Supporting Information

Heterometallic Zn_6Ti_2 Building Block Persistent in Metal-organic Frameworks Based on Asymmetrically Substituted Dicarboxylate Ligands

Hyungphil Chun

Department of Applied Chemistry, College of Science and Technology, Hanyang University, Ansan 426-791, Korea
E-mail: hchun@hanyang.ac.kr
Received January 23, 2014, Accepted February 21, 2014

Table S1. Crystal data and summary of structure refinements.

Formula	$C_{45}\ H_{31}\ N\ O_{18}\ Ti\ Zn_3$
FW	1117.72
Temp (K)	100(2)
λ (Å)	0.80003
Crystal system	Monoclinic
Space group	$P2_1/c$
a (Å)	20.563(4)
a (Å)	18.543(4)
c (Å)	28.528(6)
β (°)	106.43(3)
V (Å^3)	10433(4)
Z	4
ρ_{calc} (g cm^{-3})	0.712
μ (mm^{-1})	1.088
F(000)	2256
Crystal size (mm^3)	0.08 × 0.06 × 0.06
θ range (°)	1.70 to 30.50
h, k, l ranges	$-25 \le h \le 25$, $-23 \le k \le 23$, $-36 \le l \le 36$
Reflections collected	77087
Independent (R_{int})	21970 (0.0394)
Completeness (%)	98.4
Absorption correction	Semi-empirical
T_{max} / T_{min}	0.9376 / 0.9180
Refinement method	Full-matrix least-squares on F^2
Data / restraints / param	21970 / 1 / 659
GOF on F^2	1.030
R_1, wR_2 [$I>2\sigma(I)$]	$R_1 = 0.0809$, $wR_2 = 0.2343$
R_1, wR_2 (all data)	$R_1 = 0.0895$, $wR_2 = 0.2443$
Extinction coefficient	0.0173(9)
Largest diff. peak / hole (e/Å^3)	1.138 / -1.684

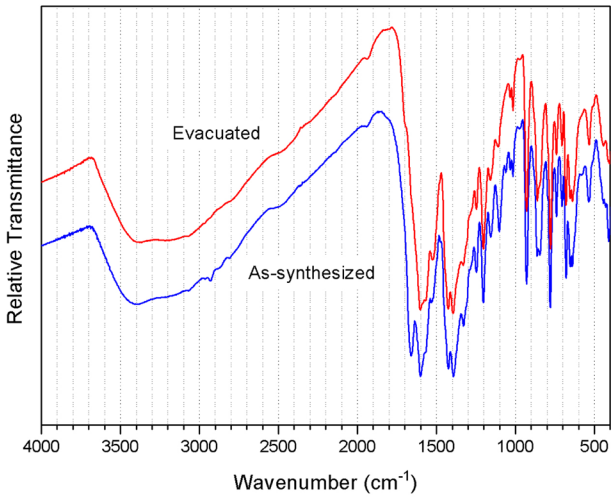

Figure S1. FT-IR spectra for as-synthesized and evacuated **1**.

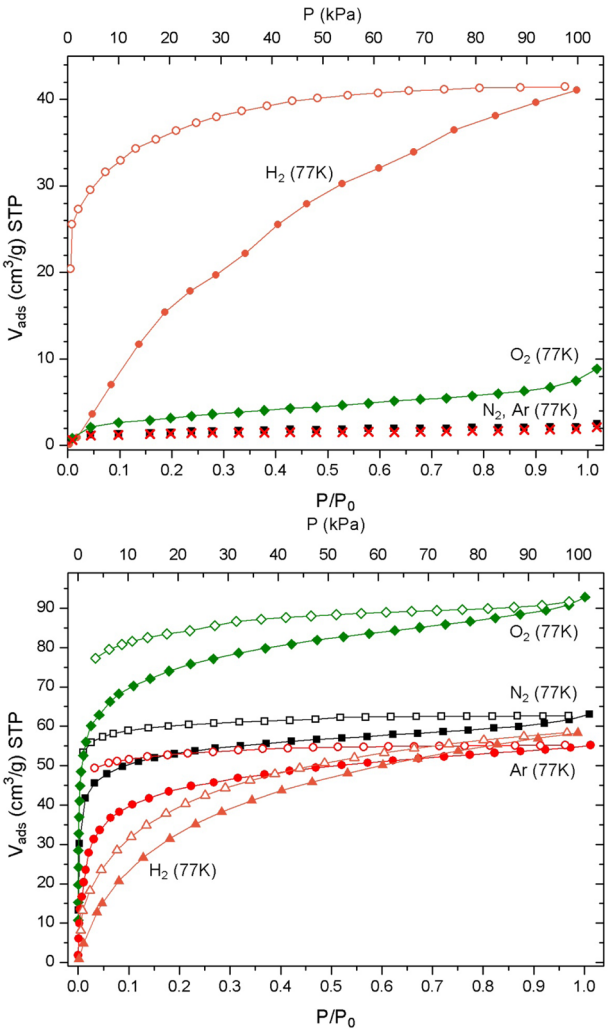

Figure S2. Complete gas sorption isotherms for **1** (top) and **1-Fe** (bottom).