Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Supplementary Information for the paper

Sieving di-branched from mono-branched and linear alkanes with ZIF-8: Experimental proof and theoretical explanation

Alexandre F. P. Ferreira[a], Marjo C. Mittelmeijer-Hazeleger[b], Miguel A. Granato[a], Vanessa F. D. Martins[a], Alírio E. Rodrigues[a], Gadi Rothenberg*[b]

[a] *Laboratory of Separation and Reaction Engineering, Associate Laboratory LSRE/LCM, Department of Chemical Engineering, Faculty of Engineering, University of Porto, Rua Dr. Roberto Frias, Porto, Portugal*

[b] *Van 't Hoff Institute for Molecular Sciences, University of Amsterdam, Science Park 904, Amsterdam, The Netherlands*

Table S1: Equilibration times of *n*-hexane, on ZIF-8 sample, at 373 K.

No.Ads	P_{eq} (kPa)	T_{eq} (h)
1	0.09	1.89
2	0.18	1.86
3	0.26	2.03
4	0.35	2.03
5	0.45	2.23
6	0.55	2.20
7	0.64	2.36
8	0.74	2.53
9	0.83	2.56
10	0.94	2.70
11	1.04	2.86
12	1.28	3.36
13	1.54	3.72
14	1.80	3.86
15	2.12	4.03
16	2.47	4.19
17	2.96	4.53
18	3.50	4.52
19	4.27	4.55
20	5.33	4.36
21	6.53	4.19
22	8.07	4.03
23	9.60	3.69
24	11.41	3.71
25	20.91	3.87
26	30.37	2.53
27	41.15	2.03
28	51.52	1.86
29	60.81	1.86
30	72.18	2.03
31	81.20	2.03
32	89.21	2.61
33	96.58	3.20
34	102.45	2.53
35	107.98	2.70

Table S2: Equilibration times of 2-methylpentane, on ZIF-8 sample, at 373 K.

No.Ads	P_{eq} (kPa)	T_{eq} (h)
1	0.23	3.04
2	0.42	3.88
3	0.61	4.38
4	0.78	4.71
5	0.95	4.88
6	1.11	5.22
7	1.58	9.37
8	2.03	10.53
9	2.53	11.69
10	3.05	12.36
11	3.64	13.87
12	4.30	13.37
13	5.07	14.71
14	6.00	14.02
15	7.11	13.21
16	8.51	8.40
17	9.87	2.36
18	17.47	7.03
19	26.99	5.62
20	36.86	11.25
21	46.30	9.25
22	57.81	14.28
23	69.10	11.67
24	79.97	16.72
25	90.64	13.90

Table S3: Equilibration times of 2,3-dimethylbutane, on ZIF-8 sample, at 373 K.

No.Ads	Pe (i)	T_{eq} (h)
1	0.54	2.52
2	1.05	4.19
3	1.54	5.86
4	1.97	6.87
5	2.42	8.23
6	2.85	8.70
7	3.24	8.19
8	3.66	9.57
9	4.05	9.54
10	4.44	9.71
11	4.81	8.36
12	5.22	10.36
13	5.60	8.19
14	5.97	10.20
15	6.32	8.52
16	7.11	18.36
17	7.95	17.86
18	8.78	17.03
19	9.68	21.52
20	11.30	25.87
21	21.48	15.83
22	29.50	23.42
23	39.40	14.43
24	47.26	15.62
25	56.49	14.23
26	65.72	16.03
27	75.07	12.83
28	84.47	8.82
29	93.60	5.63
30	102.71	10.03

Table S4: Equilibration times of 2,2-dimethylbutane, on ZIF-8 sample, at 373 K.

No.Ads	Pe (i)	T_{eq} (h)
1	0.78	2.22
2	1.46	2.41
3	4.04	4.05
4	6.32	2.89
5	8.91	2.74
6	11.15	2.22
7	24.21	2.44
8	36.74	2.25
9	47.33	2.25
10	59.07	4.83
11	70.10	2.43
12	81.12	3.83
13	91.07	3.63
14	100.54	3.63
15	108.96	3.43

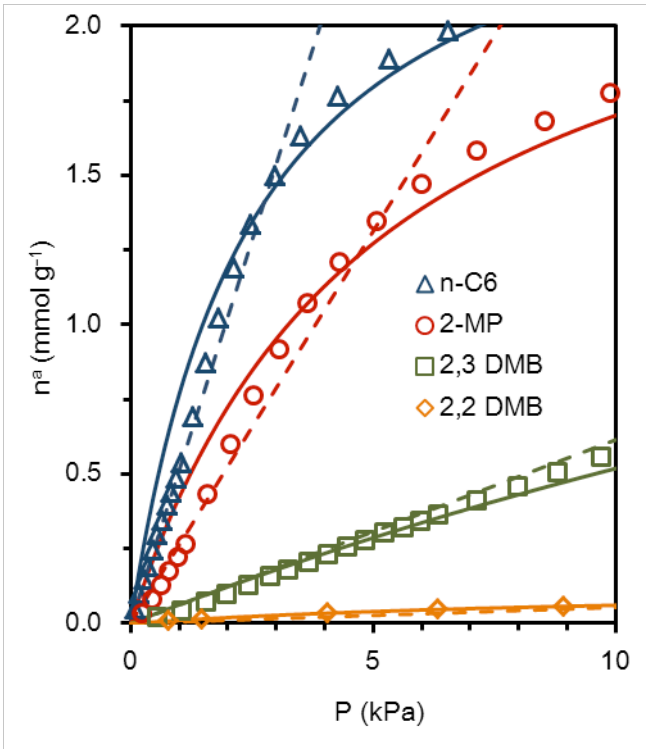

Fig. S1 - Hexane isomers adsorption isotherms, on ZIF-8, at 373 K: △ n-hexane, ○ 2-methylpentane, □ 2,3-dimethylbutane, and ◇ 2,2-dimethylbutane. Full lines are the isotherm model fits by Langmuir model (eq. 1); dashed lines are the isotherms fits by Henry Law model (eq. 2).

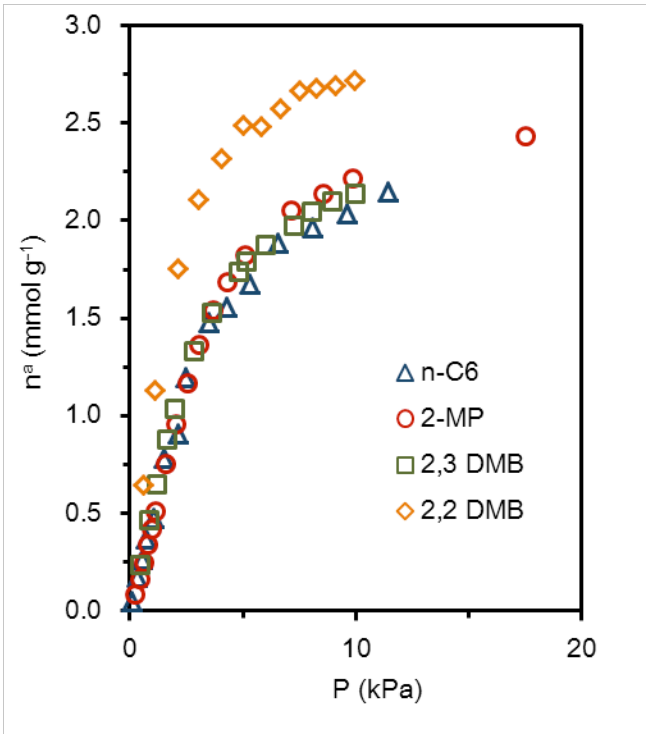

Fig. S2 - Molecular Simulation of the hexane isomers adsorption isotherms, without blocking, on ZIF-8, at 373 K: △ n-hexane, ○ 2-methylpentane, □ 2,3-dimethylbutane, and ◇ 2,2-dimethylbutane. Zoom of **Figure 7a**.

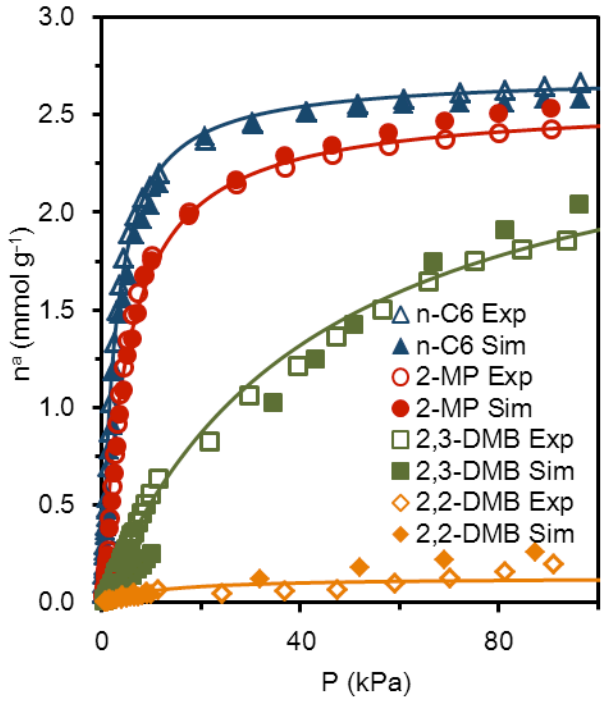

Fig. S3 - Comparison between Experimental and Molecular Simulation hexane isomers adsorption isotherms, on ZIF-8, at 373 K: △ n-hexane, ○ 2-methylpentane, □ 2,3-dimethylbutane, and ◇ 2,2-dimethylbutane.

Fig. S4 - Photograph of the experimental Set-Up: a) the volumetric introduction system, b) micro-calorimeter in a thermostatic oven, and c) general over view of the connection between the two parts of the experimental system.