Supporting Information

Synthesis, Structure Determination and Hydrogen Sorption Studies of New Metal-Organic Frameworks using Triazole and Naphthalenedicarboxylic Acid

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Table S1. Selected bond distances for Structure **1**

Bond	Length (Å)	Valence	Bond	Length (Å)	Valence
Zn1 – O2	1.912(19)	0.57	Zn2 – O3	1.982(14)	0.47
Zn1 – N1	2.060(17)	0.40	Zn2 – N3	1.997(15)	0.47
Zn1 – N9	1.969(17)	0.51	Zn2 – N6	1.998(16)	0.47
Zn1 – N12	1.989(16)	0.48	Zn2 – N7	2.062(17)	0.40
		$\Sigma s = 1.96$			$\Sigma s = 1.81$
Zn3 – O7	1.999(14)	0.45	Zn4 – O6	1.930(16)	0.54
Zn3 – N2	1.981(16)	0.49	Zn4 – N4	1.990(15)	0.48
Zn3 – N5	1.993(15)	0.48	Zn4 – N8	2.008(16)	0.46
Zn3 – N10	2.009(15)	0.46	Zn4 – N11	2.044(18)	0.42
		$\Sigma s = 1.88$			$\Sigma s = 1.90$

Table S2. Selected bond distances for Structure **2**

Bond	Length (Å)	Valence	Bond	Length (Å)	Valence
Zn1 – O2	1.992(10)	0.46	Zn2 – O6	1.960(13)	0.50
Zn1 – N1	1.994(15)	0.48	Zn2 – N2	2.010(15)	0.46
Zn1 – N6	2.036(13)	0.43	Zn2 – N4	2.004(12)	0.46
Zn1 – N11	1.967(12)	0.51	Zn2 – N9	1.996(14)	0.47
		Σs = 1.88			Σs = 1.90
Zn3 – O3	2.004(13)	0.44	Zn4 – O7	2.082(16)	0.36
Zn3 – O4	2.493(13)	0.12	Zn4 – O8	2.257(14)	0.22
Zn3 – N5	2.042(13)	0.42	Zn4 – O11	2.477(13)	0.12
Zn3 – N7	2.029(15)	0.43	Zn4 – N3	2.076(13)	0.38
Zn3 – N12	2.007(13)	0.46	Zn4 – N8	2.011(13)	0.46
			Zn4 – N10	2.071(14)	0.39
		Σs = 1.87			Σs = 1.93

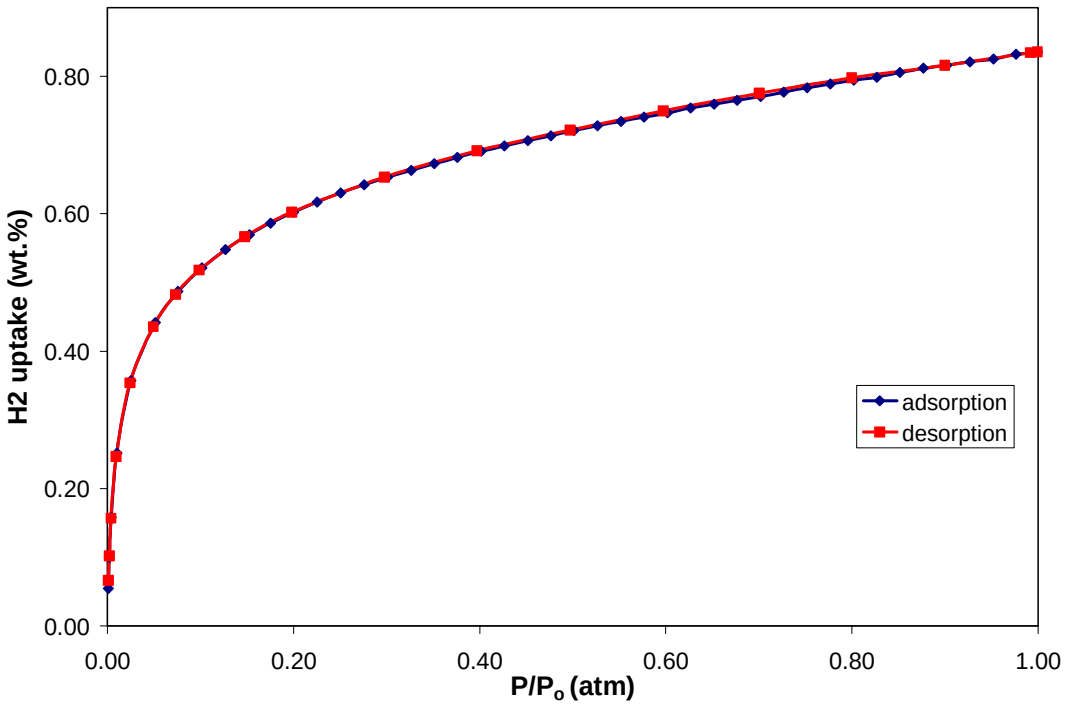

Figure S1. Hydrogen adsorption-desorption isotherm of structure **1**.

The maximum H_2 sorption capacity was estimated by using Langmuir equation (X. Lin, et al. *Angew. Chem. Int. Ed*. **2006**, 45, 7358).

$$\frac{P}{W} = \frac{1}{W_o}P + \frac{1}{W_oK}$$

W = degree of adsorption at a pressure P
W_o = saturated adsorption
K = constant

The linear regression analysis of the P/W vs. P plot was carried out, then the maximum uptake (W_o) can be determined (W_o = 1/slope).

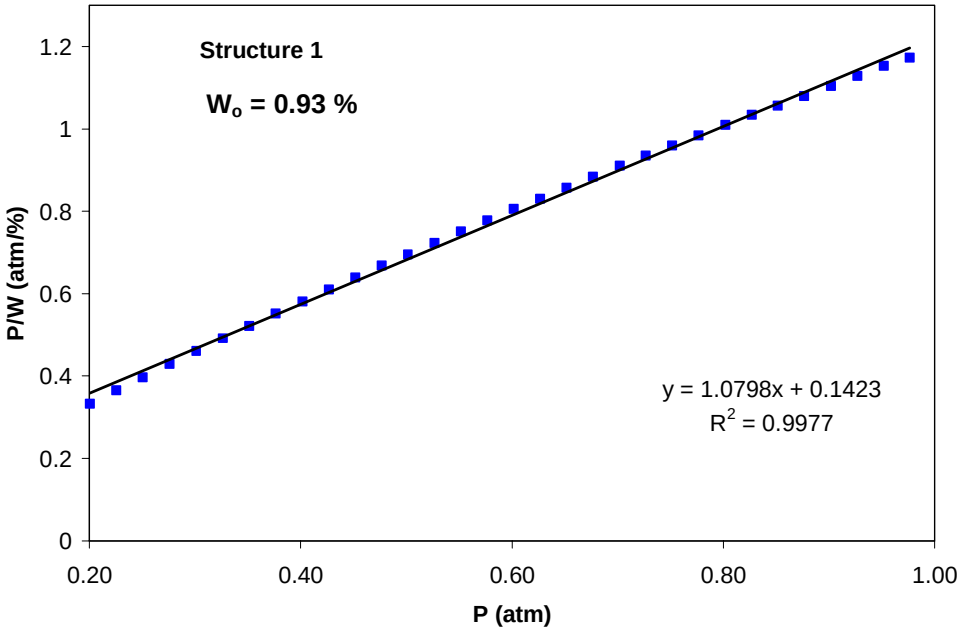

Figure S2. Langmuir fitting of H_2 adsorption of structure **1**.

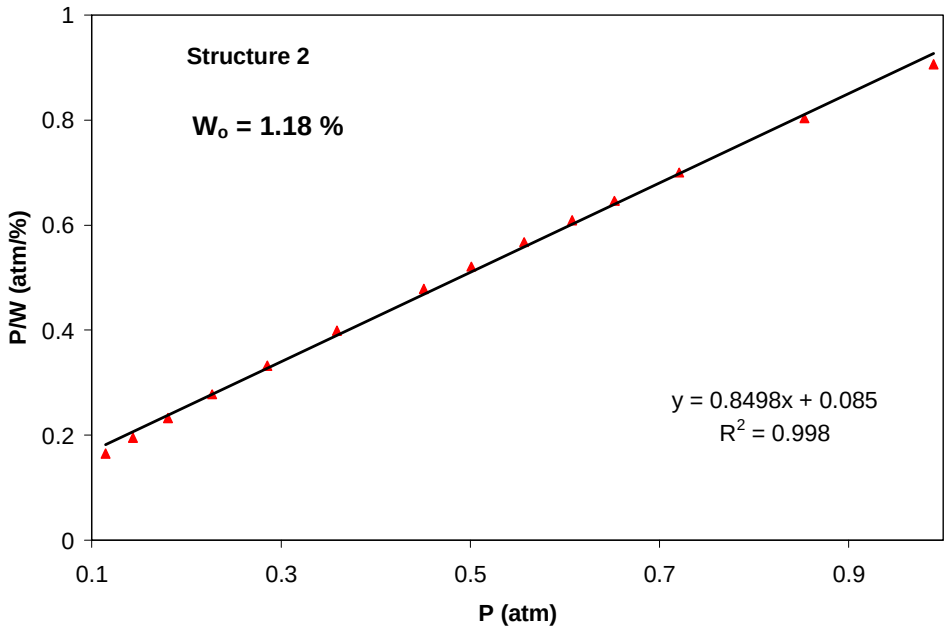

Figure S3. Langmuir fitting of H_2 adsorption of structure **2**.

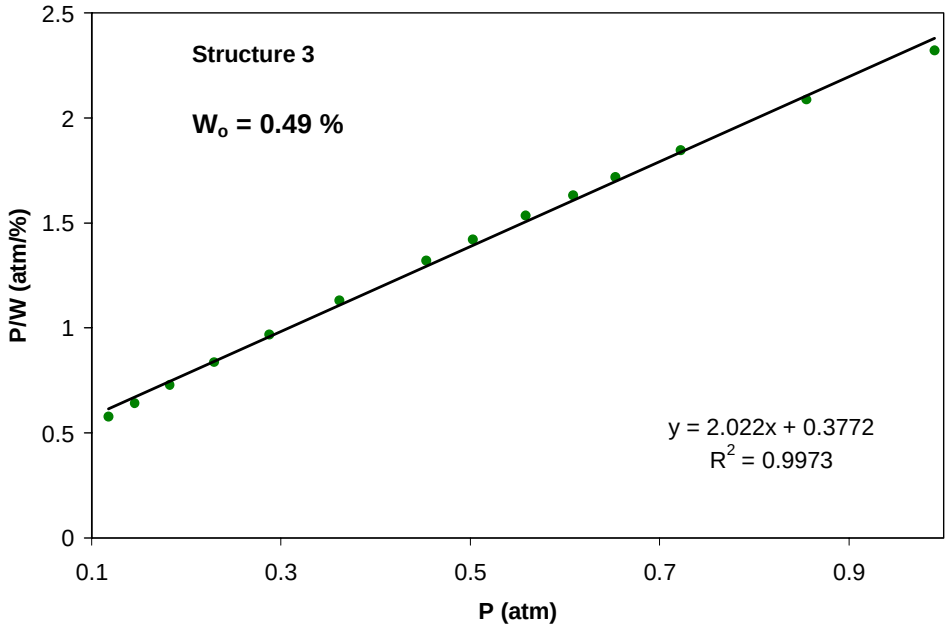

Figure S4. Langmuir fitting of H_2 adsorption of structure **3**.