Electronic Supporting Information for:

Predicting and Creating 7-connected Zn_4O vertices for the construction of exceptional metal-organic framework with nanoscale cages

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1. Materials and General Procedures.

All reagents were purchased from commercial sources and used without further purification. Thermogravimetric (TGA) analyses were investigated with a METTLER TOLEPO TGA/SDTA851 analyzer in N_2 atmosphere from 30 to 800 °C with a heating rate of 10 K min^{-1}. Elemental analysis was measured on an Elementar Vario EL III microanalyzer. IR spectra were measured from a KBr pellets on a Nicolet Nexus 470 FT-IR spectrometer in the range of 4000-400 cm^{-1}. X-ray powder diffraction (XRD) patterns were measured using a Bruker D4 powder diffractometer at 40 kV, 40 mA for Cu Kα radiation (λ = 1.5406 Å), with a scan speed of 0.2 s/step and a step size of 0.05 °(2θ). N2 or Ar sorption isothermal at 77 K were carried out on ASAP 2020 apparatus. Before gas sorption, the as-made crystal samples (about 100 mg) were exchanged with acetone (10 mL for three times) and then degased at room temperature overnight. The solid state fluorescent spectra were recorded on Hitachi F-4500 with a xenon arc lamp as the light source at room temperature. The EX Slit and EM Slit settled to be 5.0 nm and PMT Voltage: 400 V.

2. Theoretical Calculation Details

The structural model of basic zinc acetate $[Zn_4O(CH_3COO)_6]$, $[Zn_4O(CH_3COO)_7]^-$ and $[Zn_4O(CH_3COO)_6(\eta_1\text{-}CH_3COO)]^-$ were built with the Visualizer Program from Accelrys, Inc. The geometry optimization calculations were carried using the program DMOL^3.[1] The DND basis set with fine precision was used. DFT Semi-core Pseudopots (DSPP) was used for the treatments of core electrons. The GGA (PW91, BP, PBE and BLYP) functional was used respectively in the calculation. No imaginary frequency was observed for each model after geometry optimization.

3. Synthesis

$\{[(Zn_4O)_2(H_2O)_2(bptc)_{3.5}]\cdot 2CH_3NH_3\cdot xG\}_n$ (**1**) were obtained through solvothermal synthesis. A mixture of H_4bptc (0.058 g, 0.175 mmol), $Zn(CH_3COO)_2\cdot 2H_2O$ (0.089 g, 0.4 mmol), and DMF (4 mL) were placed in a 15 mL teflon-lined stainless steel autoclave and was stirred for 10 min. Then 0.3 mL of nitric acid was added and the mixture was further stirred for another 10 min. The mixture was heated at 140 °C for 3 days, followed by slowly cooling down to room temperature. Colorless rhombus crystals of compound **1** were collected by filtration (yield: 48% based on H_4pbpdc). IR (KBr, cm^{-1}): 3077 (w), 2919 (m), 2854 (m), 1664 (vs), 1629 (vs), 1575 (vs), 1417 (vs), 1360 (vs), 1253 (m), 1180 (m), 1112 (s), 1082 (s), 902 (w), 823 (w), 775 (m). 727 (m), 661 (s), 613 (m).

4. X-ray Crystallographic Study

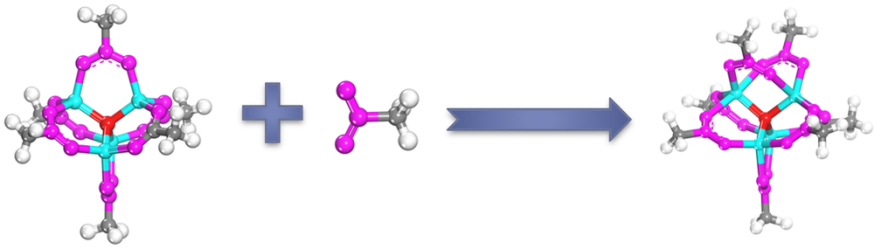
Data collection for **1** was carried out on a Bruker Apex Duo diffractometer with graphite monochromated Mo $K\alpha$ radiation (λ = 0.71073 Å) at 173 K. Data reduction was performed with SAINT, and empirical absorption corrections were applied by SADABS program. Structures were solved by direct method using SHELXS program and refined with SHELXL program.[2] Heavy atoms and other non-hydrogen atoms were directly obtained from difference Fourier map. Final refinements were performed by full-matrix least-squares methods with anisotropic thermal parameters for all non-hydrogen atoms on F^2. C-bonded H atoms were placed geometrically and refined as riding modes. The H atoms of coordinated and guest water molecules were not placed because of their disorder and the number was calculated based on the number of guest water oxygen atoms. The highest residual electron density peak (2.25) from difference Fourier map is around the Zn2 center of SBU-I with the distance of 0.84 Å. DFIX and ISOR commands were respectively used for guest molecules because they are in large disorder. Crystallographic data are listed in Table S5 and selected bond length and angles are listed in Table S6.

Table S1. Total energy and enthalpy data of CH_3COO^-, $Zn_4O(CH_3COO)_6$, $[Zn_4(CH_3COO)_7]^-$ and $[Zn_4O(CH_3COO)_8]^{2-}$ based on BP, PBE and BLYP function, respectively.

Function		Total Energy (Ha)	Free Energy @ 298.15 K (kcal/mol)	Free Energy @ 413.15 K (kcal/mol)	Enthalpy @298.15 K (kcal/mol)	Enthalpy @413.15 K (kcal/mol)
PW91	CH_3COO	-228.5433068	12.611	4.498	32.787	34.767
	Zn_4O-6	-2465.2586135	147.079	116.157	220.07	236.535
	Zn_4O-7	-2693.8735085	173.337	139.011	254.106	272.975
	Zn_4O-8	-2922.3771658	198.051	160.106	287.238	308.33
BP	CH_3COO	-228.5943223	12.539	4.415	32.741	34.724
	Zn_4O-6	-2465.6204208	145.939	114.65	219.869	236.359
	Zn_4O-7	-2694.2761491	173.256	139.23	253.339	272.005
	Zn_4O-8	-2922.8101730	199.895	163.657	284.946	305.394
PBE	CH_3COO	-228.3605402	12.711	4.643	32.769	34.751
	Zn_4O-6	-2463.0989781	149.964	120.443	219.431	235.662
	Zn_4O-7	-2691.5304179	173.972	139.812	254.323	273.169
	Zn_4O-8	-2919.8508346	200.913	163.594	288.403	309.665
BLYP	CH_3COO	-228.5663615	12.717	5.025	31.899	33.663
	Zn_4O-6	-2464.7554995	147.429	117.768	217.326	233.402
	Zn_4O-7	-2693.3841117	170.278	135.447	252.319	271.275
	Zn_4O-8	/*	/*	/*	/*	/*

*The energy didn't converge in 100 SCF steps.

Table S2. ΔG and ΔH of the formation of $[Zn_4(CH_3COO)_7]^-$ calculated by BP, PBE and BLYP function, respectively.

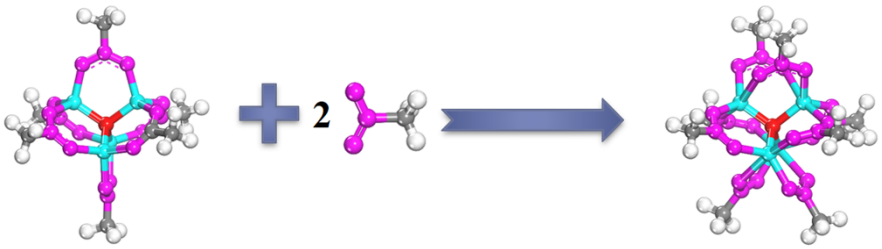


Function	T (K)	$G_{reactans}$ (kcal/mol)	$G_{product}$ (kcal/mol)	$\Delta G^{t\,\#}$ (kcal/mol)	$H_{reactans}$ (kcal/mol)	$H_{product}$ (kcal/mol)	$\Delta H^{t\,\#}$ (kcal/mol)
PW91	298.15	159.690	173.337	-31.275	252.857	254.106	-43.673
	413.15	120.655	139.011	-26.566	271.302	271.302	-43.249
BP	298.15	158.478	173.256	-23.755	252.610	253.339	-37.804
	413.15	119.065	139.230	-18.368	271.083	272.005	-37.611
PBE	298.15	162.675	173.972	-33.193	252.200	254.323	-42.367
	413.15	125.086	139.812	-29.764	270.413	273.169	-41.734
BLYP	298.15	160.146	170.278	-28.931	249.225	252.319	-35.969
	413.15	122.793	135.447	-26.409	267.065	271.275	-34.853

$^{\#}$ $\Delta G^t = (\text{Total Energy}_{product} + G_{product}) - \sum(\text{Total Energy}_{reactants} + G_{reactants})$

$\Delta H^t = (\text{Total Energy}_{product} + H_{product}) - \sum(\text{Total Energy}_{reactants} + H_{reactants})$

Table S3. ΔG and ΔH of the formation of $[Zn_4(CH_3COO)_8]^{2-}$ calculated by BP, PBE and BLYP function, respectively.



Function	T (K)	$G_{reactans}$ (kcal/mol)	$G_{product}$ (kcal/mol)	$\Delta G^{t\,\#}$ (kcal/mol)	$H_{reactans}$ (kcal/mol)	$H_{product}$ (kcal/mol)	$\Delta H^{t\,\#}$ (kcal/mol)
PW91	298.15	172.301	198.051	5.708	285.644	287.238	-18.448
	413.15	125.153	160.106	14.911	306.069	308.330	-17.781
BP	298.15	171.017	199.895	28.183	285.351	284.946	-1.100
	413.15	123.480	163.657	39.482	305.807	305.394	-1.108
PBE	298.15	175.386	200.913	6.215	284.969	288.403	-15.878
	413.15	129.729	163.594	14.553	305.164	309.665	-14.811
BLYP	298.15	172.863	/*	/*	281.124	/*	/*
	413.15	127.818	/*	/*	300.728	/*	/*

*The energy didn't converge in 100 SCF steps.

$\Delta G^t = (\text{Total Energy}_{product} + G_{product}) - \sum(\text{Total Energy}_{reactants} + G_{reactants})$

$\Delta H^t = (\text{Total Energy}_{product} + H_{product}) - \sum(\text{Total Energy}_{reactants} + H_{reactants})$

Table S4. Synthetic conditions of some other similar products. [a]

Molecular fomular	Zinc salt and amount/mmol	Solvent and acid amount/mL	Temperature /°C	Time /days	Cell parameter (a, b, c /Å, α, β, γ /°)
$[Zn_2(bptc)(H_2O)(DMF)_2]\cdot DMF\cdot H_2O$ [b]	NO_3, 0.2	DMF, 4 mL; HBF_4, 0.6 mL	90	2	14, 13, 18, 90, 96, 90
$[Zn_2(bptc)(H_2O)_2]\cdot 2.67H_2O$	NO_3, 0.6	DMF, 3 mL; EtOH, 2mL; HNO_3, 0.2 mL	90	5	19, 19, 25, 90, 90, 120
$[Zn_5(Hbptc)_3(H_2O)]\cdot 2H_3O\cdot 2\ H_2O$	OAc, 0.2	DMF, 4 mL; i-PrOH, 1mL; HNO_3, 1.2 mL	140	3	12, 31, 23, 90, 94, 90 [d]
$[Zn_3(Hbptc)_2(DMF)_2]\cdot 2\ DMF$	OAc, 0.3	DMF, 4 mL; i-PrOH, 1mL; HNO_3, 1.2 mL	140	2	17, 18, 16, 90, 109,90 [d]
$[Zn_2(bptc)(DMF)]\cdot 2\ DMF$	Cl, 0.4	DMF, 4 mL	140	2	20, 10, 18, 90, 114, 90 [d]
$[(Zn_4O)_2(H_2O)_2(bptc)_{3.5}]\cdot 2\ CH_3NH_3\cdot xG$ (**1**)	OAc, 0.4	DMF, 4 mL HNO3, 0.3 mL	140	3	52, 52, 52, 90, 90,90

[a] The molar amount of H_4bptc is 0.175 mmol for **1** and 0.2 mmol for the other compounds.

[b] Isostructure with Co-MOF-502. [3]

[c] Isostructure with Cu-MOF-505. [4]

[d] These structures are firstly synthesized by our group, which are in preparation for publishing, so the detailed crystallographic data is not given here.

Table S5. Crystal structure parameter and refinement data of **1**.

	1
Empirical formula	$C_{58}H_{45.33}N_2O_{36.17}Zn_8$
Formula weight	1871.92
Temperature (K)	173(2)
Wavelength (Å)	0.71073
Crystal system	Cubic
Space group	*I a -3*
a (Å)	52.623(3)
V (Å^3)	145726(24)
Z	48
D_c (g cm^{-3})	1.024
μ (mm^{-1})	1.607
F(000)	44960
Total collected	399468
Unique data, R_{int}	21758, 0.1504
GOF on F_2	1.096
R_1[a]. wR_2[b][I > 2σ(I)]	0.0860, 0.2331
R_1. wR_2(all data)	0.1423, 0.3012
CCDC	1037939

[a] $R_1 = \sum||F_o| - |F_c|/\sum|F_o|$.

[b] $wR_2 = [\sum w(F_o^2-F_c^2)^2/\sum w(F_o^2)^2]^{1/2}$.

Table S6. Selected bonds lengths (Å) and angles (º) for compound 1

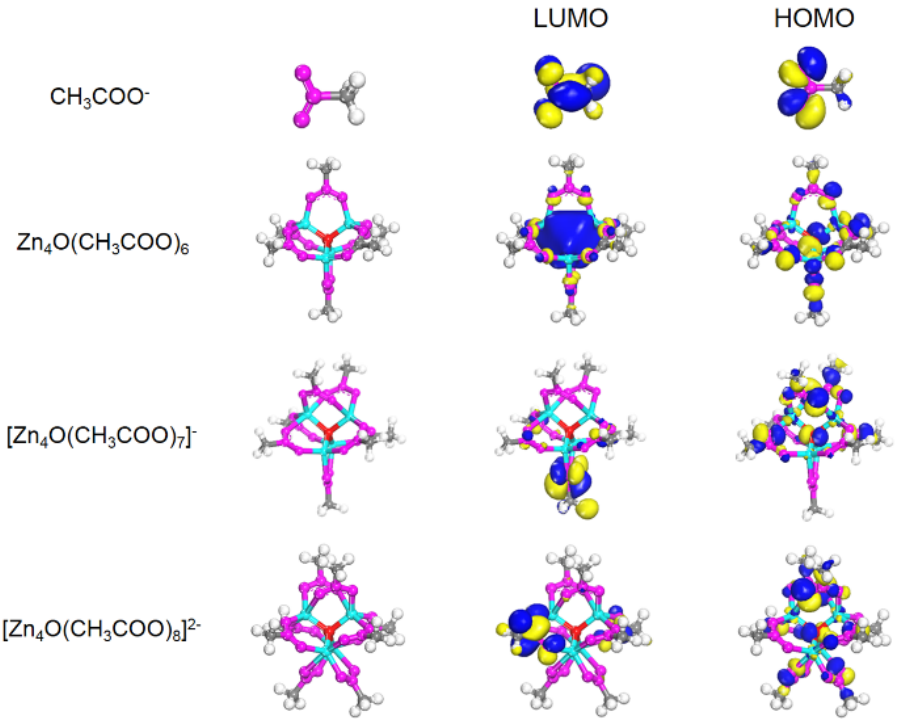
Compound **1**			
Zn(1)-O(3)#1	1.920(7)	Zn(1)-O(51)	1.956(6)
Zn(1)-O(9)	1.967(6)	Zn(1)-O(17)	2.102(7)
Zn(1)-O(1)	2.284(7)	Zn(2)-O(2)	1.895(7)
Zn(2)-O(51)	1.920(6)	Zn(2)-O(21)#2	1.920(6)
Zn(2)-O(4)#3	2.354(7)	Zn(2)-O(20)#4	2.367(8)
Zn(3)-O(19)#5	1.873(8)	Zn(3)-O(51)	1.922(6)
Zn(3)-O(27)#6	1.936(7)	Zn(3)-O(10)	1.964(6)
Zn(4)-O(18)	1.908(8)	Zn(4)-O(51)	1.922(6)
Zn(4)-O(28)#7	1.954(6)	Zn(4)-O(22)#8	1.984(7)
Zn(5)-O(50)	1.998(6)	Zn(5)-O(7)#9	2.055(7)
Zn(5)-O(11)	2.063(6)	Zn(5)-O(5)	2.080(7)
Zn(5)-O(24)#10	2.163(6)	Zn(5)-O(100)	2.231(14)
Zn(6)-O(50)	1.972(6)	Zn(6)-O(8)#11	1.994(8)
Zn(6)-O(6)	2.039(8)	Zn(6)-O(14)#12	2.046(7)
Zn(6)-O(15)#13	2.092(7)	Zn(6)-O(101)	2.159(19)
Zn(7)-O(50)	1.910(6)	Zn(7)-O(12)	1.937(7)
Zn(7)-O(26)	1.970(6)	Zn(7)-O(13)#14	1.972(6)
Zn(8)-O(25)	1.951(7)	Zn(8)-O(50)	1.909(5)
Zn(8)-O(23)#15	1.914(7)	Zn(8)-O(16)#16	1.920(8)
O(3)#1-Zn(1)-O(51)	120.5(3)	O(3)#1-Zn(1)-O(9)	119.0(3)
O(51)-Zn(1)-O(9)	119.7(2)	O(3)#1-Zn(1)-O(17)	90.1(4)
O(51)-Zn(1)-O(17)	96.9(3)	O(9)-Zn(1)-O(17)	91.6(3)
O(3)#1-Zn(1)-O(1)	88.7(4)	O(51)-Zn(1)-O(1)	88.6(3)
O(9)-Zn(1)-O(1)	84.0(3)	O(17)-Zn(1)-O(1)	174.2(3)
O(2)-Zn(2)-O(51)	119.1(3)	O(2)-Zn(2)-O(21)#2	126.3(3)
O(51)-Zn(2)-O(21)#2	114.5(3)	O(2)-Zn(2)-O(4)#3	86.3(3)
O(51)-Zn(2)-O(4)#3	95.7(3)	O(21)#2-Zn(2)-O(4)#3	89.4(3)
O(2)-Zn(2)-O(20)#4	83.7(4)	O(51)-Zn(2)-O(20)#4	96.7(3)
O(21)#2-Zn(2)-O(20)#4	89.6(3)	O(4)#3-Zn(2)-O(20)#4	166.8(3)
O(19)#5-Zn(3)-O(51)	121.7(3)	O(19)#5-Zn(3)-O(27)#6	102.5(4)
O(51)-Zn(3)-O(27)#6	107.5(3)	O(19)#5-Zn(3)-O(10)	111.3(4)
O(51)-Zn(3)-O(10)	113.1(3)	O(27)#6-Zn(3)-O(10)	97.0(4)
O(18)-Zn(4)-O(51)	111.6(3)	O(18)-Zn(4)-O(28)#7	107.9(3)
O(51)-Zn(4)-O(28)#7	113.1(3)	O(18)-Zn(4)-O(22)#8	109.8(4)
O(51)-Zn(4)-O(22)#8	109.7(3)	O(28)#7-Zn(4)-O(22)#8	104.5(3)
O(50)-Zn(5)-O(7)#9	96.7(3)	O(50)-Zn(5)-O(11)	99.8(2)
O(7)#9-Zn(5)-O(11)	162.8(3)	O(50)-Zn(5)-O(5)	103.9(3)
O(7)#9-Zn(5)-O(5)	93.0(3)	O(11)-Zn(5)-O(5)	87.9(3)
O(50)-Zn(5)-O(24)#10	99.1(2)	O(7)#9-Zn(5)-O(24)#10	86.0(3)
O(11)-Zn(5)-O(24)#10	86.6(3)	O(5)-Zn(5)-O(24)#10	157.0(3)
O(50)-Zn(5)-O(100)	176.7(4)	O(7)#9-Zn(5)-O(100)	80.2(5)

(Continued)

O(11)-Zn(5)-O(100)	83.2(4)	O(5)-Zn(5)-O(100)	77.6(4)
O(24)#10-Zn(5)-O(100)	79.6(4)	O(50)-Zn(6)-O(8)#11	104.4(3)
O(50)-Zn(6)-O(6)	97.5(3)	O(8)#11-Zn(6)-O(6)	91.0(4)
O(50)-Zn(6)-O(14)#12	104.5(3)	O(8)#11-Zn(6)-O(14)#12	151.2(4)
O(6)-Zn(6)-O(14)#12	84.3(3)	O(50)-Zn(6)-O(15)#13	106.0(3)
O(8)#11-Zn(6)-O(15)#13	86.5(4)	O(6)-Zn(6)-O(15)#13	156.3(4)
O(14)#12-Zn(6)-O(15)#13	86.6(3)	O(50)-Zn(6)-O(101)	174.8(12)
O(8)#11-Zn(6)-O(101)	79.1(11)	O(6)-Zn(6)-O(101)	78.6(12)
O(14)#12-Zn(6)-O(101)	72.0(11)	O(15)#13-Zn(6)-O(101)	77.8(12)
O(50)-Zn(7)-O(12)	111.5(3)	O(50)-Zn(7)-O(26)	114.0(2)
O(12)-Zn(7)-O(26)	107.2(3)	O(50)-Zn(7)-O(13)#14	115.5(3)
O(12)-Zn(7)-O(13)#14	103.8(3)	O(26)-Zn(7)-O(13)#14	104.0(3)
O(50)-Zn(8)-O(23)#15	119.5(3)	O(50)-Zn(8)-O(16)#16	119.3(3)
O(23)#15-Zn(8)-O(16)#16	105.9(4)	O(50)-Zn(8)-O(25)	109.0(3)
O(23)#15-Zn(8)-O(25)	99.3(4)	O(16)#16-Zn(8)-O(25)	100.3(5)
Zn(8)-O(50)-Zn(7)	109.6(3)	Zn(8)-O(50)-Zn(6)	106.7(3)
Zn(7)-O(50)-Zn(6)	108.6(3)	Zn(8)-O(50)-Zn(5)	108.2(3)
Zn(7)-O(50)-Zn(5)	116.6(3)	Zn(6)-O(50)-Zn(5)	106.6(3)
Zn(2)-O(51)-Zn(4)	109.5(3)	Zn(2)-O(51)-Zn(3)	112.0(3)
Zn(4)-O(51)-Zn(3)	111.3(3)	Zn(2)-O(51)-Zn(1)	103.4(3)
Zn(4)-O(51)-Zn(1)	118.5(3)	Zn(3)-O(51)-Zn(1)	101.7(3)

Symmetry transformations used to generate equivalent atoms: #1: 1-z, x, 0.5+y; #2: 0.5-x, y, 2-z; #3: 1-z, x, 0.5+y; #4: y, -0.5+z, 1-x; #5: y, -0.5+z, 1-x; #6: -0.5+z, 0.5+x, 0.5+y; #7: -0.5+z, 0.5+x, 0.5+y; #8: 0.5-x, y, 2-z; #9: 0.5-y, 1-z, 0.5+x; #10: -1+z, 0.5-x, 0.5+y; #11: 0.5-y, 1-z, 0.5+x; #12: x, 1-y, 1.5-z; #13: -0.5+y, -0.5+z, 0.5+x; #14: x, 1-y, 1.5-z; #15: -1+z, 0.5-x, 0.5+y; #16: -0.5+y, -0.5+z, -0.5+x.

Figure S1. The frontier molecular orbital profiles of CH_3COO^-, $Zn_4O(CH_3COO)_6$, $[Zn_4(CH_3COO)_7]^-$ and $[Zn_4O(CH_3COO)_8]^{2-}$ calculated by BP function.



The HOMO/LUMO (eV) of CH_3COO^-, $Zn_4O(CH_3COO)_6$, $[Zn_4(CH_3COO)_7]^-$ and $[Zn_4O(CH_3COO)_8]^{2-}$ based on BP, PBE and BLYP function, respectively.

Function	PW91		BP		PBE		BLYP	
	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO	HOMO	LUMO
CH_3COO^-	0.961	6.067	1.038	6.17	1.014	6.11	1.08	6.122
Zn_4O-6	-6.582	-1.441	-6.517	-1.353	-6.524	-1.409	-6.43	-1.428
Zn_4O-7	-2.827	1.893	-2.736	1.982	-2.783	1.925	-2.72	1.957
Zn_4O-8	0.247	4.651	0.256	5.071	0.212	4.532	/*	/*

*The energy didn't converge in 100 SCF steps.

Figure S2. The PXRD pattern of **1** compared with the simulated one from CIF.

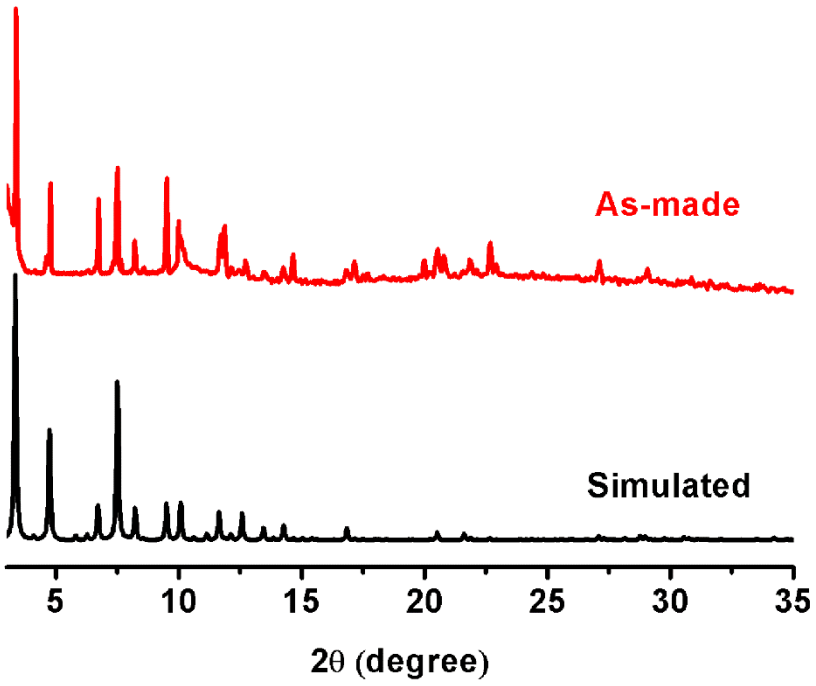


Figure S3. The coordination mode between bptc ligands and zinc atoms (Hydrogen atoms, guest water molecules as well as CH_3NH_3 are omitted for clarity). Asymmetric code: A: 1-z, x, 0.5+y; B： 1-z, x, 0.5+y; C: 0.5+y, 1-z, 0.5+x; D: 0.5+y, 1-z, 0.5+x; E: x, 1-y, 1.5-z; F: x, 1-y, 1.5-z; G: -0.5+y, -0.5+z, 0.5+x; H: -0.5+y, -0.5+z, 0.5+x; I: y, -0.5+z, 1-x; J: y, -0.5+z, 1-x; K: 0.5-x, y, 2-z; L: 0.5-x, y, 2-z; M:-1+z, 0.5+x, 0.5+y; N:-1+z, 0.5-x, 0.5+y; O: -0.5+z, 0.5+x, 0.5+y; P: -0.5+z, 0.5+x, 0.5+y.

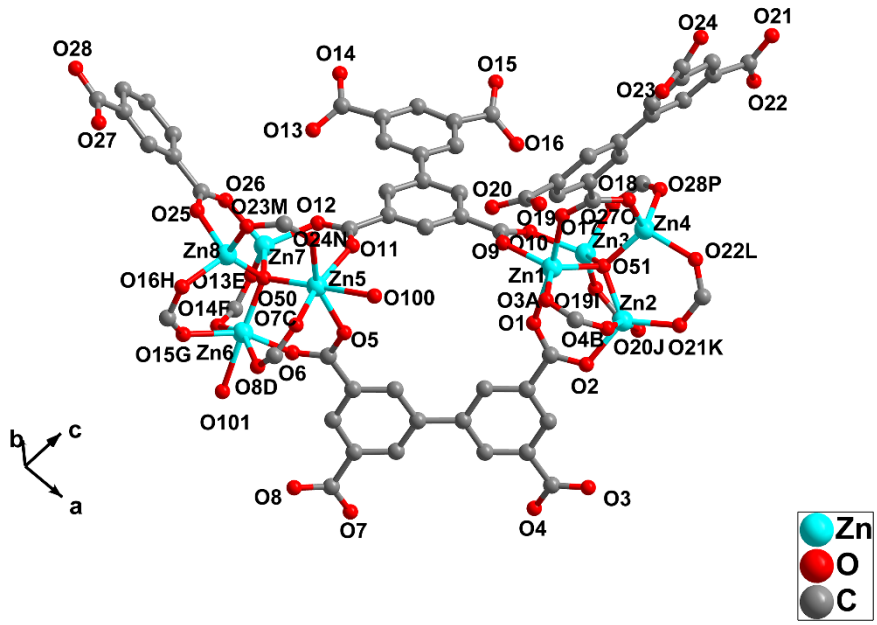


Figure S4. **1** viewing along [1, 1, 1] direction showing the channels that were filled with (a) protonated methanamine, and (b) water molecules.

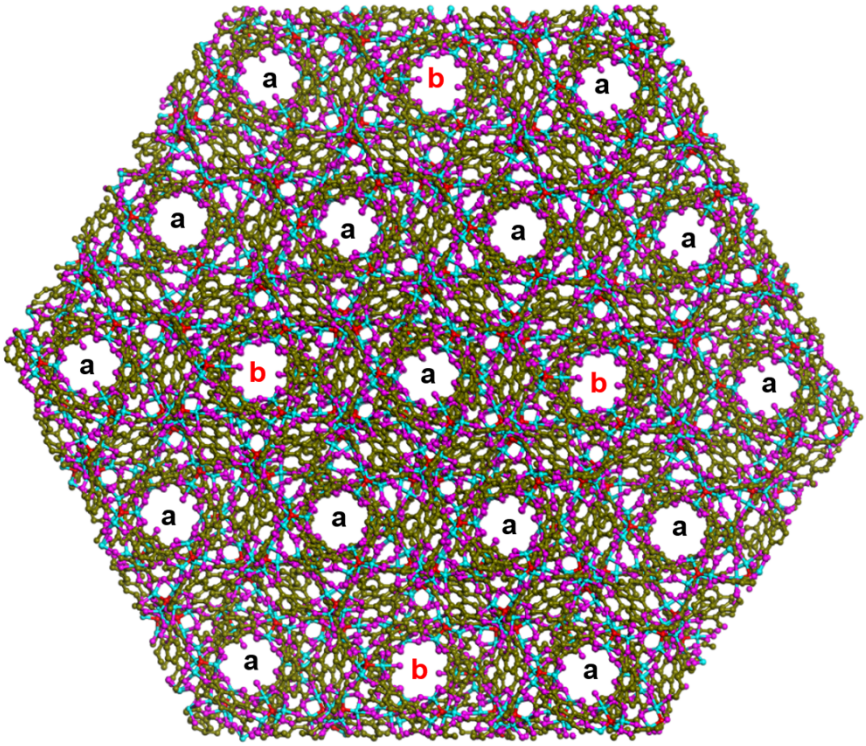
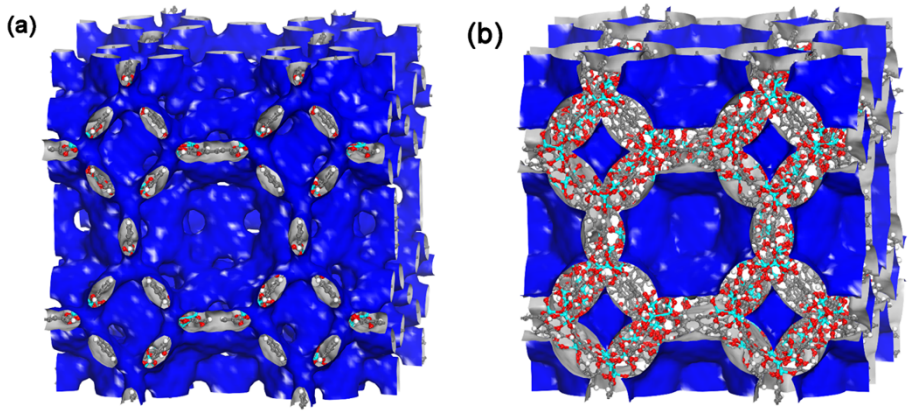


Figure S5. (a) Connolly surface area calculated with probe atomic radii of 1.4 Å, (b) the theoretical accessible surface area calculated with probe atomic radii of 1.84 Å.



	Occupied Volume (Å^3)	Free Volume (Å^3)	Surface Area (Å^2)
Connolly surface @1.4 Å	50472.45	95250.12	35806.59
Solvent Surface @1.84 Å	106434.05	39288.51	18013.18
Accessible Solvent Surface @1.84 Å	115329.41	30393.15	12141.93

Theoretical Porosity = Free Volume/ (Free Volume+ Occupied Volume)×100%

1 is therefore calculated to be 65.36 %.

Theoretical surface area = A. S. S (per unit cell)/ (D_c× Volume) × 10^4 m^2/g

The theoretical surface area of **1** is therefore calculated to be 881 m^2/g.

Figure S6. The components of 1 showing the abstraction of the (a) $Zn_4O(-CO_2)_7$ SBU as a distorted pentagonal bipyramid, (b) the ligand as two triangles, and (c) their assembly into a (3, 3, 7)- connected net

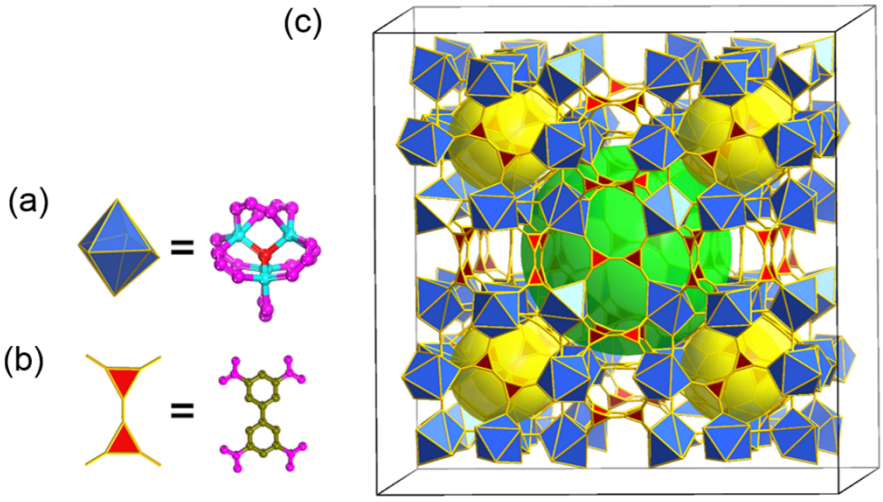


Figure S7. The TGA data of **1**: the first step weight loss (30 ~ 170 ^{o}C) could be attributed to the loss of the guest molecules; the second step weight loss (360 ~ 520 ^{o}C) corresponded to the collapse of the framework.

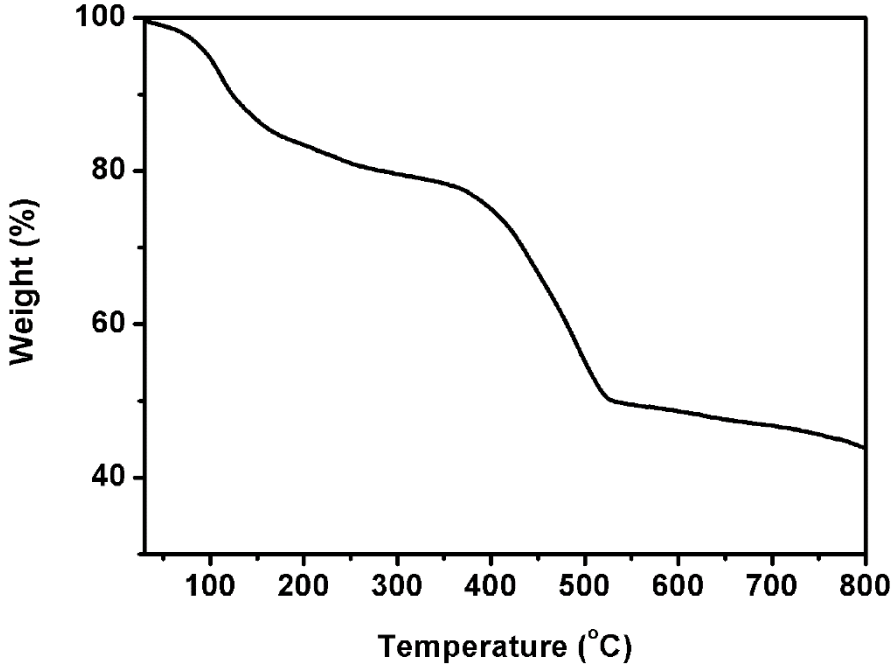


Figure S8. The PXRD pattern of **1** exposed in air for 8 hours compared with that of as-made sample showing the phase transformation.

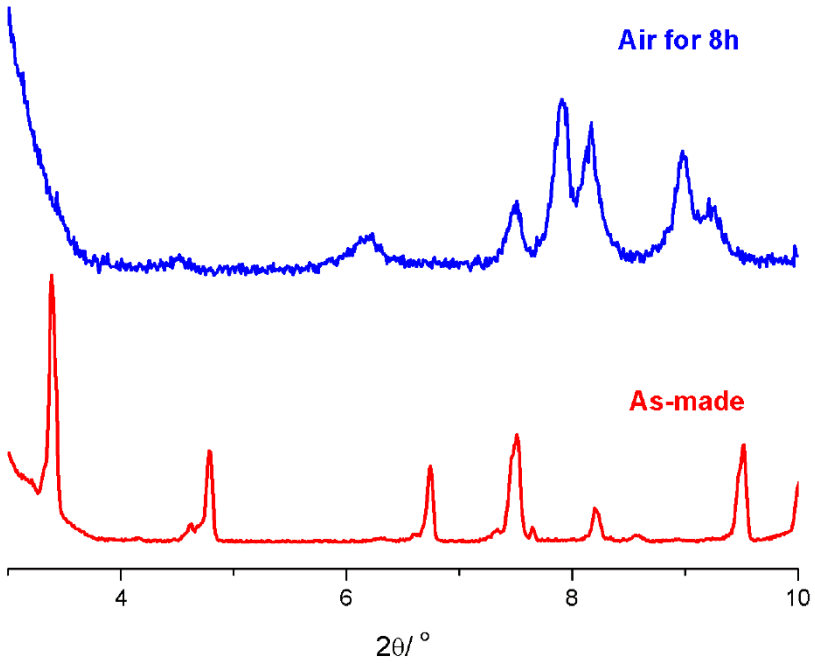
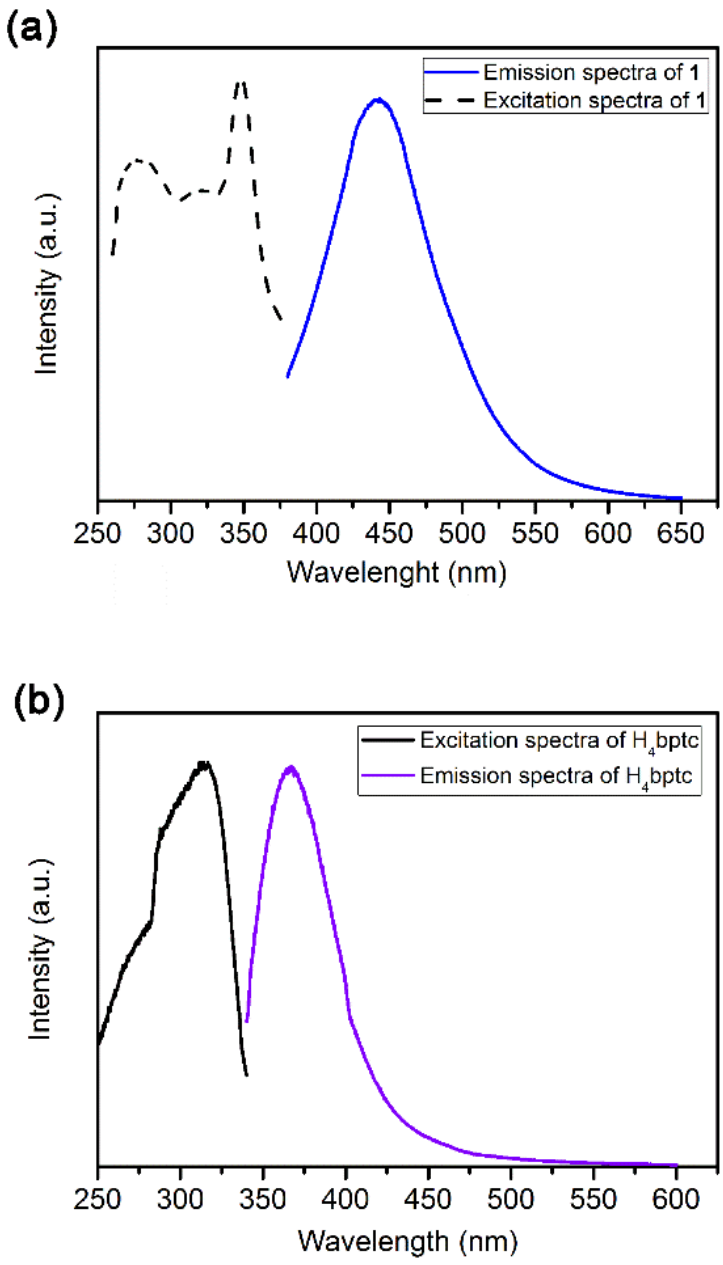


Figure S9. The photoluminescent spectra of (a) **1** and (b) the ligand.



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