Supplementary Information for:

Confined phase behavior of subcritical carbon dioxide in nanoporous media: The effects of pore size and temperature

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1. Nitrogen Sorption analysis:

Figures S1 and **S2** show the experimentally measured nitrogen adsorption and desorption isotherms using samples of MCM-41 with pore sizes of 6 and 10 nm. It is evident from the results that condensation and evaporation of nitrogen followed different paths, i.e., exhibiting the adsorption-desorption hysteresis in a specific range of relative pressures. The isotherms measured with 6 nm pores were completely reversible up to a relative pressure of approximately 0.40. The hysteresis loop started precisely at this relative pressure and continued up to 0.70. The capillary-induced condensation and evaporation occurred in this range during adsorption and desorption. The results demonstrate that the processes of adsorption, isothermal compression and decompression, and bulk phase transition all produce reversible behavior below and above this pressure range. Similar trends are observed in the case of the larger pore diameter of 10 nm, where the hysteresis loop occurs in a relative pressure range of 0.65 to 0.85, indicating an increase in nitrogen adsorption at higher pressures, as demonstrated in **Figure S2**.

When capillary condensation occurs in mesopores (such as in the present study for MCM-41), the adsorption and desorption processes follow distinctive paths, creating a hysteresis loop, as shown in **Figures S1** and **S2**. This type of hysteresis loop is called H1, which is often observed in materials possessing a homogenous distribution of thin cylindrical mesopores.

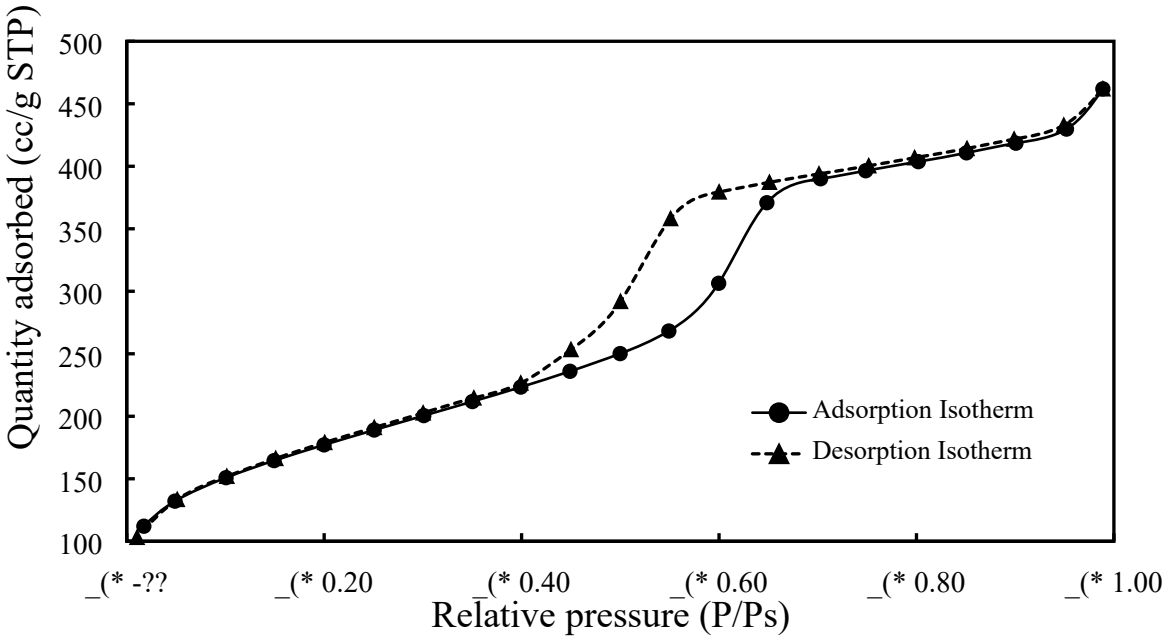

Figure S1. Nitrogen physisorption in MCM-41 (6 nm) shown by adsorption-desorption isotherms.

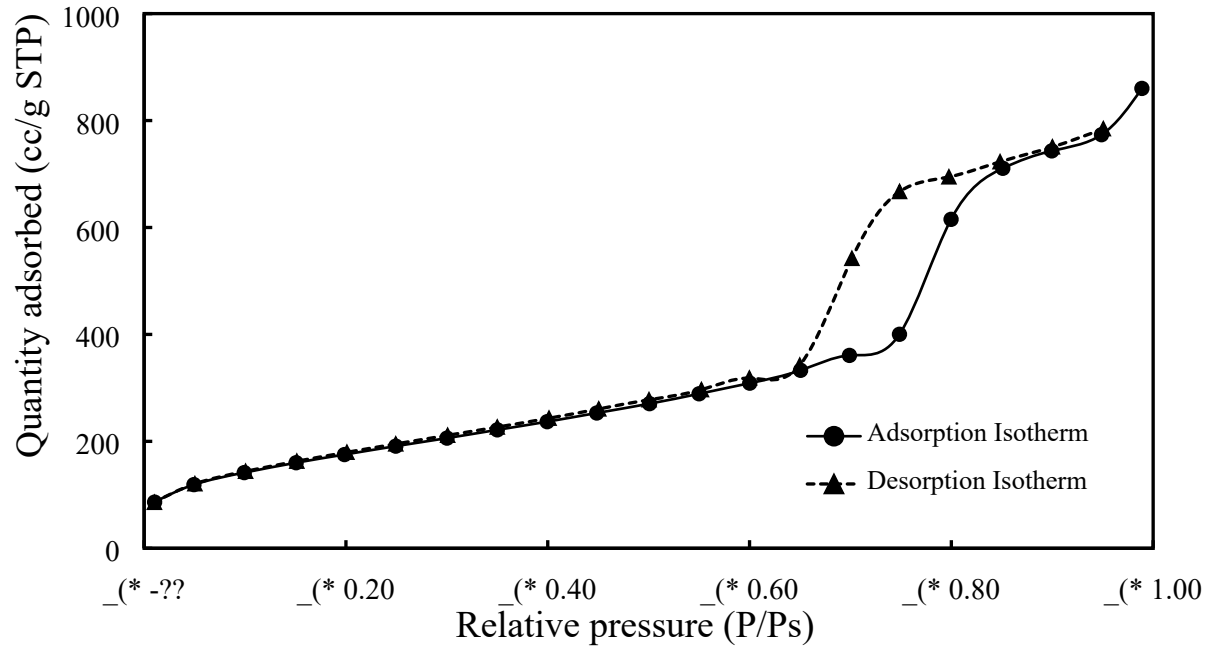

Figure S2. Nitrogen physisorption in MCM-41 (10 nm) shown by adsorption-desorption isotherms.

2. CO_2 Phase Equilibrium during Adsorption

Figures S3 and **S4** show examples of the CO_2 adsorption isotherms measured at four different equilibrium times, 2, 2.5, 3, and 3.5 hours at a temperature of 10 °C. The equilibrium condition was defined as pressure stabilization inside the core holders containing porous media after introducing CO_2. The results demonstrate that the 2-hour equilibrium time produced an inaccurate isotherm with inconsistent data points and lower capillary condensation shift for all pore sizes studied here. It is evident that increasing the equilibrium time from 2 to 2.5 hours provided sufficient time for the pressure to stabilize in the nanoporous material, significantly improving the quality of the isotherm regarding data consistency, i.e., smoothness of curves. Furthermore, well-distinguished phase shifts in the capillary condensation branches of the isotherms obtained for different MCM-41 samples revealed the effect of pore size. Extending the equilibrium time from 2.5 to 3 hours and 3.5 hours did not significantly alter the pressure profile within the core holder, almost reproducing the results obtained in the case of 2.5 hours. Although longer equilibration periods beyond 2.5 hours did not notably enhance overall isotherm quality, we adopted longer intervals to ensure ultimate pressure stabilization. This extended duration (3.5 hours) allowed for thorough equilibration of gas and liquid molecules within the confined spaces of nanopores and bulk regions. Thus, a 3.5-hour equilibrium time was deemed optimal for achieving equilibrium across all experiments conducted in this study.

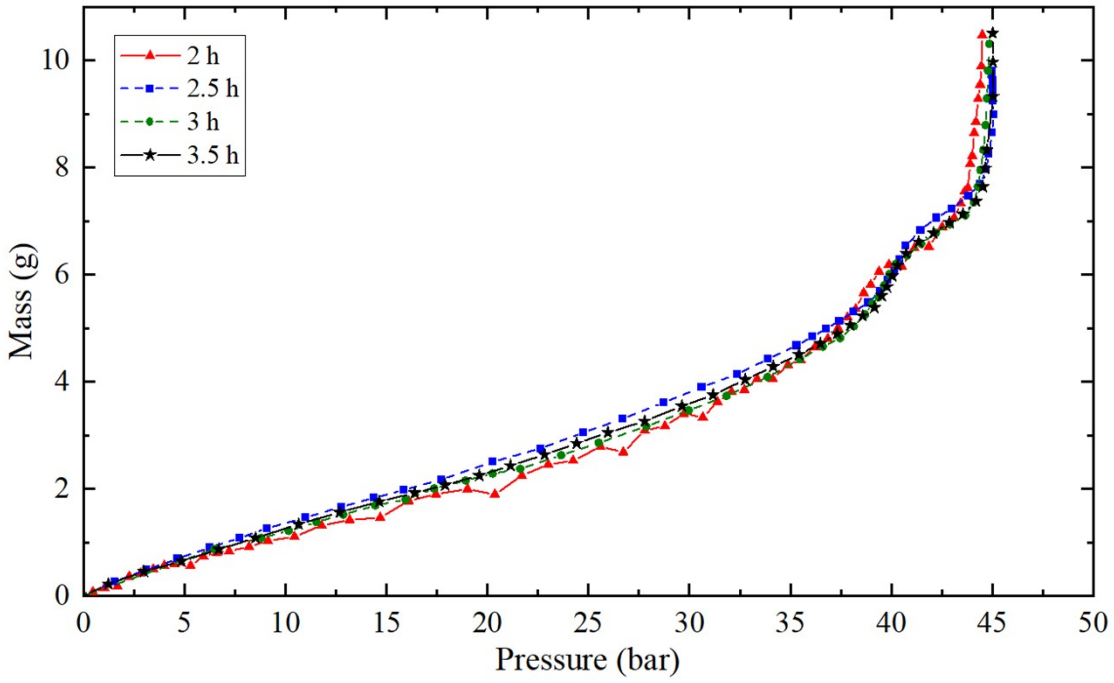

Figure S3. Experimentally measured CO_2 adsorption isotherms obtained at various equilibrium times and a temperature of 10 °C in MCM-41 of 8 nm pore diameter.

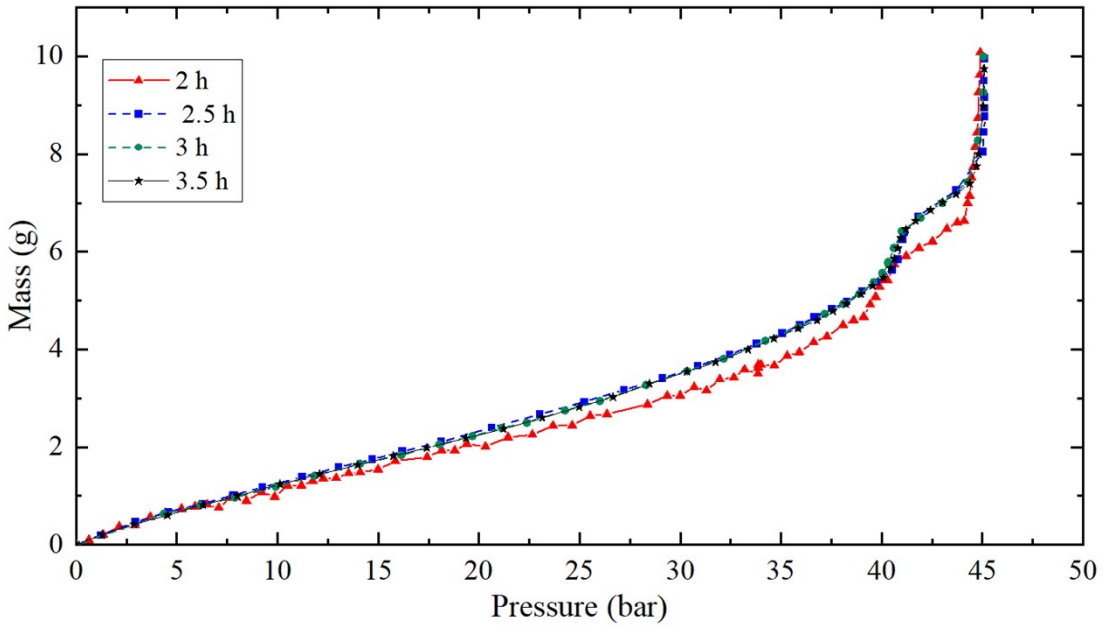

Figure S4. Experimentally measured CO_2 adsorption isotherms obtained at various equilibrium times and a temperature of 10 °C in MCM-41 of 10 nm pore diameter.

Table S1. Summary of the adsorption and desorption isotherms describing the confined and bulk phase behavior for Carbon Dioxide in MCM-41 of different pore sizes at varying temperatures.

Adsorbent	Temperature (°C)	Pm (bar)	NIST saturation Pressure (Ps) (bar)	Relative Pressure (Pm/Ps)	Pressure difference (bar)
MCM-41 (6 nm)	-23.1	14.058	17.879	0.786	3.821
	-10	21.142	26.487	0.798	5.345
	0	28.470	34.851	0.817	6.381
	10	35.881	45.022	0.797	9.141
	20	48.823	57.291	0.852	8.468
MCM-41 (8 nm)	-23.1	15.349	17.879	0.858	2.530
	-10	23.054	26.487	0.870	3.433
	0	30.939	34.851	0.888	3.912
	10	39.950	45.022	0.887	5.072
	20	52.402	57.291	0.915	4.889
MCM-41 (10 nm)	-23.1	15.619	17.879	0.874	2.260
	-10	23.358	26.487	0.882	3.129
	0	31.436	34.851	0.902	3.415
	10	40.744	45.022	0.905	4.278
	20	52.866	57.291	0.923	4.425
MCM-41 (12 nm)	-23.1	15.901	17.879	0.889	1.978
	-10	24.046	26.487	0.908	2.441
	0	31.817	34.851	0.913	3.034
	10	41.463	45.022	0.921	3.559
	20	53.289	57.291	0.930	4.002

Table S2. Experimentally measured values of pressure and mass during adsorption of CO_2 in MCM-41 at -23.1°C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.253	0.310	0.443	0.255	0.487	0.092	0.749	0.297
0.707	0.572	0.997	0.498	1.228	0.412	1.801	0.575
1.318	0.901	1.608	0.690	2.055	0.648	2.707	0.768
2.097	1.103	2.284	0.884	2.946	0.883	3.657	0.886
3.106	1.479	3.122	1.077	3.898	1.122	4.449	1.227
4.225	1.724	4.049	1.231	4.875	1.302	5.277	1.252
5.435	1.971	4.916	1.439	5.924	1.432	6.269	1.573
6.894	2.300	6.085	1.702	7.091	1.679	7.169	1.748
8.352	2.610	7.224	1.949	8.247	1.931	8.314	1.945
9.716	2.919	8.322	2.192	9.332	2.186	9.201	2.113
10.970	3.235	9.386	2.467	10.354	2.434	10.043	2.320
12.122	3.527	10.395	2.672	11.299	2.664	10.906	2.561
12.744	3.721	11.268	2.860	11.869	2.809	11.389	2.715
13.207	3.927	11.998	3.046	12.539	3.012	11.859	2.854
13.501	4.105	12.560	3.295	13.068	3.174	12.788	3.131
13.714	4.332	13.055	3.455	13.686	3.424	13.228	3.347
13.858	4.500	13.483	3.577	14.077	3.567	13.712	3.483
13.999	4.702	13.893	3.704	14.415	3.758	14.227	3.645
14.151	4.913	14.129	3.891	14.823	3.921	15.246	4.045
14.201	5.185	14.440	4.036	15.082	4.118	15.162	4.329
14.721	5.440	14.811	4.204	15.324	4.320	15.448	4.959
15.623	5.630	14.941	4.432	15.423	4.611	15.466	5.069
16.494	5.786	15.052	4.658	15.465	4.845	15.538	5.223
17.237	5.904	15.119	4.851	15.497	5.095	15.597	5.468
17.694	6.130	15.198	5.072	15.602	5.307	16.349	6.483
17.850	6.348	15.284	5.367	15.643	5.573	17.805	6.828
17.873	6.355	15.383	5.597	15.687	5.793	17.652	7.112
17.880	6.349	15.456	5.846	15.729	6.070	17.660	7.379
17.870	6.342	15.540	6.127	15.763	6.338	17.913	7.205

17.874	6.395	15.711	6.368	15.900	6.588	17.916	7.340
17.867	6.376	15.997	6.616	16.204	6.854	17.920	7.350
17.862	6.319	16.466	6.863	16.649	7.144	17.903	7.549
17.866	6.335	16.988	7.090	17.091	7.393	17.907	7.774
17.862	6.294	17.430	7.327	17.511	7.639	17.915	7.943
17.856	6.364	17.811	7.565	17.754	7.904	17.907	8.077
17.859	6.334	18.093	7.898	17.872	8.156	17.907	8.394
17.875	6.312	17.991	7.903	17.907	8.256	17.908	8.165
17.871	6.236	18.372	8.353	17.912	8.313	17.914	8.978
17.877	6.181	18.276	9.718	17.913	8.351		
17.877	6.225			17.926	8.317		
17.885	6.471			17.941	8.576		
17.907	7.145			17.956	8.993		

Table S3. Experimentally measured values of pressure and mass during desorption of CO_2 in MCM-41 at -23.1°C.

6 nm		**8 nm**		**10 nm**		**12 nm**	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
17.877	8.966	18.119	10.287	17.929	9.579	17.910	7.354
17.870	8.775	17.952	10.012	17.921	8.972	17.910	8.156
17.861	8.647	18.073	9.652	17.913	8.511	17.909	10.922
17.865	8.608	17.944	9.377	17.770	8.038	17.911	7.355
17.876	8.518	17.837	9.213	17.071	7.376	17.910	8.059
17.885	8.312	17.819	8.921	16.006	6.764	17.909	10.406
17.876	8.188	17.799	8.728	15.730	6.528	17.910	7.669
17.869	8.041	17.822	8.199	15.658	6.263	17.872	9.075
17.839	7.602	17.829	8.067	15.513	6.058	17.850	9.745
17.796	6.883	17.820	7.992	15.529	5.832	17.802	8.978
17.598	6.149	17.836	7.959	15.457	5.585	17.751	8.214
15.559	5.577	17.832	7.955	15.416	5.328	17.897	6.811
14.115	5.086	17.822	8.056	15.399	5.080	17.330	6.684
13.801	4.567	17.825	8.271	15.460	4.811	16.851	6.053
13.328	4.070	17.815	7.937	15.350	4.545	16.256	5.641

12.321	3.621	17.818	8.088	15.242	4.274	15.766	5.192
11.031	3.242	17.831	8.042	15.252	4.173	15.448	4.713
9.748	2.923	17.844	8.156	14.807	3.916	15.381	4.439
8.627	2.655	17.827	8.286	14.334	3.675	15.797	4.258
7.766	2.465	17.820	8.273	13.726	3.428	15.273	4.031
6.971	2.307	17.815	7.898	13.243	3.214	15.488	4.016
6.271	2.135	17.795	7.845	12.626	3.001	14.769	3.778
5.656	2.000	16.745	7.223	11.970	2.793	14.288	3.516
5.081	1.877	15.630	6.500	11.372	2.612	13.753	3.258
4.599	1.774	15.372	5.783	10.740	2.455	13.478	3.224
4.175	1.654	15.196	5.093	10.104	2.302	12.676	3.052
3.790	1.550	14.967	4.415	9.500	2.158	11.897	2.850
3.463	1.479	14.173	3.784	8.971	2.012	11.474	2.757
3.167	1.403	12.844	3.432	8.386	1.885	10.788	2.621
2.906	1.323	11.430	2.955	7.872	1.771	10.147	2.494
2.677	1.236	10.250	2.624	7.397	1.692	9.545	2.360
2.473	1.184	9.218	2.359	6.935	1.591	9.107	2.221
2.291	1.120	8.275	2.145	6.501	1.490	8.568	2.086
2.128	1.078	7.419	1.935	6.101	1.403	7.982	1.965
1.980	1.025	6.641	1.770	5.707	1.369	7.456	1.866
1.847	0.962	5.952	1.580	5.357	1.257	7.009	1.810
1.703	0.924	5.310	1.443	4.977	1.178	6.566	1.744
1.583	0.855	4.801	1.331	4.687	1.112	6.130	1.680
1.461	0.824	4.299	1.205	4.355	1.032	5.830	1.581
1.346	0.791	3.870	1.102	4.057	0.984	5.394	1.510
1.250	0.731	3.495	1.036	3.711	0.918	5.040	1.431
1.153	0.702	3.166	0.991	3.326	0.843	4.816	1.405
1.051	0.642			2.998	0.753	4.493	1.304
				2.643	0.662	4.234	1.194
				2.331	0.539	3.986	1.097
				2.067	0.501	3.772	1.009
				1.835	0.500		
				1.587	0.445		
				1.355	0.358		

				1.140	0.291		

Table S4. Experimentally measured values of pressure and mass during adsorption of CO_2 in MCM-41 at -10 °C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.501	0.316	0.709	0.249	0.911	0.313	1.119	0.273
1.307	0.615	1.630	0.481	2.046	0.540	2.510	0.530
2.460	0.953	2.765	0.726	3.190	0.792	3.869	0.766
3.786	1.254	3.937	0.969	4.383	1.011	5.214	0.964
5.201	1.518	5.136	1.176	5.587	1.190	6.341	1.126
6.716	1.772	6.287	1.373	6.645	1.382	7.534	1.312
8.168	2.029	7.385	1.549	7.693	1.522	8.570	1.449
9.945	2.312	8.978	1.814	9.129	1.711	9.769	1.599
11.737	2.605	10.474	2.053	10.478	1.922	10.892	1.772
13.212	2.835	11.873	2.278	11.813	2.100	11.908	1.914
14.618	3.068	13.167	2.501	13.149	2.395	12.957	2.078
16.039	3.320	14.780	2.789	14.553	2.628	14.193	2.259
17.383	3.513	16.283	3.031	15.909	2.835	15.322	2.416
18.632	3.826	17.725	3.357	17.185	3.063	16.491	2.631
19.749	4.089	18.985	3.645	18.329	3.308	17.541	2.826
20.351	4.283	19.947	3.875	19.396	3.541	18.523	2.996
20.719	4.448	20.547	4.035	20.283	3.717	19.480	3.200
20.987	4.612	21.085	4.188	21.110	3.984	20.350	3.367
21.240	4.799	21.591	4.353	21.803	4.210	21.226	3.578
21.465	4.984	22.105	4.534	22.411	4.414	21.962	3.778
21.795	5.126	22.575	4.712	22.982	4.630	22.626	3.965
22.402	5.304	22.723	4.880	23.141	4.856	23.002	4.110
23.194	5.427	22.814	5.042	23.206	4.998	23.319	4.261
23.971	5.546	22.903	5.202	23.270	5.151	23.562	4.477
24.706	5.661	22.966	5.363	23.310	5.356	23.705	4.670
25.373	5.780	23.037	5.538	23.347	5.535	23.849	4.907
25.915	5.910	23.111	5.718	23.398	5.741	23.973	5.105

26.213	6.075	23.176	5.897	23.433	5.981	24.057	5.314
26.332	6.268	23.245	6.065	23.509	6.194	24.188	5.559
26.383	6.428	23.348	6.229	23.658	6.365	24.284	5.725
26.438	6.654	23.592	6.457	24.024	6.588	24.460	5.979
26.470	6.801	23.952	6.633	24.455	6.749	24.636	6.171
26.480	6.891	24.383	6.795	24.879	6.938	24.961	6.426
26.473	6.935	24.848	6.942	25.341	7.119	25.316	6.644
26.469	6.952	25.310	7.080	25.768	7.280	25.656	6.814
26.468	7.008	25.751	7.248	26.068	7.499	25.670	6.808
26.463	7.022	26.102	7.449	26.136	7.597	25.674	6.838
26.493	7.009	26.172	7.503	26.173	7.575	25.700	6.826
26.496	7.046	26.186	7.522	26.173	7.609	25.704	6.826
26.505	7.088	26.192	7.531	26.188	7.602	25.704	6.825
26.498	7.092	26.206	7.535	26.196	7.608	25.729	6.830
26.501	7.128	26.206	7.523	26.200	7.655	25.712	6.801
26.517	7.209	26.219	7.520	26.212	7.627	25.710	6.813
26.504	7.265	26.210	7.513	26.218	7.685	25.723	6.800
26.519	7.318	26.211	7.524	26.228	7.702	25.720	6.798
26.527	7.440	26.218	7.531	26.244	7.743	25.733	6.816
26.515	7.423	26.206	7.529	26.225	7.772	25.720	6.874
26.497	7.336	26.194	7.513	26.224	7.756	25.714	6.849
26.479	7.246	26.177	7.519	26.224	7.836	25.757	6.870
26.482	7.202	26.183	7.532	26.258	7.995	26.444	7.417
26.478	7.183	26.176	7.557	26.397	8.763	26.502	8.332
26.483	7.213	26.193	7.600	26.453	9.584	26.526	9.239
26.497	7.266	26.440	8.158	26.482	10.551	26.587	10.211
26.521	7.344	26.551	9.154	26.520	11.495	26.645	11.224

Table S5. Experimentally measured values of pressure and mass during desorption of CO_2 in MCM-41 at -10 °C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
26.517	7.720	26.499	9.244	26.583	10.055	26.510	9.946
26.528	7.667	26.451	8.672	26.550	9.377	26.457	9.126
26.475	7.610	26.343	8.193	26.479	8.794	26.465	8.293
26.487	7.579	26.281	7.902	26.358	8.394	26.431	7.474
26.493	7.549	26.268	7.813	26.354	8.231	25.628	6.951
26.501	7.534	26.217	7.777	26.360	8.160	25.624	6.918
26.489	7.497	26.227	7.777	26.363	8.112	25.625	6.926
26.478	7.441	26.235	7.774	26.369	8.101	25.633	6.909
26.471	7.384	26.231	7.766	26.346	8.049	25.630	6.913
26.459	7.331	26.251	7.771	26.341	8.036	25.622	6.921
26.458	7.272	26.237	7.762	26.340	8.023	25.617	6.920
26.467	7.230	26.219	7.755	26.328	7.980	25.613	6.904
26.458	7.133	26.218	7.752	26.344	7.991	25.614	6.883
26.401	6.829	26.211	7.722	26.304	7.897	25.631	6.888
26.274	6.394	26.209	7.708	26.312	7.881	25.621	6.887
25.577	5.954	26.205	7.701	26.313	7.855	25.622	6.875
23.822	5.617	26.198	7.699	26.239	7.773	25.587	6.862
22.137	5.288	26.179	7.675	25.126	7.212	24.500	6.257
21.418	4.917	26.180	7.667	23.797	6.685	24.117	5.665
21.105	4.633	26.173	7.660	23.450	6.050	23.813	5.065
20.734	4.353	26.058	7.549	23.333	5.469	23.518	4.479
20.190	4.118	24.715	7.011	23.182	4.928	22.791	4.024
19.462	3.883	23.580	6.578	22.294	4.424	21.495	3.607
18.639	3.685	23.143	6.096	20.974	3.961	20.031	3.242
17.778	3.484	22.947	5.612	19.772	3.643	18.501	2.935
16.923	3.306	22.788	5.120	18.520	3.342	17.181	2.683
16.076	3.140	22.545	4.736	17.400	3.085	15.876	2.439
15.256	2.988	21.782	4.384	16.299	2.878	14.767	2.268
14.447	2.842	20.858	4.077	15.227	2.695	13.762	2.109
13.670	2.704	19.937	3.817	14.174	2.502	12.820	1.954

12.923	2.572	18.997	3.575	13.088	2.312	11.911	1.813
12.163	2.454	18.005	3.340	12.150	2.179	11.067	1.705
11.481	2.344	17.030	3.135	11.221	2.015	10.251	1.571
10.845	2.252	16.048	2.935	10.396	1.906	9.513	1.480
10.237	2.153	15.115	2.756	9.631	1.759	8.807	1.389
9.654	2.040	14.216	2.597	8.896	1.673	8.161	1.304
9.120	1.962	13.344	2.453	8.249	1.535	7.575	1.226
8.615	1.876	12.517	2.302	7.704	1.454	7.031	1.130
8.150	1.784	11.723	2.152	7.223	1.403	6.563	1.053
7.695	1.740	10.954	2.031	6.757	1.304	6.133	0.998
7.273	1.674	10.225	1.905	6.305	1.223	5.736	0.959
6.882	1.613	9.555	1.786	5.908	1.184	5.366	0.889
6.520	1.562	8.938	1.718	5.533	1.144	5.025	0.856
6.049	1.478	8.348	1.615	5.168	1.097	4.696	0.816
5.591	1.381	7.805	1.529	4.830	1.023	4.392	0.760
5.183	1.320	7.295	1.448	4.518	0.932	4.101	0.724
4.813	1.264	6.709	1.346	4.231	0.919	3.847	0.673
4.480	1.213	6.128	1.233	3.961	0.882	3.615	0.609
4.177	1.138	5.602	1.142	3.715	0.822	3.359	0.597
3.895	1.072	5.130	1.067	3.474	0.774	3.162	0.573
3.583	0.997	4.697	0.994	3.265	0.711	2.977	0.605
3.309	0.937	4.308	0.925	3.001	0.650	2.796	0.532
3.067	0.893	3.956	0.853	2.760	0.620	2.589	0.469
2.835	0.904	3.585	0.771	2.538	0.586	2.394	0.420
2.642	0.850	3.253	0.699	2.351	0.539	2.219	0.415
2.457	0.775	2.972	0.646	2.170	0.530	2.047	0.383
2.300	0.749	2.705	0.632	2.012	0.489	1.908	0.383
2.062	0.716	2.470	0.580	1.864	0.459	1.774	0.354
1.879	0.641	2.266	0.519	1.622	0.420	1.645	0.373
1.593	0.622	2.077	0.489	1.419	0.357	1.393	0.292
1.372	0.561	1.839	0.454	1.197	0.331	1.186	0.256
1.087	0.456	1.638	0.411	1.013	0.298	0.965	0.227
0.881	0.398	1.389	0.389	0.822	0.271	0.796	0.203
0.736	0.349	1.188	0.351	0.664	0.233	0.623	0.171

0.592	0.284	0.948	0.299	0.556	0.212	0.499	0.128
0.473	0.230	0.777	0.243	0.456	0.137	0.406	0.153
0.399	0.182	0.645	0.205	0.370	0.106	0.325	0.101
0.083	0.009	0.523	0.163	0.072	0.009	0.247	0.080
		0.429	0.121			0.052	0.015
		0.140	0.026			0.000	0.000

Table S6. Experimentally measured values of pressure and mass during adsorption of CO_2 in MCM-41 at 0 °C.

6 nm		**8 nm**		**10 nm**		**12 nm**	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
0.559	0.336	0.837	0.305	0.883	0.242	1.169	0.232
1.555	0.638	1.952	0.542	2.294	0.439	2.629	0.432
2.792	0.909	3.150	0.744	3.711	0.639	4.131	0.616
4.518	1.210	4.655	0.971	5.406	0.899	5.960	0.858
6.483	1.498	6.221	1.195	7.062	1.073	7.461	1.023
8.421	1.752	7.785	1.399	8.570	1.298	8.509	1.131
10.185	1.983	9.419	1.611	10.009	1.461	9.600	1.262
12.114	2.218	11.487	1.862	11.852	1.717	11.143	1.431
14.094	2.465	13.409	2.094	13.531	1.894	12.592	1.606
15.966	2.695	15.219	2.312	15.112	2.104	13.997	1.758
17.496	2.881	16.764	2.614	16.459	2.290	15.384	1.937
19.278	3.106	18.528	2.951	18.116	2.514	17.055	2.134
21.184	3.353	20.589	3.224	20.383	2.822	19.487	2.442
22.849	3.592	22.259	3.481	21.776	3.054	21.161	2.694
23.859	3.747	23.268	3.667	23.162	3.262	22.667	2.910
24.860	3.905	24.121	3.811	24.180	3.447	23.773	3.083
25.944	4.095	25.009	4.009	25.176	3.636	24.813	3.238
26.863	4.274	25.815	4.162	26.115	3.781	25.815	3.415
27.556	4.433	26.662	4.325	26.891	3.976	26.611	3.550
28.122	4.616	27.340	4.462	26.888	3.950	26.603	3.522
28.535	4.791	27.958	4.602	27.763	4.105	27.648	3.725

29.024	5.007	28.730	4.798	28.646	4.331	28.584	3.928
29.791	5.208	29.408	4.973	29.477	4.550	29.508	4.142
30.981	5.370	30.037	5.149	30.251	4.799	30.490	4.426
32.222	5.544	30.478	5.342	30.954	5.069	31.122	4.681
33.296	5.704	30.746	5.600	31.229	5.330	31.485	4.986
34.212	5.882	30.921	5.900	31.386	5.655	31.688	5.268
34.689	6.086	31.088	6.141	31.508	6.044	31.895	5.553
34.863	6.329	31.279	6.393	31.639	6.299	32.185	5.853
34.959	6.602	31.632	6.609	32.015	6.534	32.508	6.150
35.016	6.846	32.268	6.799	32.716	6.802	33.020	6.478
		32.988	6.988	33.535	7.041	33.677	6.702
		33.736	7.171	34.316	7.316	34.037	6.846
		34.379	7.368	34.815	7.617	34.043	6.833
		34.839	7.650	34.937	7.785	34.060	6.842
		34.919	7.782	34.943	7.822	34.062	6.811
		34.933	7.836	34.962	7.913	34.060	6.851
		34.943	7.880	34.968	8.011	34.078	6.841
		34.941	7.916	35.020	8.426	34.089	6.824
		34.954	8.010	35.096	9.228	34.834	8.522
		34.956	8.096			34.992	339.884
		35.101	9.020				

Table S7. Experimentally measured values of pressure and mass during desorption of CO_2 in MCM-41 at 0 °C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
34.894	8.685	34.898	9.863	34.854	9.055	34.884	9.764
34.853	8.034	34.866	9.343	34.833	8.757	34.841	9.215
34.793	7.406	34.854	8.848	34.808	8.580	34.806	8.657
34.675	6.784	34.788	8.356	34.798	8.392	34.791	8.128
34.323	6.149	34.720	8.043	34.773	8.204	34.657	7.203
32.239	5.667	34.701	7.824	34.775	8.156	34.074	6.934
29.795	5.262	34.672	7.708	34.758	8.121	34.068	6.943
28.445	4.821	34.682	7.687	34.759	8.011	34.052	6.940
27.358	4.387	34.675	7.695	34.455	7.592	34.049	6.934
25.568	3.979	34.680	7.715	32.317	6.792	34.042	6.946
23.870	3.670	34.676	7.719	31.289	5.947	34.048	6.926
22.146	3.393	34.682	7.719	30.926	5.131	34.034	6.917
20.417	3.142	34.660	7.674	29.034	4.458	32.971	6.550
18.821	2.927	34.637	7.651	26.621	3.897	31.923	5.640
17.318	2.739	34.640	7.649	24.691	3.496	31.332	4.853
15.900	2.558	34.638	7.644	22.710	3.148	29.624	4.171
14.588	2.384	34.362	7.289	20.779	2.839	27.195	3.599
13.366	2.239	32.483	6.747	18.856	2.509	24.642	3.129
12.245	2.099	31.038	6.193	17.129	2.263	22.053	2.722
11.226	1.984	30.589	5.584	15.455	2.061	19.972	2.432
10.308	1.884	29.936	5.100	13.997	1.862	18.028	2.150
9.439	1.786	28.427	4.680	12.645	1.715	16.216	1.916
8.612	1.686	26.769	4.316	11.388	1.562	14.530	1.706
7.920	1.610	25.057	4.022	10.105	1.363	13.032	1.514
7.283	1.526	23.295	3.753	8.974	1.240	11.664	1.362
6.721	1.447	21.742	3.530	7.977	1.073	10.388	1.219
6.214	1.406	20.214	3.315	6.761	0.962	9.298	1.101
5.751	1.371	18.729	3.102	5.732	0.851	8.309	0.970
5.333	1.330	17.283	2.796	4.907	0.743	7.204	0.859
4.944	1.282	15.951	2.557	4.209	0.659	6.307	0.740

4.590	1.227	14.719	2.410	3.626	0.575	5.479	0.653
4.269	1.182	13.570	2.274	2.847	0.441	4.638	0.591
3.982	1.148	12.499	2.159	2.269	0.381	3.940	0.516
		11.511	2.046	1.735	0.267	3.349	0.424
		10.451	1.899			2.856	0.342
		9.501	1.783			2.452	0.320
		8.644	1.661			1.880	0.230
		7.549	1.549			1.461	0.203
		6.608	1.428			1.090	0.117
		5.797	1.348			0.830	0.087
		5.094	1.269			0.650	0.070
		4.471	1.177			0.518	0.045
		3.561	1.030				
		2.865	0.932				
		2.173	0.824				
		1.676	0.758				

Table S8. Experimentally measured values of pressure and mass during adsorption of CO_2 in MCM-41 at +10°C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.169	0.304	1.228	0.220	1.297	0.210	1.655	0.228
2.817	0.582	2.990	0.456	2.877	0.423	3.217	0.376
4.685	0.842	4.848	0.648	4.528	0.607	4.817	0.540
6.632	1.107	6.687	0.866	6.292	0.815	6.455	0.701
8.585	1.346	8.519	1.081	8.002	1.000	8.059	0.855
10.965	1.618	10.647	1.336	10.121	1.241	10.176	1.043
13.290	1.877	12.681	1.560	12.094	1.447	12.042	1.225
15.423	2.103	14.646	1.759	13.968	1.630	13.958	1.402
17.296	2.275	16.401	1.922	15.742	1.818	15.696	1.571
18.834	2.435	17.907	2.069	17.419	1.986	17.293	1.714
20.526	2.614	19.599	2.247	19.360	2.184	19.155	1.903
22.080	2.792	21.135	2.430	21.223	2.373	20.916	2.075
23.727	2.983	22.828	2.639	23.141	2.601	22.761	2.264
25.368	3.178	24.415	2.846	24.985	2.820	24.580	2.468
26.820	3.346	25.970	3.050	26.661	3.028	26.561	2.697
28.404	3.537	27.786	3.264	28.466	3.299	28.276	2.888
30.004	3.749	29.633	3.544	30.334	3.546	29.920	3.102
31.399	3.938	31.176	3.753	31.749	3.738	31.248	3.277
32.740	4.146	32.768	4.038	33.363	3.996	32.599	3.458
33.967	4.343	34.152	4.283	34.651	4.226	33.991	3.670
35.059	4.570	35.427	4.508	35.853	4.434	35.315	3.889
36.065	4.814	36.489	4.710	36.783	4.596	36.244	4.056
36.867	5.039	37.322	4.897	37.571	4.788	37.398	4.242
37.664	5.195	37.972	5.060	38.236	4.930	38.083	4.399
38.574	5.334	38.584	5.231	38.961	5.139	38.772	4.529
39.525	5.435	39.153	5.388	39.545	5.303	39.548	4.735
40.430	5.566	39.524	5.611	40.085	5.462	40.142	4.895
41.256	5.676	39.788	5.773	40.438	5.658	40.653	5.034
42.058	5.796	40.045	5.978	40.634	5.853	41.089	5.312

42.780	5.911	40.309	6.170	40.789	6.075	41.297	5.478
43.403	6.066	40.731	6.401	40.947	6.278	41.521	5.678
43.754	6.243	41.357	6.612	41.199	6.458	41.767	5.870
43.966	6.451	42.090	6.778	41.686	6.628	42.112	6.073
44.112	6.654	42.871	6.975	42.425	6.855	42.481	6.276
44.206	6.863	43.541	7.135	43.026	7.011	42.923	6.445
44.329	7.141	44.200	7.374	43.687	7.180	43.572	6.658
44.442	7.416	44.526	7.644	44.371	7.402	44.292	6.876
44.542	7.760	44.656	7.988	44.716	7.750	44.609	6.981
44.627	8.116	44.741	8.330	44.812	8.001	44.616	6.984
44.876	9.593	45.038	9.331	45.043	8.976	44.628	7.001
45.071	11.188	45.030	9.976	45.089	9.748	44.634	7.008
		45.015	10.513			45.069	7.640
						45.180	9.530

Table S9. Experimentally measured values of pressure and mass during desorption of CO_2 in MCM-41 at +10°C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
45.202	11.572	45.083	10.844	45.096	9.916	45.133	9.587
45.072	10.897	44.982	10.153	44.957	9.024	45.057	8.785
44.925	10.117	44.902	9.375	44.776	8.058	44.992	8.151
44.763	9.402	44.686	8.567	43.675	7.201	44.936	7.671
44.567	8.695	44.366	7.658	41.607	6.509	44.881	7.412
44.326	7.974	43.155	7.165	40.451	5.919	44.872	7.226
44.026	7.305	41.189	6.502	39.574	5.264	44.819	7.197
43.566	6.623	39.760	5.942	37.626	4.786	44.510	7.016
42.871	5.966	38.921	5.529	35.352	4.319	42.362	6.310
40.971	5.673	37.667	5.020	32.919	3.878	41.054	5.478
38.573	5.381	35.867	4.571	30.434	3.472	39.486	4.765
36.175	4.964	33.905	4.185	28.229	3.165	36.740	4.138
36.002	4.751	31.904	3.783	26.092	2.813	33.701	3.620
33.377	4.123	29.896	3.472	24.064	2.608	30.577	3.138
31.368	3.852	27.872	3.103	22.110	2.302	28.174	2.849
29.144	3.519	25.493	2.750	20.568	2.128	25.727	2.524
26.947	3.196	23.433	2.469	19.078	1.915	23.504	2.293
24.811	2.893	21.472	2.282	17.680	1.831	21.389	2.043
22.768	2.611	19.543	2.068	16.333	1.705	19.638	1.876
20.844	2.432	17.848	1.857	15.141	1.562	18.100	1.712
19.030	2.235	16.259	1.669	14.004	1.433	16.658	1.585
17.360	2.043	14.800	1.525	12.951	1.356	15.321	1.446
15.782	1.876	13.465	1.399	12.005	1.235	14.061	1.352
14.375	1.707	12.215	1.267	11.090	1.175	12.912	1.218
13.093	1.584	11.122	1.133	10.199	1.080	11.851	1.144
11.897	1.434	10.125	1.045	9.453	1.008	10.857	1.017
10.837	1.282	9.212	0.989	8.756	0.971	9.952	0.964
9.886	1.231	8.360	0.864	8.125	0.904	9.115	0.880
9.025	1.141	7.577	0.820	7.536	0.767	8.374	0.824
8.250	1.050	6.918	0.711	7.005	0.778	7.639	0.765

7.548	0.963	6.310	0.619	6.511	0.734	7.029	0.718
6.913	0.859	5.769	0.567	6.060	0.700	6.459	0.635
6.337	0.846	5.275	0.515	5.633	0.628	5.944	0.622
5.788	0.790	4.824	0.354	5.215	0.544	5.472	0.578
5.322	0.722	4.424	0.411	4.855	0.556	5.044	0.514
4.863	0.714	4.051	0.360	4.532	0.527	4.619	0.492
4.459	0.620	3.727	0.216	4.229	0.442	4.270	0.432
4.090	0.602	3.404	0.322	3.890	0.483	3.940	0.442
3.757	0.582	3.110	0.151	3.566	0.390	3.644	0.408
3.458	0.548	2.847	0.196	3.274	0.387	3.377	0.378
3.185	0.515	2.610	0.205	3.027	0.391	3.077	0.348
2.928	0.512	2.398	0.116	2.800	0.326	2.808	0.314
2.692	0.514	2.203	0.062	2.595	0.294	2.566	0.303
2.460	0.486	2.023	0.150	2.381	0.364	2.354	0.268
2.153	0.443	1.864	0.142	2.176	0.310	2.158	0.237
1.785	0.410	1.716	0.111	1.988	0.292	1.979	0.226
1.493	0.383	1.514	0.072	1.702	0.256	1.795	0.246
1.163	0.348	1.295	0.078			1.635	0.203
0.865	0.279					1.476	0.206
0.586	0.248					1.259	0.165
						1.053	0.148
						0.886	0.114
						0.722	0.137

Table S10. Experimentally measured values of pressure and mass during adsorption of CO_2 in MCM-41 at +20 °C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.135	0.255	1.748	0.297	1.512	0.212	1.513	0.163
2.662	0.486	3.555	0.492	3.292	0.406	3.168	0.307
4.710	0.741	5.606	0.684	5.260	0.594	5.058	0.470
6.951	0.978	7.547	0.842	7.149	0.785	6.881	0.595
9.306	1.205	9.434	1.013	9.240	0.941	8.681	0.732
11.412	1.389	11.255	1.156	10.909	1.108	10.448	0.870
13.789	1.595	13.423	1.325	13.016	1.254	12.538	1.030
15.938	1.766	15.327	1.475	14.984	1.438	14.484	1.162
17.887	1.916	17.316	1.620	16.713	1.562	16.402	1.307
20.050	2.088	19.496	1.787	18.944	1.730	18.764	1.471
22.293	2.258	21.593	1.944	21.083	1.915	21.015	1.646
24.452	2.430	23.610	2.086	23.138	2.069	23.160	1.812
26.428	2.584	25.762	2.297	25.106	2.234	25.206	1.980
28.148	2.715	27.471	2.425	27.131	2.418	27.252	2.153
29.800	2.834	29.107	2.623	29.026	2.589	29.312	2.321
31.691	2.989	30.958	2.756	31.243	2.789	31.442	2.500
33.654	3.150	33.014	3.117	33.314	3.027	33.456	2.687
35.350	3.286	34.575	3.264	35.030	3.159	35.099	2.824
36.968	3.422	35.988	3.414	36.641	3.363	36.683	2.990
38.513	3.565	37.380	3.571	38.138	3.481	38.133	3.163
39.989	3.718	38.664	3.707	39.506	3.626	39.526	3.300
41.306	3.850	39.836	3.840	40.721	3.750	40.720	3.429
42.552	3.980	40.872	3.980	42.067	3.900	41.940	3.571
43.747	4.109	42.045	4.119	43.246	4.122	42.956	3.679
44.834	4.239	43.065	4.254	44.286	4.223	43.847	3.764
45.850	4.371	44.073	4.378	45.282	4.349	44.818	3.891
46.852	4.523	45.233	4.558	46.334	4.504	45.932	4.076
47.944	4.724	46.096	4.700	47.172	4.633	46.692	4.194
48.757	4.872	47.016	4.862	47.745	4.727	47.474	4.338

49.616	5.033	47.970	5.044	48.555	4.868	48.273	4.454
50.475	5.182	48.815	5.212	49.363	5.030	48.928	4.538
51.436	5.345	49.846	5.427	50.020	5.163	49.615	4.664
53.204	5.663	51.310	5.864	50.653	5.292	50.285	4.854
54.265	5.859	51.969	6.131	51.252	5.447	50.932	5.002
54.914	5.994	52.380	6.335	51.774	5.593	52.064	5.295
55.399	6.097	52.788	6.527	52.205	5.736	52.508	5.383
55.990	6.245	53.617	6.764	52.529	5.857	52.823	5.537
56.692	6.474	54.689	7.044	52.780	6.006	53.096	5.651
56.975	6.702	55.331	7.218	52.986	6.133	53.318	5.786
57.030	6.842	55.638	7.306	53.213	6.256	53.527	5.881
57.049	6.947	55.908	7.386	53.497	6.375	53.806	6.023
57.084	7.088	56.269	7.490	53.948	6.521	54.505	6.289
57.114	7.221	56.533	7.599	54.355	6.629	55.327	6.612
57.153	7.374	56.793	7.724	54.790	6.754	55.705	6.682
57.180	7.552	56.927	7.862	55.153	6.842	56.234	6.926
57.201	7.748	56.999	8.020	55.602	6.993	56.747	7.086
57.239	7.951	57.038	8.133	55.995	7.087	57.002	7.164
		57.051	8.273	56.442	7.265	57.044	7.158
		57.001	8.316	56.794	7.466	57.071	7.165
		57.040	8.387	57.009	7.706	57.057	7.154
		57.066	8.461	57.055	7.835	57.072	7.187
		57.086	8.550	57.080	7.925	57.048	7.220
		57.083	8.663	57.061	7.970	57.062	7.219
		57.099	8.828	57.065	8.034	57.080	7.195
		57.083	9.180	57.045	8.140	57.107	7.180
				57.063	8.249	57.226	7.224
				57.078	8.348	57.340	7.379
				57.099	8.447	57.492	7.935
						57.504	8.752
						57.560	9.544
						57.580	10.227

Table S11. Experimentally measured values of pressure and mass during desorption of CO_2 in MCM-41 at +20 °C.

6 nm		8 nm		10 nm		12 nm	
Pressure	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**	**Pressure**	**Mass**
bar	**g**	**bar**	**g**	**bar**	**g**	**bar**	**g**
57.314	9.459	57.288	9.568	57.290	8.358	57.369	9.759
57.231	8.099	57.269	8.815	56.974	7.647	57.289	9.005
56.601	6.743	56.935	7.885	55.663	7.064	57.222	8.477
54.835	6.256	56.083	7.539	54.544	6.713	57.158	7.922
52.640	5.786	54.969	7.200	53.495	6.332	57.101	7.629
51.066	5.481	53.905	6.909	52.930	5.964	57.041	7.402
49.717	5.210	53.008	6.636	52.293	5.753	56.935	7.306
48.411	4.915	52.352	6.304	50.961	5.345	55.200	6.637
47.201	4.662	51.653	5.971	49.906	5.214	54.124	6.194
45.681	4.389	50.743	5.700	48.910	4.971	53.118	5.677
44.317	4.164	49.698	5.419	47.964	4.852	52.300	5.299
42.930	3.953	48.640	5.194	46.813	4.682	51.224	5.012
41.500	3.748	47.490	4.957	45.685	4.470	50.013	4.776
40.103	3.695	46.268	4.727	44.583	4.280	48.679	4.517
38.635	3.511	45.031	4.526	43.499	4.166	47.487	4.271
37.282	3.487	43.712	4.311	42.401	3.995	46.268	4.166
35.889	3.331	42.417	4.107	41.238	3.900	44.978	3.905
34.547	3.181	41.117	3.919	40.093	3.730	43.550	3.681
33.196	3.032	39.729	3.728	38.977	3.573	42.271	3.564
31.817	2.887	38.461	3.573	37.861	3.488	40.785	3.414
30.537	2.822	37.004	3.397	36.682	3.407	39.387	3.268
29.268	2.697	35.538	3.218	35.592	3.282	38.026	3.128
28.053	2.720	34.103	3.054	34.311	3.190	36.635	2.970
26.897	2.616	32.656	2.903	33.051	3.044	35.229	2.852
25.742	2.512	31.283	2.760	31.678	2.936	33.916	2.768
24.643	2.405	29.962	2.612	30.188	2.760	32.628	2.656
23.588	2.306	28.237	2.451	28.983	2.641	31.377	2.528
22.571	2.214	26.844	2.312	27.806	2.510	29.685	2.364
21.458	2.115	25.391	2.183	26.356	2.380	28.440	2.268
20.515	2.027	23.980	2.079	24.929	2.244	27.276	2.152

19.624	1.952	22.513	1.943	23.387	2.096	25.752	2.043
18.758	1.880	21.102	1.835	21.894	1.966	24.600	1.921
17.930	1.811	19.789	1.737	20.273	1.815	23.497	1.844
17.005	1.733	18.439	1.620	18.659	1.679	22.431	1.786
16.255	1.674	17.101	1.522	16.887	1.527	21.099	1.654
15.554	1.619	15.826	1.412	15.830	1.439	20.137	1.575
14.885	1.565	14.613	1.314	14.794	1.327	19.186	1.482
14.229	1.500	13.593	1.244	13.820	1.252	18.258	1.459
13.611	1.451	12.650	1.173	12.909	1.170	17.284	1.349
13.013	1.397	11.771	1.105	12.165	1.092	16.436	1.292
12.444	1.351	10.910	1.041	11.415	1.020	15.602	1.248
11.906	1.306	10.046	1.008	10.735	0.962	14.833	1.193
11.372	1.258	9.270	0.944	10.116	0.906	14.074	1.132
10.879	1.227	8.544	0.898	9.522	0.856	13.300	1.039
10.419	1.190	7.897	0.843	8.931	0.821	12.639	0.985
9.969	1.154	7.297	0.801	8.419	0.766	11.951	0.949
9.423	1.103	6.735	0.768	7.937	0.725	11.344	0.943
8.934	1.061	6.190	0.721	7.477	0.689	10.659	0.904
8.502	1.026	5.696	0.700	7.052	0.697	9.888	0.809
8.074	0.990	5.245	0.656	6.479	0.603	9.172	0.756
7.687	0.953	4.830	0.631	5.867	0.555	8.491	0.692
7.193	0.909	4.440	0.602	5.312	0.570	7.892	0.652
6.638	0.858	4.095	0.583	4.814	0.478	7.324	0.618
6.128	0.809	3.779	0.575	4.372	0.433	6.748	0.573
5.655	0.757			3.985	0.414	6.127	0.526
5.240	0.718			3.637	0.383	5.597	0.479
4.858	0.669			3.217	0.325	5.114	0.452
4.518	0.636			2.827	0.315	4.667	0.394
4.118	0.597			2.436	0.258	4.278	0.384
3.713	0.548			2.107	0.223	3.877	0.350
3.275	0.496			1.779	0.225	3.549	0.355
2.900	0.457			1.512	0.194	3.132	0.323
2.523	0.412			1.292	0.164	2.732	0.280
2.203	0.372			1.115	0.183	2.328	0.244

1.930	0.336			0.912	0.139	1.998	0.195
1.704	0.309			0.758	0.081	1.660	0.182
1.419	0.267			0.634	0.074	1.382	0.159
1.189	0.237			0.541	0.056	1.172	0.141
1.012	0.206			0.469	0.066	0.996	0.111
0.871	0.186			0.365	0.037	0.800	0.085
0.762	0.167			0.264	0.041	0.657	0.062
0.573	0.121			0.146	0.022	0.545	0.051
0.382	0.082			0.000	0.000	0.456	0.040
0.191	0.046					0.393	0.054
0.000	0.000					0.308	0.054
						0.247	0.015
						0.139	0.025
						0.000	0.000