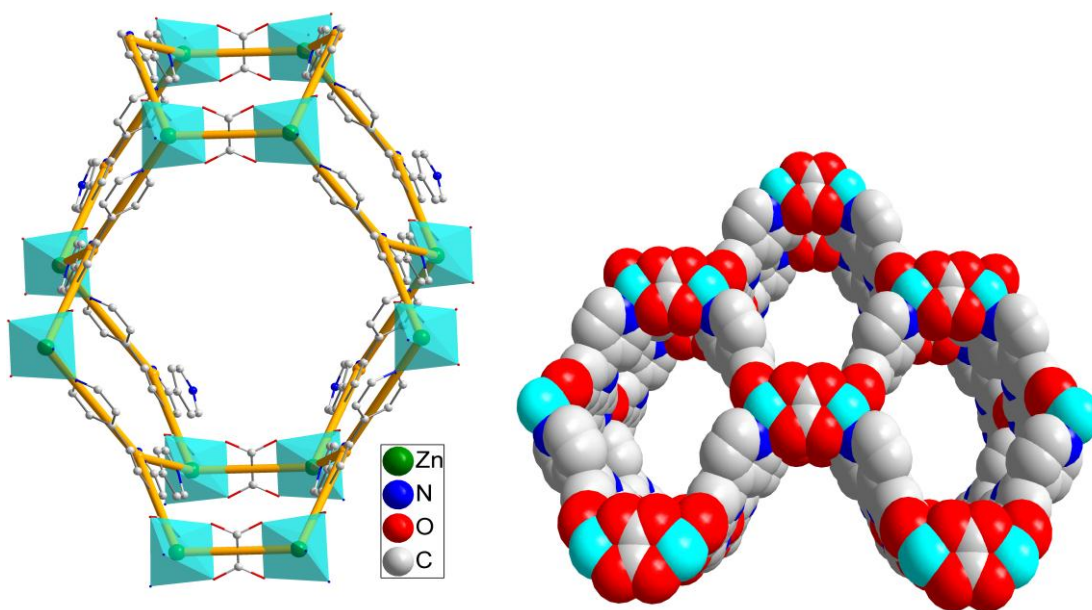
Fig. S2. Left: a single **fsc** unit cage of **3**. Right: the space filling mode of a single 3D

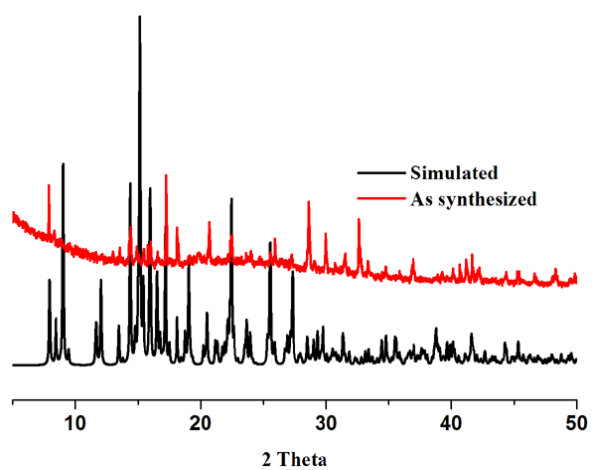**fsc** net in **3** (gray: C; blue: N; red: O; turquiose: Zn).

Fig. S3. topological representation of the 2-fold interpenetrating network of **3** (each color represents a network).
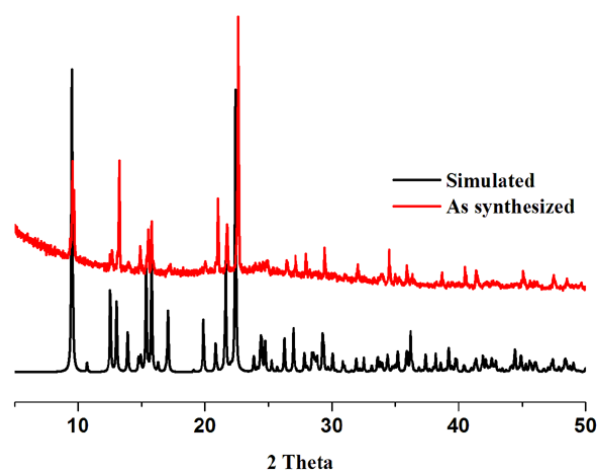

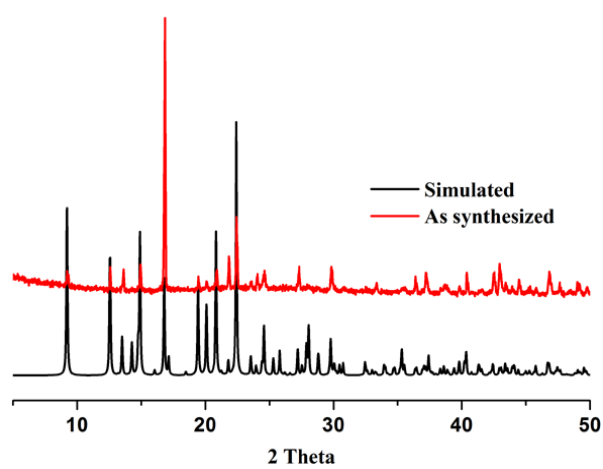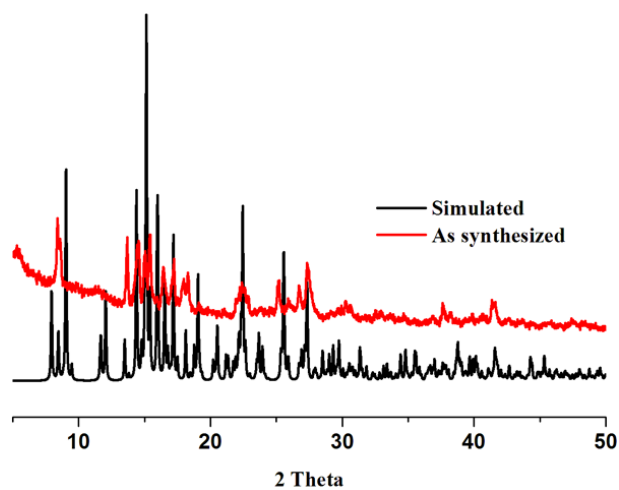**Fig. S4.** The emission spectra of **Hctpy** and **1-3** in the solid state at room temperature.
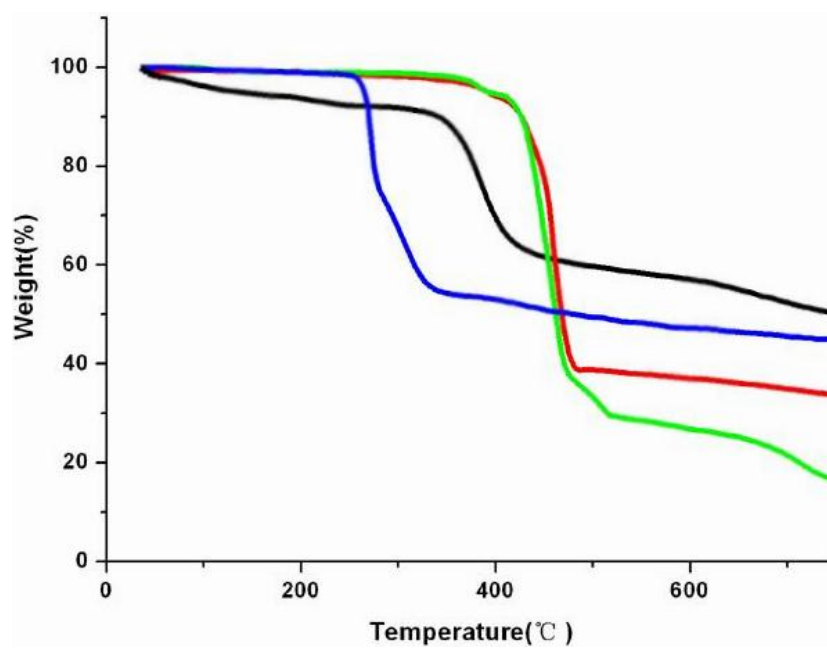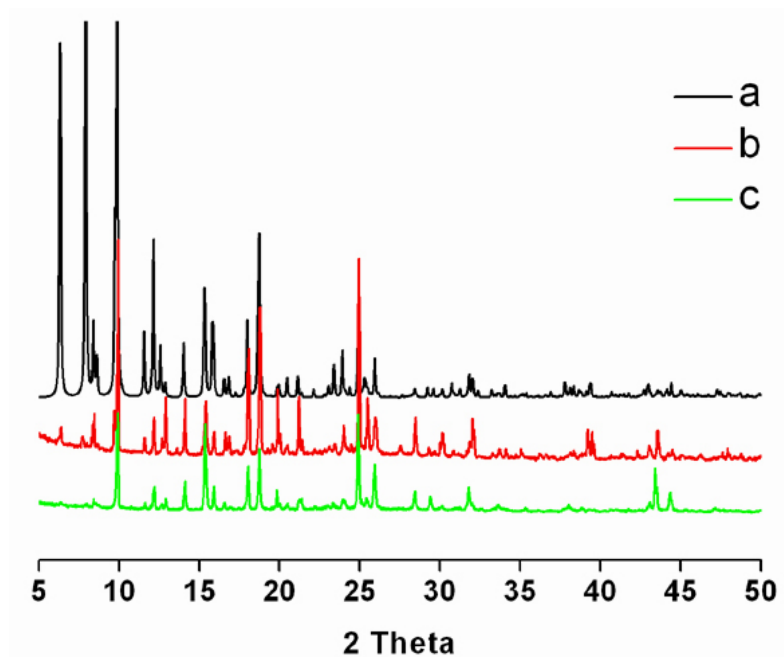
(a)

(b)

(c)

(d)

Fig. S5. PXRD patterns of compounds **1**, **2**, **4** and white powder (a-d) simulated from the X-ray single-crystal structure and as-synthesized.
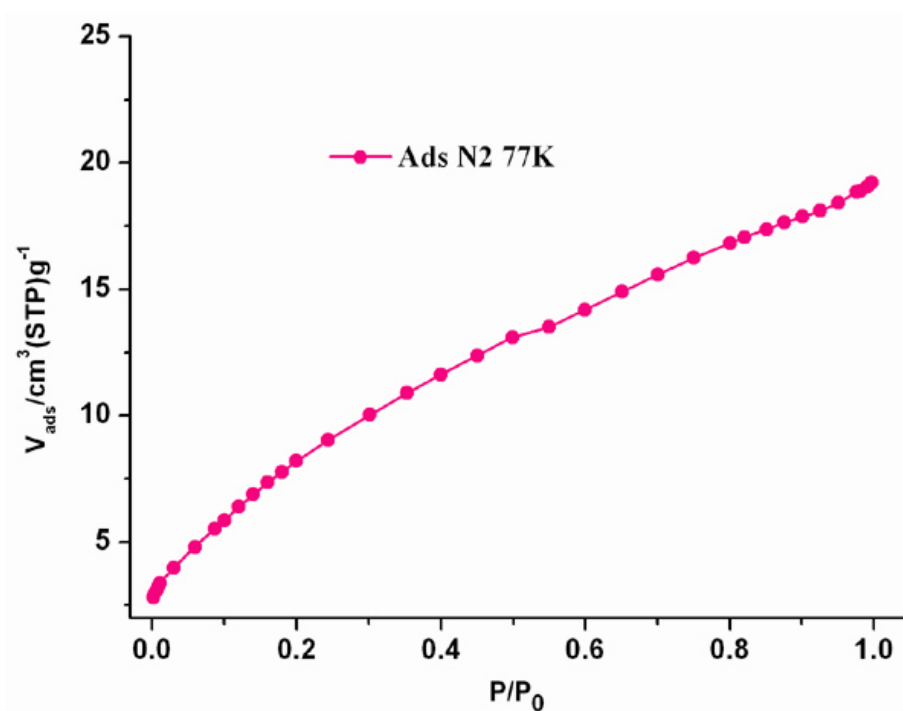

Fig. S6. TGA curves for 1-4（red: 1; green: **2**; black: **3**; blue: **4）.**

Fig. S7. PXRD patterns for **3:** (a) simulated from the single crystal data; (b) synthesized powder samples; c) dehydrated samples.

Fig. S8. N_2 adsorption isotherm (77 K) of **3a** (activated at 140℃).