Electronic Supplementary Material (ESI) for CrystEngComm

Metal-Organic Framework with Two Different Types of Rigid Triscarboxylates: Net Topology and Gas Sorption Behavior

Dongwook Kim and Myoung Soo Lah*

Interdisciplinary School of Green Energy, Ulsan National Institute of Science & Technology, Ulsan, 689-798, Korea. Fax: 82 52 217 2019; Tel: 82 52 217 2931; E-mail: mslah@unist.ac.kr

Table S1. Crystal data and structure refinement for **1**.

Empirical formula	$C_{23}H_{17}N_1O_{10}Zn_2$	
Formula weight	598.12	
Temperature	100(2) K	
Wavelength	0.67000 Å	
Crystal system	Cubic	
Space group	*Fd*-3*c*	
Unit cell dimensions	a = 62.779(7) Å	α = 90°
	b = 62.779(7) Å	β = 90°
	c = 62.779(7) Å	γ = 90°
Volume	247422(49) $Å^3$	
Z	192	
Density (calculated)	0.771 Mg/m^3	
Absorption coefficient	0.785 mm^{-1}	
F(000)	57984	
Crystal size	0.50 × 0.50 × 0.50 mm^3	
Theta range for data collection	1.22 to 24.00°	
Index ranges	-75<=h<=76, -75<=k<=76, -74<=l<=72	
Reflections collected	356572	
Independent reflections	9637 [R(int) = 0.0538]	
Completeness to theta = 24.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.6949 and 0.6949	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9637 / 0 / 298	
Goodness-of-fit on F^2	1.188	
Final R indices [I>2sigma(I)]	R1 = 0.0850, wR2 = 0.2807	
R indices (all data)	R1 = 0.1064, wR2 = 0.3095	
Largest diff. peak and hole	0.496 and –0.345 $e·Å^{-3}$	

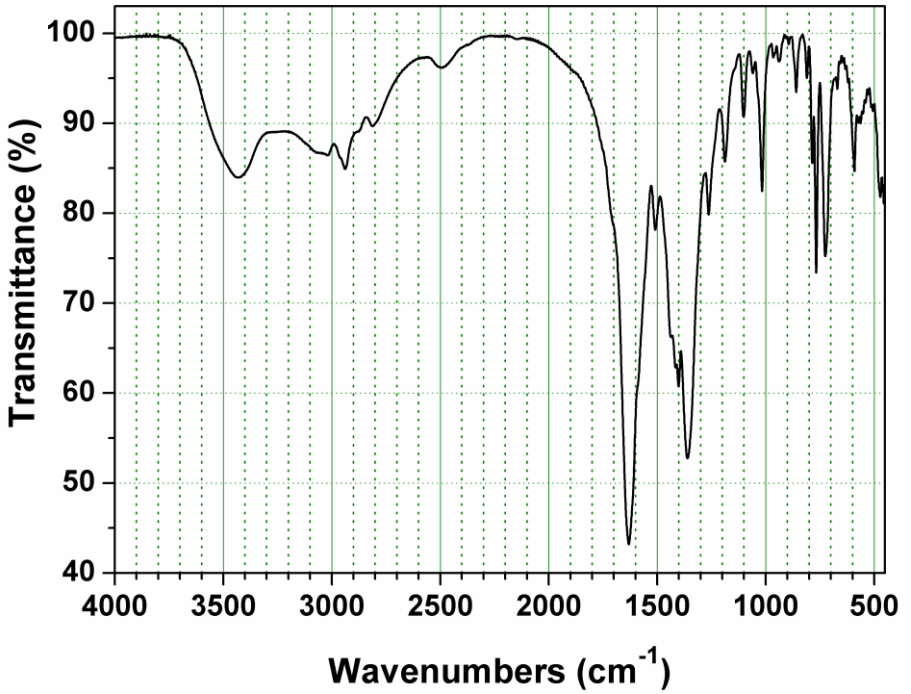

Figure S1. The IR spectrum of **1**.

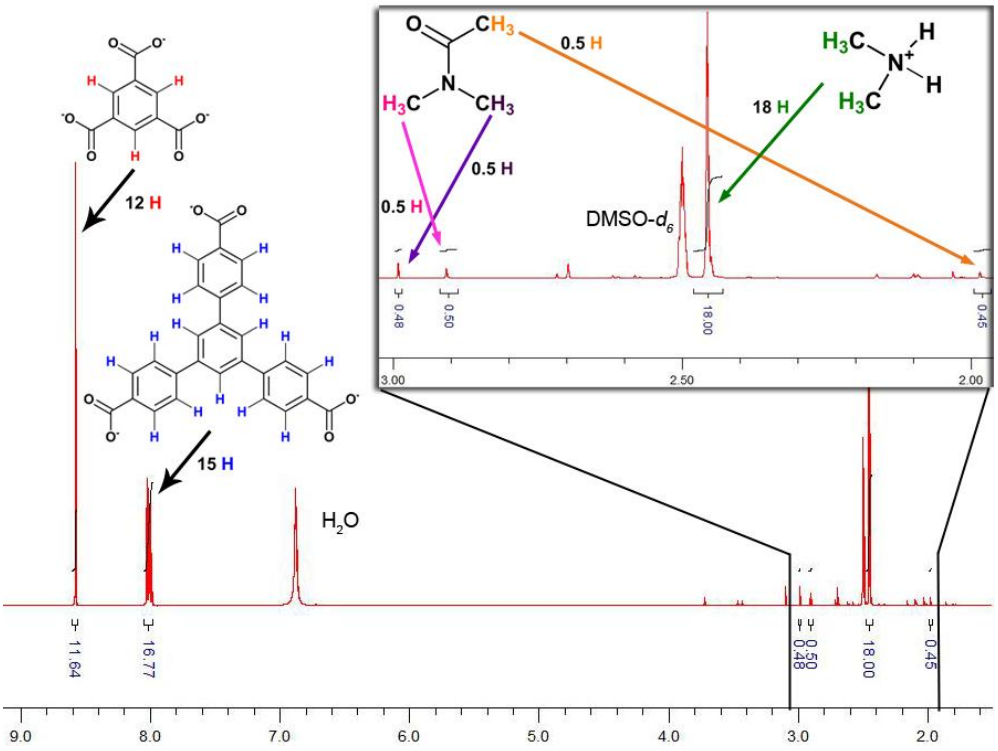

Figure S2. The ^{1}H NMR spectrum of **1a** digested in DCl/D_2O/dmso-d_6 solution.

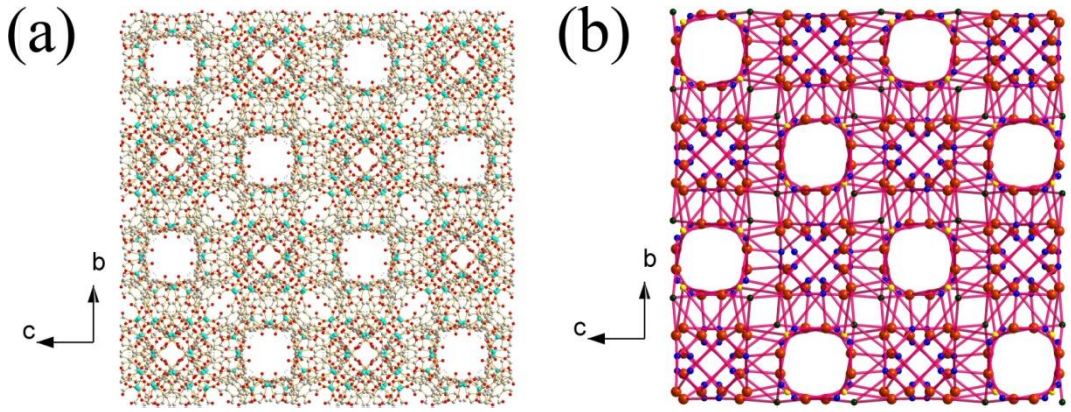

Figure S3. Ball-and-stick (a) and the corresponding network drawing (b) of **1** viewed along the crystallographic *a*-axis.

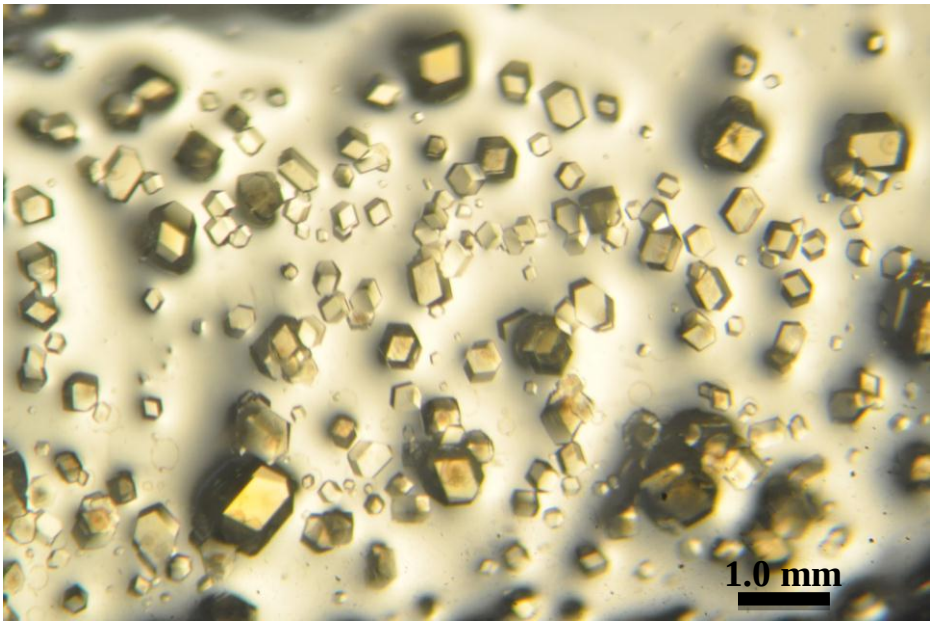

Figure S4. An optical microscopic photograph of the as-synthesized crystals of **1** in a capillary tube.

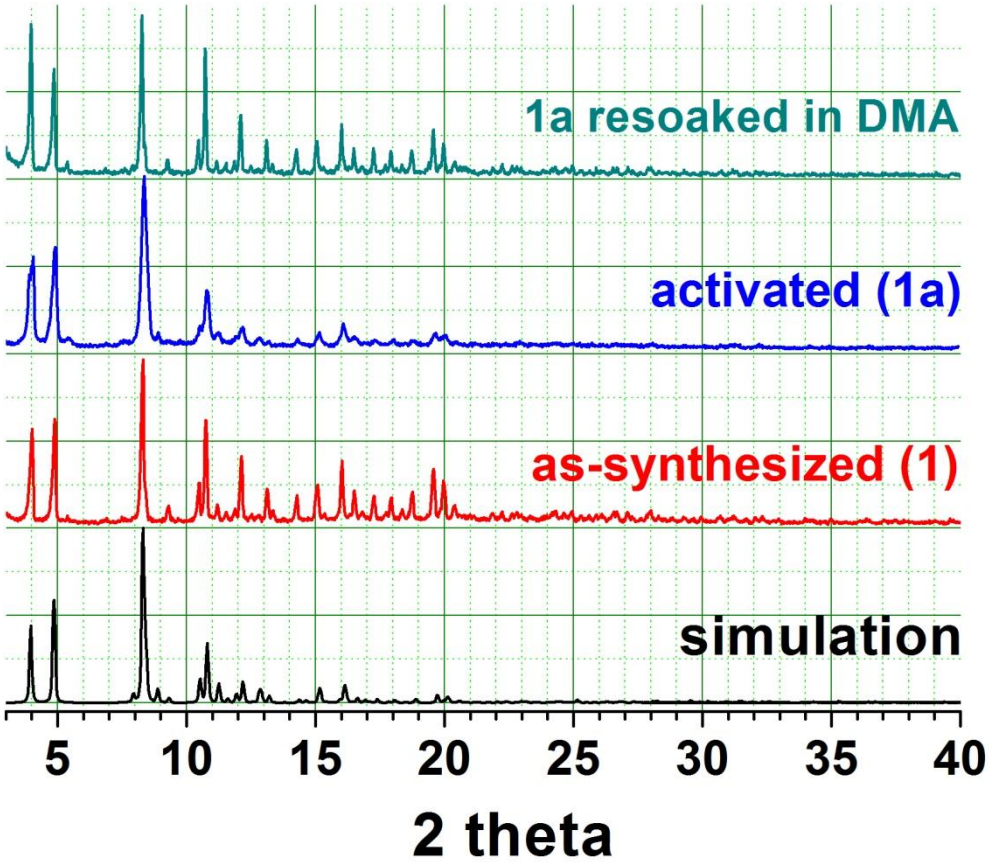

Figure S5. The PXRD patterns of **1**. (a) A simulation from the single crystal structure of **1** (black), (b) as-synthesized **1** (red), (c) activated **1a** (blue), and (d) **1a** resoaked in DMA (green).

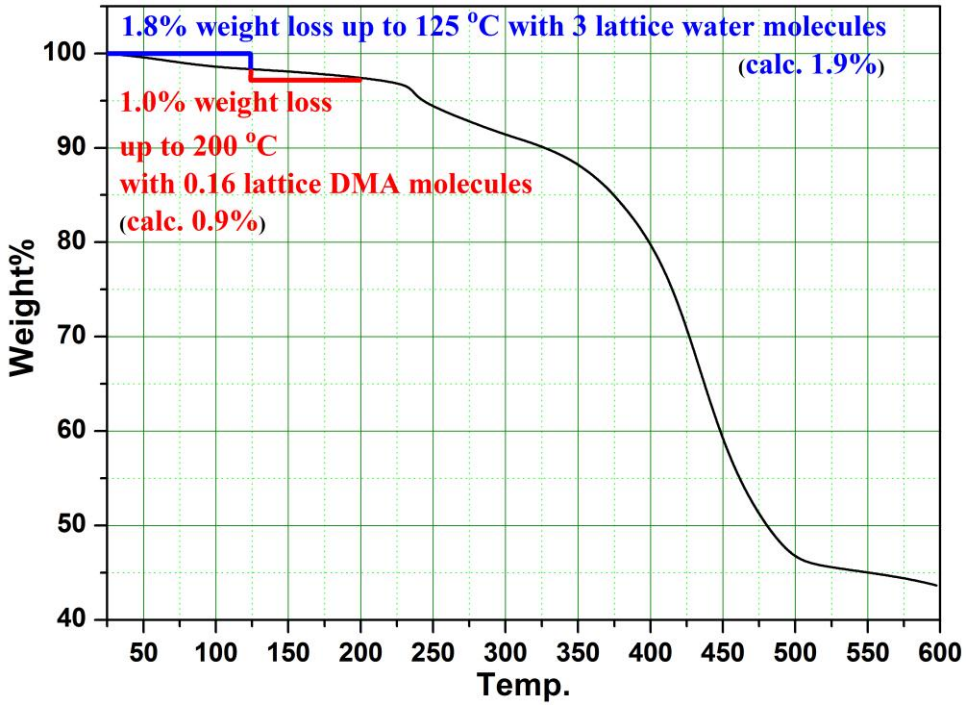

Figure S6. TGA of **1a**.

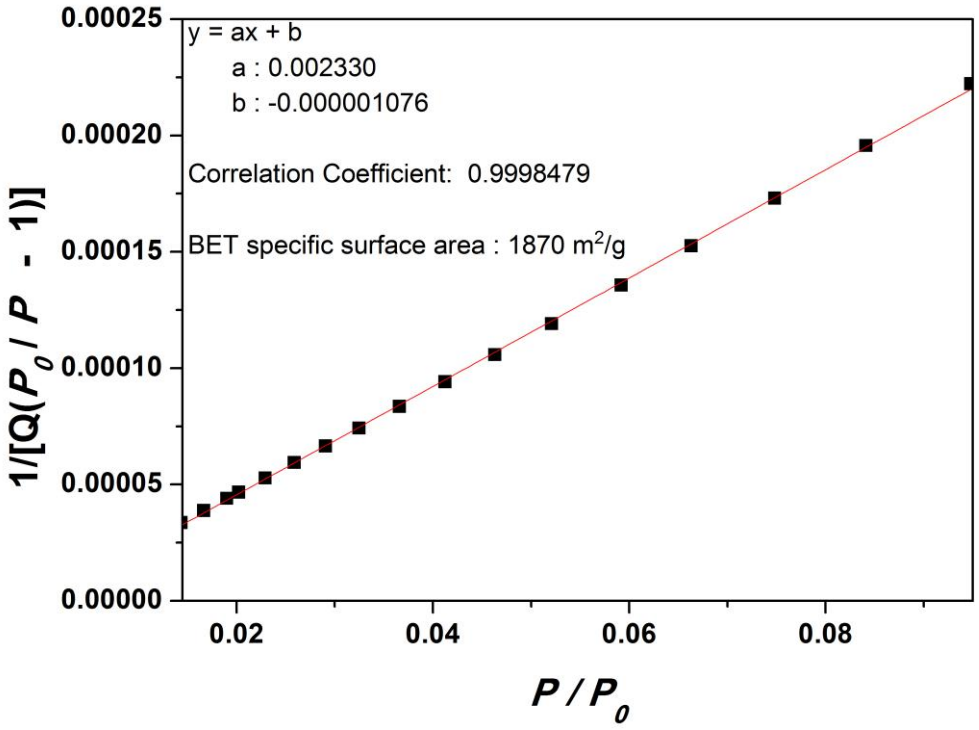

Figure S7. BET specific surface area from the N_2 adsorption isotherm on **1a** at 77 K.

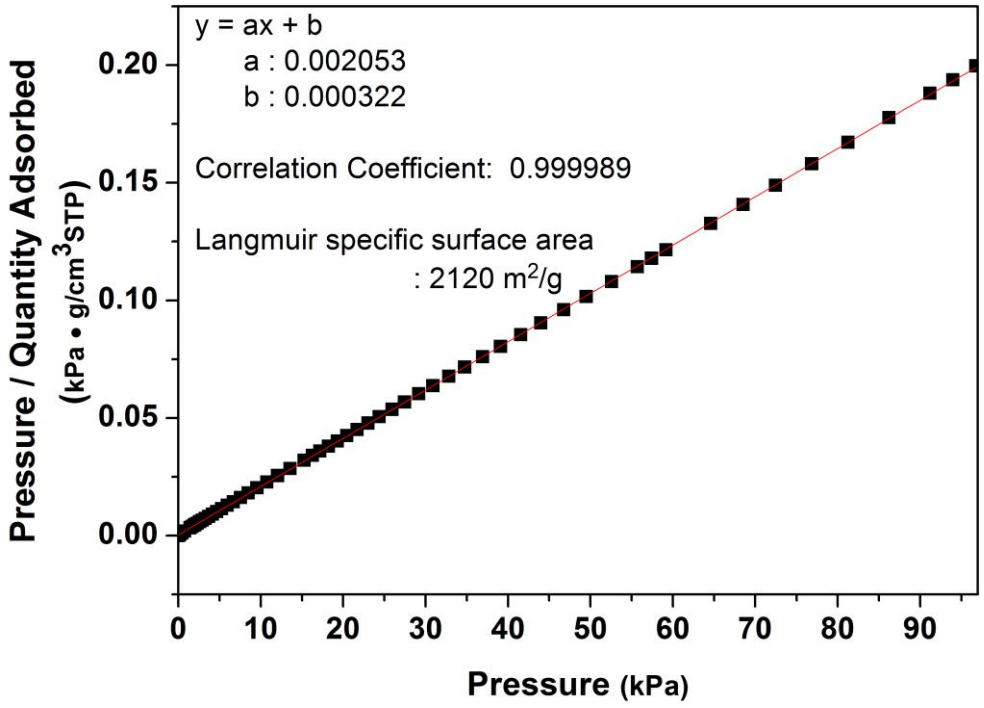

Figure S8. Langmuir specific surface area from the N_2 adsorption isotherm on **1a** at 77 K.