Electronic supplementary information (ESI)

Dynamic porous metal-organic frameworks: synthesis, structure and sorption property

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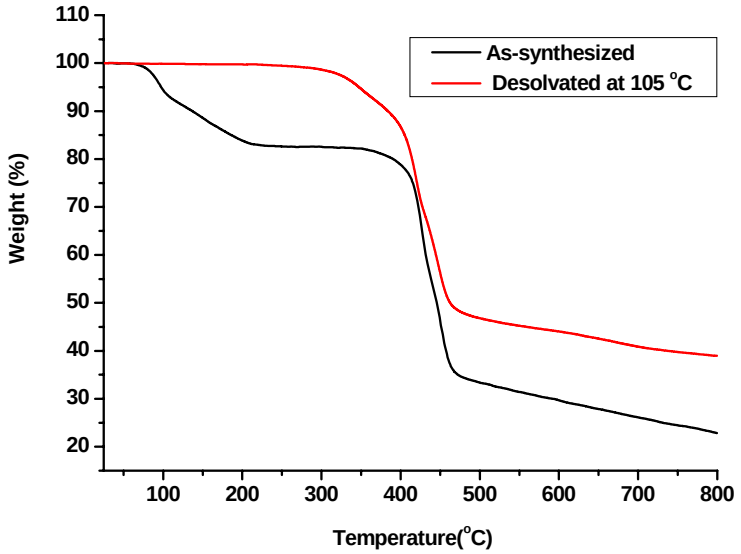
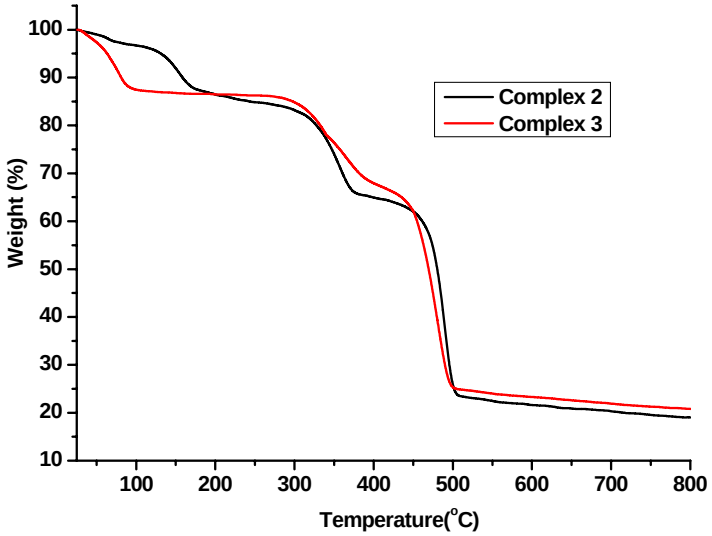


(a)



(b)

Figure S1. TGA curves for complex **1** (a), complexes **2** and **3** (b).

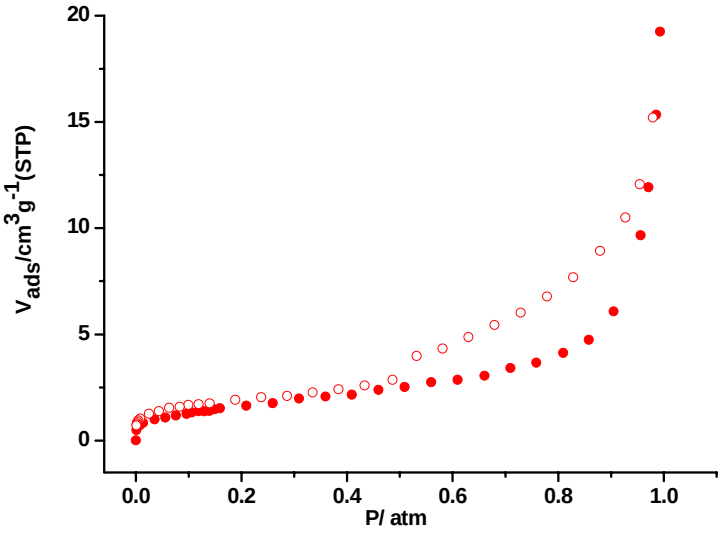
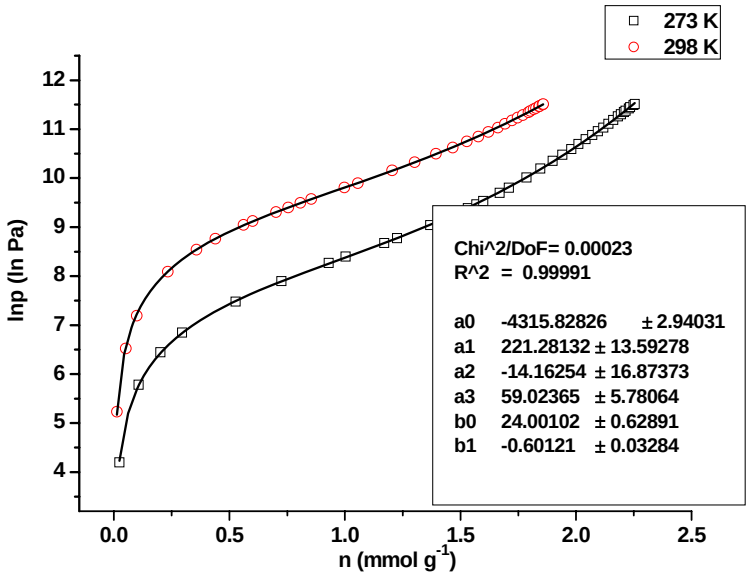
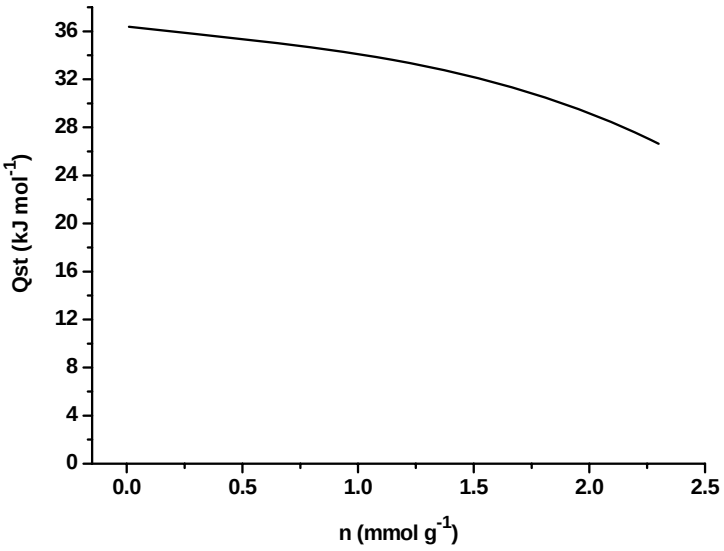


Figure S2. N_2 adsorption isotherms for desolvated **1** at 77 K: filled shape, adsorption; open shape, desorption.



(a)



(b)

Figure S3. (a) The calculated virial equation isotherms parameters fit to the experimental CO_2 data of desolvated **1**. (b) The isosteric adsorption enthalpy for desolvated **1**.

Estimation of the isosteric heats of gas adsorption

A virial-type [1] expression comprising the temperature-independent parameters a_i and b_i was employed to calculate the enthalpies of adsorption for CO_2 (at 273 and 298 K) on desolvated **1**. In each case, the data were fitted using the equation:

$$\ln P = \ln N + 1/T \sum_{i=0}^{m} a_i N^i + \sum_{j=0}^{n} b_j N^j$$

Here, P is the pressure expressed in Pa, N is the amount adsorbed in mmol g^{-1}, T is the temperature in K, a_i and b_j are virial coefficients, and m, n represent the number of coefficients required to adequately describe the isotherms (m and n were gradually increased until the contribution of extra added a and b coefficients was deemed to be statistically insignificant towards the overall fit, and the average value of the squared deviations from the experimental values was minimized). The values of the virial coefficients a_0 through a_m were then used to calculate the isosteric heat of adsorption using the following expression.

$$Q_{st} = -R \sum_{i=0}^{m} a_i N^j$$

Q_{st} is the coverage-dependent isosteric heat of adsorption and R is the universal gas constant.

[1] Rowsell, J. L. C.; Yaghi, O. M. *J. Am. Chem. Soc.* **2006**, *128*, 1304.

Indexing result of the powder pattern of the desolvated solid of 1

*** CONVENTIONAL CELL (METRIC SYMMETRY) ***

MONOCLINIC P

a = 19.902(24), b = 6.412(8), c = 12.645(10) Å

α = 90.00, β = 118.12(5), γ = 90.00 °; V = 1423.30 Å^3

H	K	L	SST-OBS	SST-CALC	DELTA	2TH-OBS	2TH-CALC	D-OBS
-1	0	1	0.003836	0.003839	-0.000003	7.102	7.105	12.4365
-2	0	1	0.006753	0.006760	-0.000007	9.427	9.432	9.3737
2	0	0	0.007744	0.007703	0.000042	10.097	10.070	8.7530
0	1	0	0.014375	0.014431	-0.000056	13.772	13.799	6.4246
-1	0	2		0.015292			14.207	
-2	0	2	0.015345	0.015356	-0.000011	14.232	14.237	6.2182
0	0	2		0.019079			15.879	
0	1	1	0.019214	0.019200	0.000014	15.935	15.930	5.5570
-3	0	2		0.019272			15.959	
-2	1	1	0.021253	0.021190	0.000063	16.765	16.740	5.2837
1	1	1		0.023982			17.818	
-4	0	1	0.024153	0.024155	-0.000001	17.882	17.882	4.9563
-4	0	2	0.027011	0.027038	-0.000028	18.919	18.929	4.6869
-3	0	3	0.034561	0.034552	0.000010	21.428	21.425	4.1434
2	1	2	0.052631	0.052638	-0.000007	26.525	26.527	3.3576
-5	1	1	0.052862	0.053059	-0.000197	26.585	26.635	3.3502
-5	1	2		0.053087			26.642	
-2	0	4		0.061169			28.638	
-4	0	4	0.061379	0.061425	-0.000046	28.689	28.700	3.1091
4	1	1		0.061436			28.702	
-1	2	1		0.061561			28.732	

NUMBER OF OBS. LINES = 13

NUMBER OF CALC. LINES = 21

M(13)= 13 AV.EPS.= 0.0000372

F 13 = 16.(0.013383, 62)

M CF. J.APPL.CRYST. 1(1968)108

F CF. J.APPL.CRYST. 12(1979)60

0 LINES ARE UNINDEXED

M-TEST= 13 UNINDEXED IN THE TEST= 0