Electronic Supplementary Information

A 2D Metal-thiacalix[4]arene Porous Coordination Polymer with 1D Channels: Gas Absorption/Separation and Frequency Response

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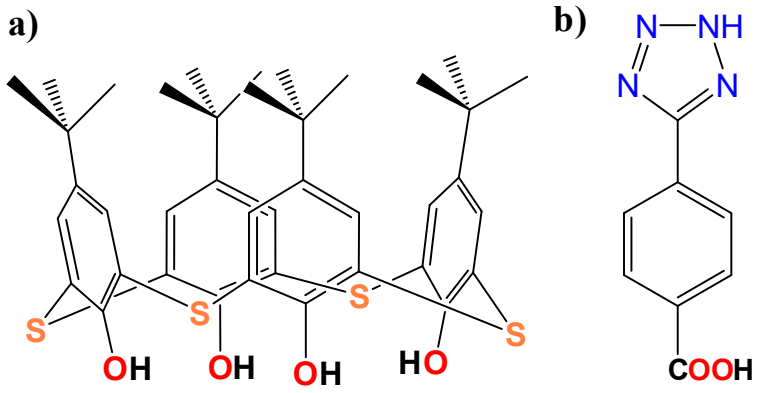

H_4TC4A **H_2L**

Scheme S1. (a) *p-tert*-Butylthiacalix[4]arene (H_4TC4A); (b) 4-(2H-tetrazol-5-yl)benzoic acid (H_2L).

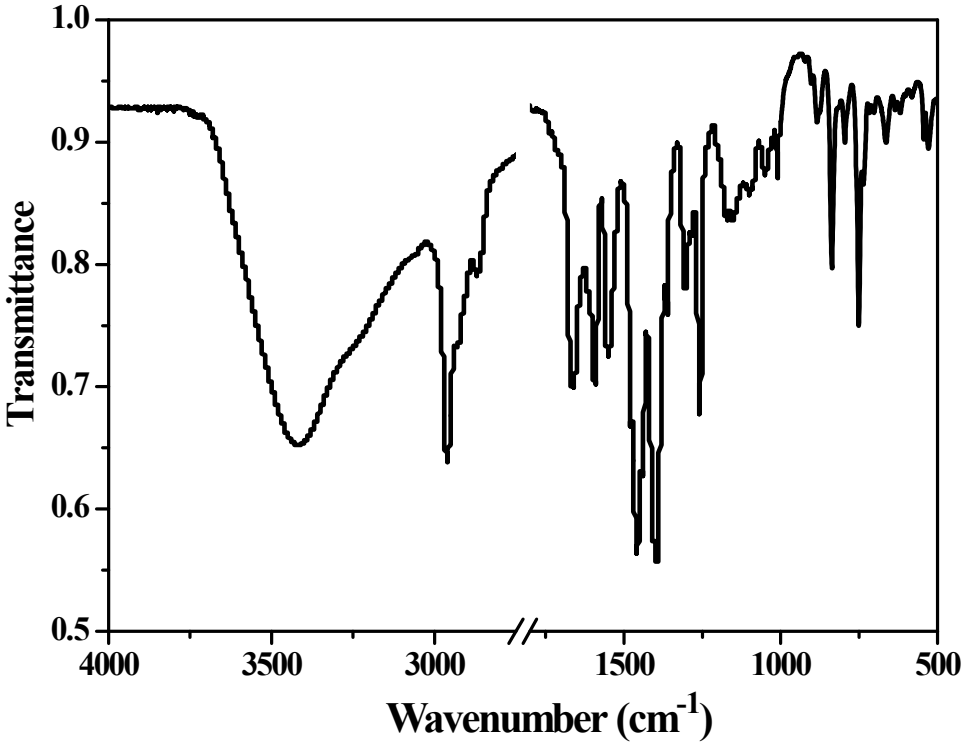

Fig. S1 FT-IR spectra of **1**

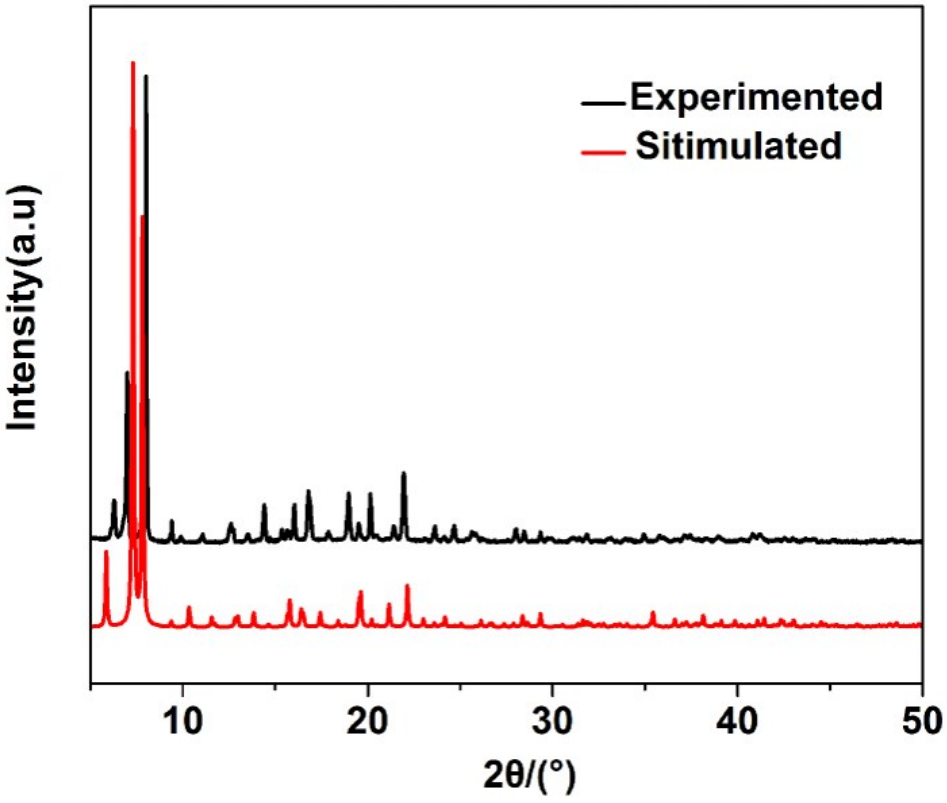

Fig. S2 PXRD patterns of **1**

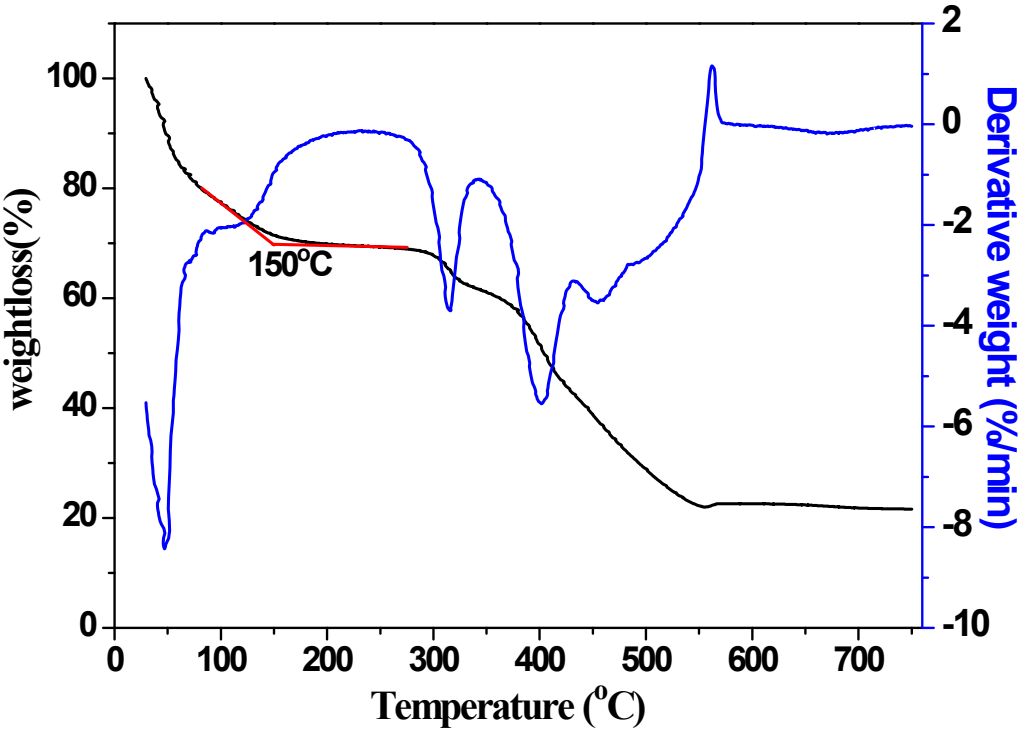

Fig. S3 TGA experiment of **1**

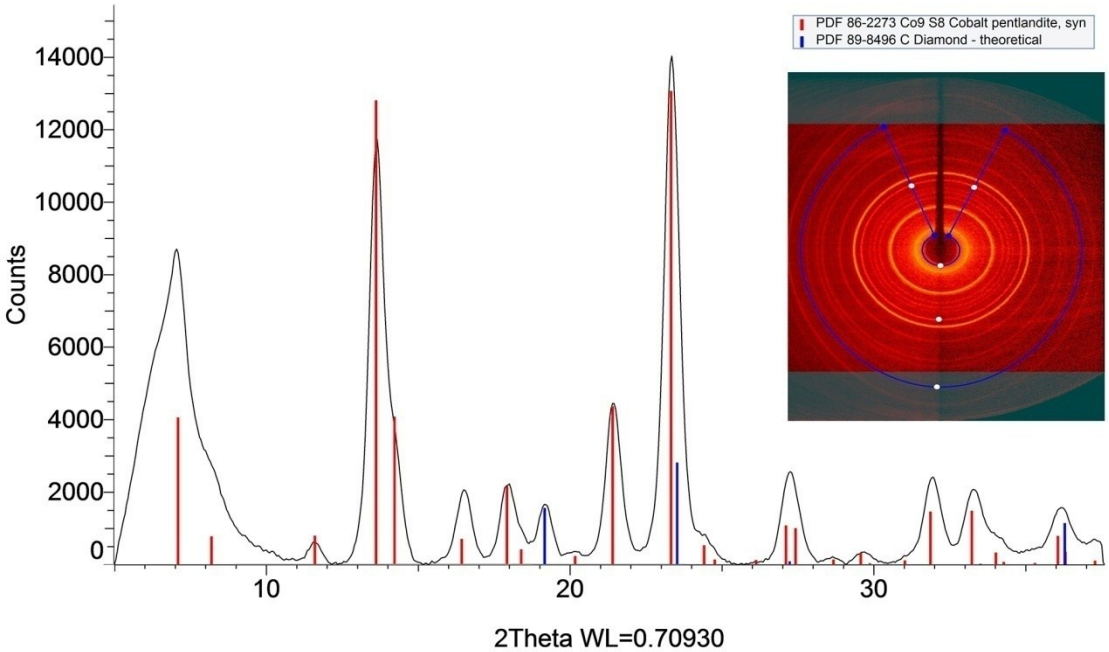

Fig. S4 PXRD analysis of residue after thermogravimetry measurement for **1**

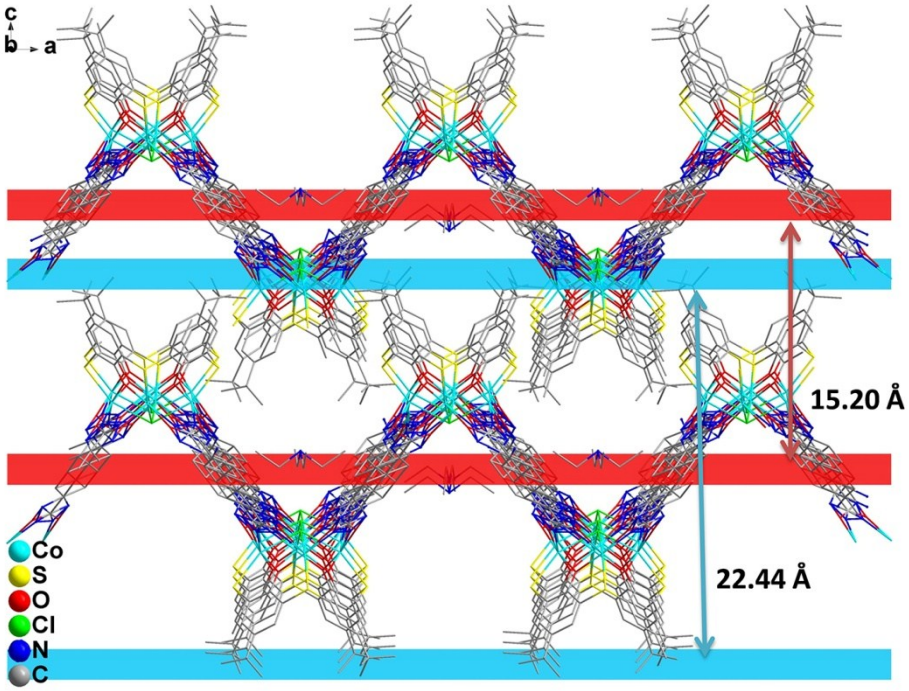

Fig. S5 Representation of the thickness of the layers and the centre distance between adjacent two layer.

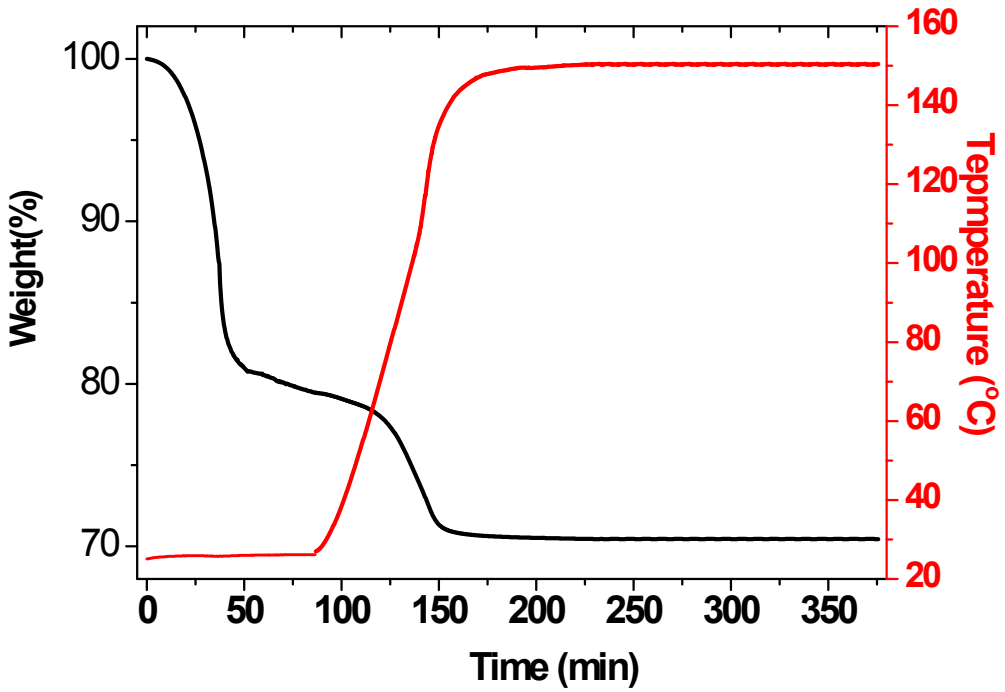

Fig. S6 Temperature programmed desorption (TPD, heating rate 3 °C/min, in vacuum for 90min, maintained at 150 °C for 220 min) of **1**.

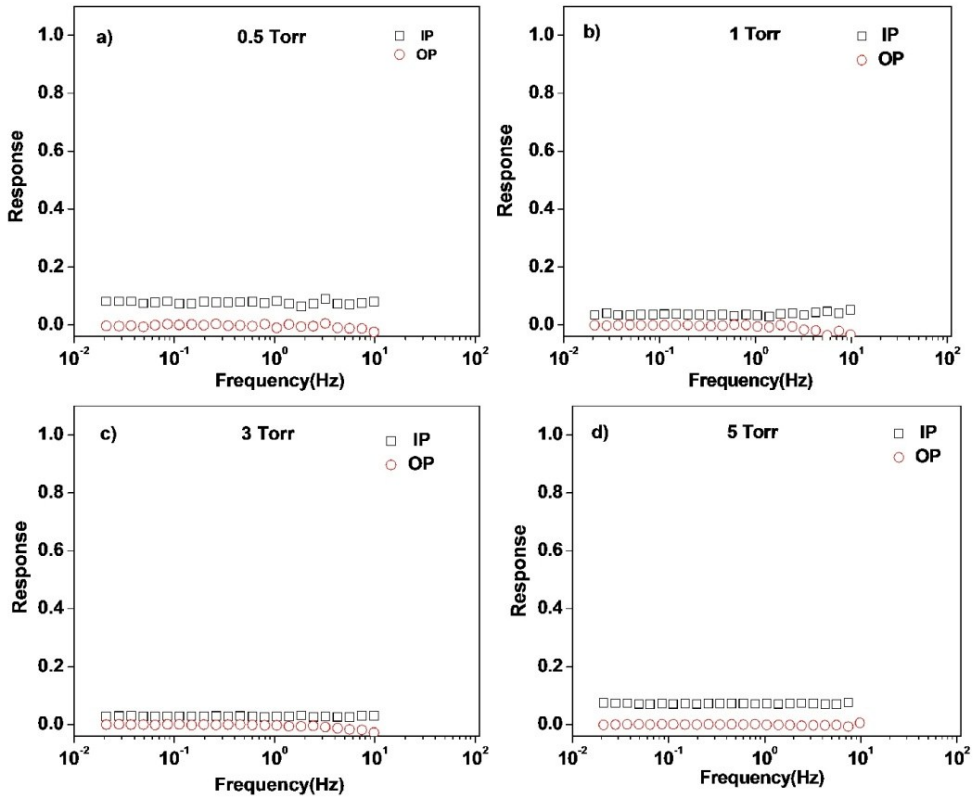

Fig. S7 Frequency response (FR) spectra of C_2H_6 for **1'** at different pressure (0.5, 1, 3, 5 Torr) at 273K, 0–100Hz.

Table S1 Crystal data and structural refinement parameters for **1**

Formula	$C_{83}H_{118}ClCo_4N_{15}O_{15}S_4$
Mr	1965.33
Crystal system	tetragonal
space group	$P42_12$ (No.90)
Temperature (K)	150
a(Å)	17.0886(5)
b(Å)	17.0886(5)
c(Å)	15.0638(5)
α(°)	90
β(°)	90
γ(°)	90
Volume(Å^3)	4398.9(3)
Z	2
D_c(g/cm^3)	1.484
μ(mm^{-1})	0.939
Reflections collected	46014
Unique data(R_{int})	3888
GOF on F^2	1.08
R_1 [I>2sigma(I)]	0.0377
wR_2	0.1061

$^aR_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$; $^bwR_2 = \{\Sigma[w(F_0^2-F_c^2)^2]/\Sigma[w(F_0^2)^2]\}^{1/2}$*

Table S2 Selected bond lengths (Å) for **1**

Co(1)-O(1)	1.994(3)
Co(1)-O(2)2#	2.025(10)
Co(1)-N(3)	2.135(13)
Co(1)-N(4)#1	2.097(12)
Co(1)-S(1))#1	2.5450(14)
Co(1)-Cl(1)	2.5973(12)
Co(1)-O(1)#1	2.002(3)
Co(1)-O(3) 3#	2.019(11)
Co(1)-N(4)4#	2.097(12)

#1: -1/2+y,3/2-x,z; #2: y,x,-z; #3: -1/2+x,3/2-y,-z; #4: -1/2+y,3/2-x,z.