

Electronic Supporting Information for

A Combined Experimental and Quantum Chemical Study of CO₂ Adsorption in the Metal-Organic Framework CPO-27 with Different Metals

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1. Surface area and pore volume data for CPO-27-M

Table S1. Comparison of experimentally determined pore volumes (at $p/p_0=0.5$) for CPO-27 samples in this study with values calculated on basis of crystal structure determinations.

Sample	BET surface area / m ² g ⁻¹	Langmuir surface area / m ² g ⁻¹	Pore volume / cm ³ g ⁻¹	Calc. pore volume / cm ³ g ⁻¹
CPO-27-Co, standard and high pressure data	1284	1354	0.48	0.51
CPO-27-Ni, high pressure data	1218	1312	0.47	0.48
CPO-27-Mn, standard and high pressure data	1302	1384	0.59	0.55
CPO-27-Mg, standard pressure data	1743	1876	0.66	0.65
CPO-27-Mg, high pressure data	1542	1711	0.63	0.65
CPO-27-Zn, standard pressure	947	1005	0.36	0.46

2. Experimental sorption data

Table S2. High pressure sorption isotherm data for CO₂ on CPO-27-Co at 278 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.1891	1.6334E-4	3295	0.01212
0.367	3.2743E-4	2945.7	0.01227
0.5438	4.8886E-4	2596.8	0.01238
0.7274	6.5244E-4	2239.4	0.01244
0.9028	8.1371E-4	1881.3	0.01245
1.0986	9.7972E-4	1526.3	0.0124
1.2928	0.00114	1174.1	0.01228
1.4757	0.0013	827.82	0.01203
1.6766	0.00146	691.08	0.01185
1.879	0.00162	557.84	0.01161
2.0965	0.00178	430.01	0.01128
2.31	0.00194	308.46	0.01075
2.5374	0.0021	202.72	0.00999
2.7954	0.00227	157.97	0.00944
3.0362	0.00242	117.65	0.00883
3.3112	0.00259	82.562	0.00813
3.5883	0.00274	75.688	0.00793
3.8866	0.0029	68.506	0.00775
4.1868	0.00306	61.641	0.00756
4.5272	0.00322	55.032	0.00737
4.8873	0.00338	48.755	0.00717
5.266	0.00353	42.804	0.00697
5.7094	0.00369	37.207	0.00676
6.1565	0.00384	32.024	0.00654
6.6477	0.004	27.282	0.00631
7.1699	0.00415	21.627	0.00598
7.7751	0.0043	17.855	0.00571
8.4023	0.00445	15.221	0.00547
9.1163	0.0046	13.296	0.00527
9.8961	0.00475	11.846	0.00508
10.759	0.00489	10.702	0.00491
11.716	0.00503	9.7807	0.00476
12.781	0.00517		
13.928	0.00531		
15.221	0.00544		
16.626	0.00557		
18.198	0.0057		
19.865	0.00583		
21.719	0.00595		
23.664	0.00607		

25.775	0.00619
27.991	0.00631
30.239	0.00642
32.674	0.00652
35.124	0.00663
37.733	0.00673
40.396	0.00683
43.058	0.00693
45.869	0.00703
48.914	0.00713
51.92	0.00722
54.78	0.00731
57.758	0.00739
60.849	0.00748
63.73	0.00756
66.868	0.00765
69.849	0.00772
72.921	0.0078
76.088	0.00788
79.312	0.00796
82.584	0.00803
85.765	0.0081
88.933	0.00817
92.191	0.00825
95.328	0.00831
98.233	0.00837
101.4	0.00844
118.54	0.00874
135.98	0.00902
154.86	0.00929
174.32	0.00954
194.28	0.00977
215.65	0.00998
236.76	0.01016
256.99	0.01031
283.62	0.01049
311.15	0.01065
369.12	0.01091
429.09	0.01114
490.32	0.01133
553.29	0.01148
617.42	0.01161
681.49	0.01171
745.63	0.01181
811.28	0.01189
877.49	0.01196

943.15	0.01202
1008.2	0.01207
1267.9	0.01221
1515.1	0.01229
1750.1	0.01233
1972.4	0.01235
2184.1	0.01236
2383.2	0.01236
2571.5	0.01233
2786.5	0.01228
3000.8	0.01221
3213.7	0.01213
3425.5	0.01205
3635.7	0.01192

Table S3. High pressure sorption isotherm data for CO₂ on CPO-27-Co at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.4748	1.5617E-4	4787.5	0.01052
0.98	3.1342E-4	4264.3	0.01089
1.5038	4.6946E-4	3735.3	0.01111
2.0203	6.232E-4	3197.2	0.01128
2.4974	7.7618E-4	2657.4	0.01133
2.9983	9.3503E-4	2291.3	0.01132
3.494	0.00109	1930	0.01126
3.9999	0.00125	1570.8	0.01114
4.546	0.0014	1215.2	0.01092
5.077	0.00156	869.94	0.01055
5.6348	0.00171	734.83	0.01031
6.2074	0.00186	602.43	0.01002
6.8235	0.00201	476.27	0.00962
7.4563	0.00217	355.33	0.00906
8.1187	0.00232	245.01	0.00834
8.8173	0.00247	193.63	0.00788
9.5256	0.00262	147.01	0.00735
10.252	0.00277	105.52	0.00676
11.04	0.00292	70.308	0.00608
11.863	0.00306	63.018	0.0059
12.724	0.0032	56.151	0.00572
13.632	0.00334	49.786	0.00552
14.604	0.00349	43.946	0.00531
15.661	0.00363	38.668	0.00509
16.715	0.00377	33.917	0.00487
17.906	0.00391	29.706	0.00463
19.128	0.00405	24.372	0.00425
20.457	0.00418	20.719	0.00393

21.83	0.00431	18.036	0.00365
23.286	0.00444	15.967	0.00339
24.898	0.00457	14.316	0.00317
26.557	0.00469	12.98	0.00296
28.345	0.00481	11.857	0.00277
30.249	0.00493	10.884	0.0026
32.249	0.00505	10.059	0.00244
34.38	0.00516	9.3162	0.00229
36.585	0.00527		
38.945	0.00538		
41.414	0.00548		
43.97	0.00559		
46.663	0.00569		
49.503	0.00578		
52.459	0.00588		
55.385	0.00597		
58.623	0.00606		
61.83	0.00614		
65.074	0.00623		
68.504	0.00631		
71.853	0.00639		
75.291	0.00646		
78.568	0.00653		
82.158	0.0066		
85.639	0.00667		
88.964	0.00673		
92.317	0.00679		
95.74	0.00686		
99.46	0.00692		
103.32	0.00698		
122.5	0.00727		
142.36	0.00753		
162.29	0.00777		
182.51	0.00799		
203.71	0.00821		
224.72	0.0084		
246.55	0.00858		
263.12	0.00871		
289.37	0.00889		
316.42	0.00907		
372.56	0.00938		
430.5	0.00965		
489.92	0.00989		
551.06	0.01009		
613.63	0.01026		
676.67	0.01041		

741.46	0.01054
806.44	0.01066
870.83	0.01076
935.51	0.01085
1001.3	0.01094
1255.5	0.01116
1502.7	0.01131
1734.5	0.0114
1959.1	0.01148
2168	0.01152
2373.1	0.01153
2592.5	0.01154
2813.7	0.01154
3033.8	0.0115
3408.2	0.0114
3778.5	0.01134
4152.8	0.01112
4528.4	0.01097
4913	0.01065
5302.4	0.00999

Table S4. High pressure sorption isotherm data for CO₂ on CPO-27-Co at 313 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
0.8466	1.4514E-4	4522.5	0.01045
1.6999	2.9178E-4	3977.2	0.01072
2.5631	4.351E-4	3429.2	0.01092
3.4498	5.8453E-4	2878	0.01095
4.3686	7.3355E-4	2508.7	0.01093
5.2834	8.814E-4	2140.9	0.01089
6.2081	0.00103	1777.1	0.01076
7.1333	0.00117	1417.9	0.01054
8.1092	0.00131	1067.3	0.0102
9.0769	0.00146	729.22	0.00962
10.06	0.0016	598.32	0.00928
11.12	0.00174	473.04	0.00884
12.177	0.00188	350.91	0.00826
13.266	0.00202	239.17	0.00753
14.38	0.00216	187.53	0.00709
15.54	0.00229	140.44	0.00658
16.75	0.00243	99.389	0.00597
17.995	0.00256	91.196	0.0058
19.312	0.0027	83.013	0.00563
20.673	0.00284	75.387	0.00546
22.069	0.00297	68.232	0.00527
23.541	0.0031	61.544	0.00507

25.062	0.00323	55.417	0.00487
26.656	0.00336	49.785	0.00466
28.312	0.00348	44.612	0.00443
30.085	0.00361	39.889	0.0042
31.867	0.00373	35.589	0.00396
33.838	0.00386	31.674	0.00372
35.73	0.00397	28.104	0.00346
37.786	0.00409	23.609	0.00309
39.961	0.0042	20.241	0.00278
42.136	0.00431	17.58	0.0025
44.379	0.00442	15.434	0.00226
46.814	0.00453	13.661	0.00204
49.369	0.00463	12.171	0.00185
51.975	0.00473	10.888	0.00168
54.557	0.00483	9.7818	0.00153
57.398	0.00493		
60.268	0.00502		
63.211	0.00511		
66.303	0.0052		
69.303	0.00528		
72.291	0.00536		
75.526	0.00544		
78.745	0.00551		
82.064	0.00559		
85.446	0.00566		
88.931	0.00573		
92.51	0.0058		
96.176	0.00586		
99.648	0.00593		
103.49	0.00599		
122.65	0.00628		
142.36	0.00653		
163.38	0.00678		
184.47	0.00699		
205.51	0.00719		
227.66	0.00737		
248.93	0.00753		
275.88	0.00773		
303.04	0.0079		
359.54	0.00822		
416.91	0.00851		
476.41	0.00876		
536.6	0.00899		
598.86	0.00919		
660.75	0.00936		
724.16	0.00952		

787.81	0.00965
851.85	0.00978
916.7	0.00989
982.7	0.00999
1048.5	0.01008
1253.6	0.01031
1568.7	0.01056
1869.8	0.01071
2153.5	0.01081
2420	0.01087
2671	0.01091
2906.5	0.01092
3135.7	0.01093
3513.2	0.01093
3894	0.01088
4277.7	0.01076
4666.5	0.01056
5058	0.01018

Table S5. High pressure sorption isotherm data for CO₂ on CPO-27-Co at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
2.147	1.2076E-4	4632.3	0.00956
4.2722	2.3832E-4	4077.2	0.00969
6.4959	3.5945E-4	3517.6	0.00974
8.7375	4.7988E-4	2958.5	0.0097
10.956	5.9742E-4	2582.6	0.00963
13.229	7.1557E-4	2210	0.00949
15.49	8.3099E-4	1843.1	0.00929
17.761	9.4493E-4	1480.5	0.00899
20.045	0.00106	1126.3	0.00856
22.405	0.00117	785.91	0.00792
24.729	0.00128	653.26	0.00758
27.091	0.00139	524.5	0.00716
29.511	0.0015	401.55	0.00665
31.94	0.00161	285.63	0.00598
34.514	0.00172	230.53	0.00555
36.962	0.00182	181.5	0.00505
39.596	0.00193	137.9	0.00447
42.189	0.00203	100.44	0.00378
44.766	0.00213	71.592	0.00304
47.555	0.00224	65.036	0.00284
50.258	0.00233	58.757	0.00263
53.134	0.00244	52.795	0.00243
55.929	0.00253	47.043	0.00221
58.858	0.00263	41.54	0.002

61.814	0.00273	36.239	0.00178
64.631	0.00281	31.123	0.00156
67.505	0.0029	26.193	0.00133
70.502	0.00299	19.962	0.00103
73.534	0.00308	15.375	8.0153E-4
76.568	0.00316	11.929	6.2214E-4
79.692	0.00325	9.3041	4.8215E-4
82.734	0.00333		
85.952	0.00341		
89.144	0.00348		
92.137	0.00356		
95.304	0.00363		
98.59	0.0037		
101.68	0.00377		
118.75	0.00409		
136.52	0.0044		
155.69	0.00468		
175.57	0.00494		
195.91	0.00516		
217.03	0.00538		
238.1	0.00556		
257.99	0.00572		
284.58	0.00592		
311.7	0.0061		
368.77	0.00642		
427.79	0.0067		
487.72	0.00696		
549.46	0.00718		
611.35	0.00738		
673.48	0.00756		
736.47	0.00773		
800.72	0.00789		
865.09	0.00803		
930.34	0.00816		
995.97	0.00827		
1061.1	0.00839		
1267.4	0.00867		
1478.9	0.00891		
1817.1	0.0092		
2127.7	0.00939		
2419.4	0.00952		
2698	0.00959		
2958.8	0.00965		
3205.5	0.00967		
3593.3	0.00969		
3982.2	0.00964		

4376.6	0.00958
4776.7	0.00945
5182.9	0.00921

Table S6. High pressure sorption isotherm data for CO₂ on CPO-27-Co at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
4.062	7.938E-5	4473.4	0.00786
8.1689	1.5795E-4	3907.1	0.00802
12.296	2.3495E-4	3340.5	0.00804
16.35	3.0928E-4	2774.6	0.00795
20.48	3.8442E-4	2400.7	0.00779
24.577	4.5856E-4	2027.9	0.00756
28.761	5.3309E-4	1660.5	0.00725
32.851	6.0575E-4	1300.1	0.00682
37.018	6.7842E-4	951.85	0.00621
41.158	7.4983E-4	815.41	0.00588
45.37	8.2104E-4	682.46	0.0055
49.535	8.9101E-4	555.09	0.00505
53.882	9.6264E-4	433.67	0.00449
57.865	0.00103	316.47	0.00378
62.177	0.0011	211.84	0.00292
66.26	0.00117	163.33	0.0024
70.393	0.00123	118.81	0.00183
74.646	0.0013	76.947	0.00123
78.74	0.00136	67.983	0.00109
82.62	0.00142	58.953	9.371E-4
86.597	0.00148	50.101	7.8839E-4
90.533	0.00154	41.552	6.3779E-4
94.212	0.00159	33.029	4.8615E-4
97.914	0.00165	24.665	3.3171E-4
101.94	0.0017	14.509	1.3975E-4
121.88	0.00197	8.6519	2.5013E-5
142.68	0.00223		
163.58	0.00248		
184.74	0.00271		
205.25	0.00292		
226.75	0.00312		
248.88	0.00332		
275.1	0.00354		
301.37	0.00374		
356.07	0.00411		
412.46	0.00444		
470.88	0.00473		
530.4	0.005		
592.26	0.00524		

654.42	0.00546
716.67	0.00566
780.54	0.00583
844.18	0.00599
908.61	0.00615
973.15	0.00628
1036.9	0.00641
1336.3	0.00689
1617.7	0.00723
1890	0.0075
2148.8	0.00768
2393.8	0.00782
2624.2	0.00793
2843.4	0.00803
3051.3	0.00809
3439.1	0.00815
3830.7	0.00814
4227	0.00808
4628.1	0.00782
5036.6	0.00745

Table S7. High pressure sorption isotherm data for CO₂ on CPO-27-Co at 473 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
6.8743	2.608E-5	4491.1	0.00516
13.656	5.1276E-5	3918.9	0.00516
20.195	7.5276E-5	3347.9	0.00503
26.803	9.9585E-5	2776.3	0.00476
33.313	1.2354E-4	2399.9	0.00449
39.754	1.4724E-4	2025.1	0.00415
46.288	1.7131E-4	1655.7	0.00373
52.973	1.9507E-4	1292.7	0.00322
59.716	2.194E-4	939.12	0.0026
66.041	2.4198E-4	798.24	0.00229
72.193	2.6413E-4	660.1	0.00196
78.067	2.8506E-4	524.31	0.00161
84.289	3.0696E-4	390.6	0.00122
90.303	3.2813E-4	256.7	8.0588E-4
96.139	3.4843E-4	189.45	5.8182E-4
101.71	3.6761E-4	124.42	3.508E-4
131.6	4.7152E-4	60.666	1.1846E-4
161.22	5.7245E-4	47.784	6.7226E-5
190.11	6.6981E-4	34.346	1.4194E-5
218.34	7.6134E-4		
245.88	8.5019E-4		
267.03	9.1557E-4		

299.27	0.00102
331.52	0.00112
396.7	0.00131
461.86	0.0015
527.57	0.00168
593.9	0.00185
660.29	0.00202
726.52	0.00217
792.08	0.00232
858.43	0.00246
924.46	0.0026
990.91	0.00273
1057	0.00286
1351.8	0.00336
1633.8	0.00375
1903.3	0.00407
2156.3	0.00431
2398.1	0.00451
2625.9	0.00469
2842.1	0.00481
3048.6	0.00493
3440.4	0.0051
3836.7	0.00519
4237.4	0.00521
4640.5	0.00519
5055.7	0.00495

Table S8. High pressure sorption isotherm data for CH₄ on CPO-27-Co at 278 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.2605	1.6795E-4	9849.2	0.00711
18.128	4.1743E-4	9172	0.00737
28.835	6.5975E-4	8509.1	0.00756
39.57	8.9796E-4	7864.1	0.00774
50.223	0.00113	7232.1	0.00788
60.876	0.00135	6612.1	0.00803
71.528	0.00157	6002.5	0.00814
82.451	0.00178	5408.5	0.00821
91.96	0.00197	4838.5	0.00826
101.34	0.00214	4456.2	0.00827
117.6	0.00243	4081.8	0.00829
134.26	0.00269	3729.1	0.00827
151.32	0.00295	3158.4	0.00822
168.8	0.00319	2596.6	0.00809
185.52	0.00341	2044.8	0.00786
203.38	0.00362	1514.5	0.0075

220.32	0.00381	1000.5	0.00688
237.52	0.00399	507.31	0.00562
254.22	0.00415	331.66	0.0047
278.44	0.00436	185.7	0.00335
303.28	0.00456	152.22	0.0029
409.77	0.00523	121.59	0.00242
523.24	0.00575	93.075	0.00192
641.78	0.00616	80.345	0.00168
762.92	0.00648	68.064	0.00144
886.11	0.00674	56.222	0.00119
1013.3	0.00697	44.612	9.4112E-4
1357.8	0.00742		
1710.8	0.00772		
2068.4	0.00794		
2428.8	0.00811		
2790.4	0.0082		
3154.7	0.00829		
3517.9	0.00834		
3881.6	0.00836		
4242.9	0.00833		
4606.3	0.00833		
4968.5	0.00831		
5335.4	0.00826		
5914	0.00814		
6495.8	0.00805		
7076.2	0.00793		
7653.9	0.00775		
8231.4	0.00761		
8811.9	0.00743		
9391.6	0.00728		
9975	0.00705		
10559	0.00682		

Table S9. High pressure sorption isotherm data for CH₄ on CPO-27-Co at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
14.018	1.8508E-4	9633.2	0.00728
27.86	3.6571E-4	8935.5	0.00746
41.632	5.4289E-4	8251.8	0.00759
55.294	7.1607E-4	7592.9	0.00767
68.565	8.8103E-4	6953.2	0.00776
82.246	0.00105	6328.5	0.00785
93.738	0.00119	5728.4	0.00786
105	0.00132	5145.9	0.0079
124.44	0.00154	4579.4	0.0079
144.19	0.00175	4204.2	0.00788

163.19	0.00196	3834.6	0.00784
181.81	0.00214	3486	0.00779
201.12	0.00233	2917.1	0.00765
219.8	0.0025	2351.3	0.00741
240.3	0.00268	1797.7	0.00705
256.36	0.00282	1270	0.00648
281.43	0.00302	771.36	0.0055
306.98	0.00321	582.28	0.00488
414.58	0.0039	390.76	0.00396
527.82	0.00446	231.04	0.0028
645.73	0.00492	190.64	0.00243
766.43	0.00529	153.44	0.00205
889.66	0.0056	117.89	0.00166
1012.6	0.00587	83.608	0.00126
1360.4	0.00641	68.533	0.00108
1716.1	0.00679	53.671	8.8937E-4
2075	0.00706	39.094	7.0361E-4
2438.3	0.00727		
2803	0.00742		
3168.8	0.00754		
3535.1	0.00764		
3904.9	0.00769		
4275.6	0.00773		
4643.8	0.00777		
5013.4	0.00778		
5603.8	0.00775		
6192.5	0.00769		
6784.3	0.0076		
7375.9	0.00754		
7968	0.00748		
8557.1	0.00735		
9145.2	0.00727		
9742.8	0.00717		
10344	0.00705		

Table S10. High pressure sorption isotherm data for CH₄ on CPO-27-Co at 313 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
10.718	9.8244E-5	9690.9	0.00699
26.446	2.4134E-4	9138.2	0.00707
42.172	3.8278E-4	8578.8	0.00718
57.638	5.1986E-4	8035.1	0.00727
72.986	6.5446E-4	7519.1	0.00733
87.815	7.8227E-4	7009.6	0.00735
101.04	8.935E-4	6502.4	0.00738
123.34	0.00108	6030.7	0.00738

145.51	0.00126	5564.7	0.00737
166.92	0.00143	5105.7	0.00736
187.97	0.00159	4660.8	0.00731
209.48	0.00175	4268.8	0.00726
229.21	0.00189	3902.9	0.00719
250.37	0.00203	3549.9	0.0071
276.57	0.00221	2969.8	0.00691
303.23	0.00238	2398.2	0.00664
414.17	0.00301	1854.8	0.00624
529.48	0.00355	1326.7	0.00562
648.27	0.00402	825.05	0.00461
770.69	0.00441	368.32	0.00281
893.57	0.00474	168.51	0.00148
1016.9	0.00503	115.87	0.00105
1362.9	0.00563	65.516	6.2675E-4
1717.3	0.00606	48.969	4.8099E-4
2077	0.00638		
2440.8	0.00662		
2807.6	0.00681		
3174.7	0.00695		
3545.6	0.00705		
3916.6	0.00714		
4286.4	0.00721		
4656.7	0.00726		
5029.7	0.0073		
5626.3	0.00728		
6221.6	0.00728		
6819.1	0.00727		
7417.4	0.00723		
8015.2	0.00716		
8616.6	0.00706		
9217.1	0.00696		
9819.4	0.00691		
10417	0.00683		

Table S11. High pressure sorption isotherm data for CH₄ on CPO-27-Co at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
12.627	6.1014E-5	9259.3	0.00639
31.005	1.4975E-4	8543	0.0064
49.154	2.3642E-4	7843.6	0.00645
67.038	3.2104E-4	7186.1	0.00644
84.471	4.0273E-4	6434.7	0.00641
99.796	4.7551E-4	5802.5	0.00636
114.46	5.4144E-4	5185.8	0.00629
139.6	6.5376E-4	4594.3	0.0062

164.17	7.6847E-4	4204.8	0.0061
188.98	8.7608E-4	3837.1	0.006
211.62	9.7158E-4	3487.6	0.00587
234.87	0.00107	2910.1	0.0056
258	0.00116	2338.7	0.00521
287.67	0.00129	1779.4	0.00467
317.76	0.00141	1250.6	0.00392
439.5	0.00186	746.66	0.00282
562.04	0.00228	551.32	0.00224
685.63	0.00266	347.78	0.00151
811.01	0.003	164.59	7.5234E-4
935.45	0.0033	118.26	5.3889E-4
1061.1	0.00357	73.011	3.3017E-4
1411.9	0.00418	53.382	2.3614E-4
1768.3	0.00466	34.217	1.4302E-4
2132	0.00504		
2498.1	0.00533		
2867.7	0.00557		
3238.9	0.00576		
3613.2	0.00593		
3987.8	0.00607		
4364.3	0.00616		
4739.2	0.00624		
5116.8	0.00629		
5720	0.00639		
6326.5	0.00644		
6932.7	0.00649		
7542.8	0.00646		
8149.2	0.00647		
8759.5	0.00648		
9376.1	0.00639		
9989.3	0.00631		

Table S12. High pressure sorption isotherm data for CH₄ on CPO-27-Co at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
13.79	3.6987E-5	8797.4	0.00525
33.988	9.0792E-5	8116.1	0.00527
53.907	1.4283E-4	7437.1	0.00528
73.313	1.9328E-4	6770.3	0.00521
92.739	2.4322E-4	6140.9	0.00517
109.57	2.8654E-4	5525.8	0.00508
138.12	3.5748E-4	4918.4	0.00496
165.4	4.3003E-4	4521.3	0.00485
191.61	4.9214E-4	4138.2	0.00474
216.25	5.5309E-4	3762.1	0.00459

243.23	6.185E-4	3169.1	0.0043
260.81	6.5701E-4	2590.8	0.00392
292.8	7.3505E-4	2018.9	0.00344
324.78	8.0942E-4	1478	0.00284
457.01	0.0011	948.99	0.00206
587.8	0.00138	739.16	0.00168
718.63	0.00164	533.35	0.00126
848.29	0.00189	326.44	7.9709E-4
980.19	0.00211	126.98	3.1119E-4
1110.9	0.00233	76.507	1.8351E-4
1471.1	0.00284	48.1	1.0838E-4
1834.5	0.00326		
2200.8	0.00363		
2571.7	0.00393		
2944.7	0.00418		
3318.8	0.00439		
3695.7	0.00456		
4072.3	0.00471		
4449.3	0.00484		
4827.5	0.00495		
5207.4	0.00504		
5818.1	0.00513		
6428.3	0.00517		
7041.4	0.00518		
7654.3	0.00522		
8266.7	0.00523		
8885.1	0.00521		
9502.4	0.0052		

Table S13. High pressure sorption isotherm data for CH₄ on CPO-27-Co at 473 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
15.108	1.4938E-5	9519.9	0.00335
37.154	3.647E-5	8786.2	0.00333
58.887	5.7723E-5	8077.9	0.00333
79.444	7.7789E-5	7391.2	0.00329
99.725	9.7132E-5	6717.2	0.00322
117.27	1.1594E-4	5944.6	0.00314
148.9	1.4606E-4	5311.9	0.003
178.31	1.7024E-4	4698.2	0.00285
206.81	1.9898E-4	4296.8	0.00273
234.95	2.2618E-4	3908.3	0.0026
260.3	2.4688E-4	3538.3	0.00247
296.19	2.8107E-4	2935.6	0.00221
331.38	3.1345E-4	2346.3	0.00191
475.16	4.4337E-4	1764.2	0.00156

618.1	5.6944E-4	1200.5	0.00117
757.75	6.8724E-4	646.49	7.2562E-4
897.78	8.011E-4	425.29	5.3058E-4
1034.1	9.1194E-4	203.3	3.2561E-4
1413.7	0.00119	145.89	2.6643E-4
1792.3	0.00145	89.572	2.1433E-4
2172.2	0.00167	58.532	1.8126E-4
2553.6	0.00189	27.941	1.5044E-4
2936.2	0.00208		
3320.8	0.00224		
3703.5	0.0024		
4088.9	0.00253		
4474.5	0.00264		
4862	0.00275		
5250.9	0.00284		
5871.7	0.00298		
6493.3	0.00308		
7116.9	0.00317		
7741.6	0.00323		
8367.8	0.00328		
8992.2	0.00331		
9621.4	0.0033		
10254	0.00329		

Table S14. High pressure sorption isotherm data for N₂ on CPO-27-Co at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
5.7608	4.3525E-5	5482.8	0.0063
17.012	1.2735E-4	4793.1	0.0062
28.088	2.0844E-4	4296.8	0.0061
39.065	2.8753E-4	3804.3	0.00597
50.116	3.6563E-4	3329.1	0.00582
61.068	4.4166E-4	2870.5	0.00563
71.894	5.1525E-4	2427.5	0.00539
82.344	5.853E-4	1890.8	0.005
92.992	6.552E-4	1365.4	0.00443
102.22	7.1648E-4	859.79	0.00358
127.42	8.7492E-4	663.81	0.00309
152.46	0.00102	474.88	0.0025
176.69	0.00117	291.23	0.00174
200.13	0.0013	243.9	0.00151
223.04	0.00142	197.78	0.00127
246.93	0.00154	154.02	0.00102
264.27	0.00163	111.8	7.5951E-4
292.77	0.00177	70.853	4.9525E-4
321.41	0.0019	39.377	2.7626E-4

448.42	0.00241	16.803	1.1198E-4
576.92	0.00285	7.254	4.0224E-5
705	0.00322		
833.35	0.00353		
960.36	0.0038		
1086.6	0.00403		
1427.2	0.00451		
1775.2	0.0049		
2127.1	0.00519		
2483.1	0.00543		
2840.7	0.00561		
3201.7	0.00577		
3562.4	0.00589		
3925.5	0.00599		
4290	0.00608		
4653.5	0.00616		
5018.6	0.00624		
5604.1	0.00631		
6192	0.00638		

Table S15. High pressure sorption isotherm data for N₂ on CPO-27-Co at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
6.8815	1.7615E-5	5344	0.00471
20.561	5.2571E-5	4628	0.00452
34.268	8.7342E-5	4122	0.00434
47.794	1.2141E-4	3621.7	0.00413
61.092	1.5475E-4	3143.5	0.00388
74.199	1.8722E-4	2587.7	0.00355
86.858	2.1845E-4	2039.1	0.00313
99.255	2.4887E-4	1501.7	0.0026
110.18	2.7889E-4	974.61	0.00192
139.88	3.47E-4	764.78	0.00159
169.32	4.1612E-4	558.02	0.00123
197.92	4.8281E-4	349.71	8.2254E-4
225.19	5.4585E-4	149.25	3.761E-4
253.55	6.0791E-4	98.909	2.539E-4
286.49	6.8153E-4	77.372	2.0047E-4
319.3	7.5274E-4	56.063	1.4696E-4
455.46	0.00103	35.003	9.3616E-5
589.02	0.00129	10.635	3.0745E-5
721.09	0.00152	3.2773	1.0963E-5
850.51	0.00173		
977.83	0.00193		
1118	0.00213		
1469.7	0.00257		

1825.8	0.00294
2184.1	0.00325
2546.3	0.00352
2909.2	0.00376
3275.2	0.00395
3641.3	0.00413
4008.8	0.00427
4379.2	0.00442
4750.5	0.00455
5122	0.00465
5717.5	0.0048
6077.5	0.00487

Table S16. High pressure sorption isotherm data for N₂ on CPO-27-Co at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.524	1.0211E-5	5597.3	0.00355
22.071	3.0029E-5	4888.2	0.00336
36.491	4.9253E-5	4378.3	0.00319
50.912	6.8452E-5	3880	0.00301
64.699	8.6878E-5	3401.8	0.00281
78.405	1.0518E-4	2938.7	0.00259
91.697	1.2238E-4	2377.7	0.00228
103.88	1.3895E-4	1821.9	0.00191
136.32	1.8175E-4	1274.2	0.00147
167.88	2.2347E-4	734.61	9.5646E-4
197.93	2.6104E-4	519.25	7.189E-4
226.67	2.9822E-4	301.72	4.6334E-4
254.2	3.3E-4	89.052	1.9221E-4
288.86	3.757E-4	66.417	1.614E-4
323.52	4.185E-4	44.041	1.3069E-4
480.07	6.0447E-4	21.845	9.9654E-5
633.46	7.7443E-4	5.7859	7.6146E-5
783.43	9.3459E-4		
929.94	0.00108		
1073.7	0.00122		
1435.6	0.00154		
1800.3	0.00182		
2166.6	0.00207		
2534.4	0.00229		
2902.6	0.0025		
3272.7	0.0027		
3643.3	0.00287		
4016.4	0.00303		
4389.5	0.00317		
4763	0.0033		

5138.3	0.0034
5735.4	0.00358
6337.3	0.0037

Table S17. High pressure sorption isotherm data for N₂ on CPO-27-Co at 473 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.9848	3.7383E-6	5807.1	0.00185
23.362	1.1201E-5	5082.1	0.00172
38.607	1.8621E-5	4378.3	0.00158
53.724	2.5979E-5	3873.9	0.00147
68.076	3.2928E-5	3392.8	0.00133
82.748	4.0026E-5	2921.7	0.00119
96.773	4.6876E-5	2464.2	0.00104
109.68	5.4532E-5	1889.4	8.3304E-4
143.5	7.0385E-5	1318.2	6.113E-4
175.82	8.5432E-5	752.39	3.6925E-4
206.94	1.0152E-4	526.11	2.6533E-4
238.16	1.1521E-4	296	1.5498E-4
266.67	1.313E-4	234.11	1.2121E-4
303.61	1.4652E-4	174.6	9.2938E-5
478.01	2.2959E-4	117.11	6.2289E-5
647.73	3.0775E-4	60.743	3.384E-5
812.61	3.856E-4	26.484	1.5433E-5
974.02	4.5348E-4	5.9346	2.6707E-6
1131	5.206E-4		
1509.6	6.7273E-4		
1888.3	8.169E-4		
2268	9.4714E-4		
2647.4	0.00109		
3029.4	0.0012		
3410.6	0.00131		
3792.5	0.00141		
4173.7	0.00151		
4557	0.0016		
4940.4	0.00169		
5324.6	0.00177		
5935.3	0.00188		
6550	0.00198		

Table S18. High pressure sorption isotherm data for CO₂ on CPO-27-Mg at 278 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
0.02074	2.06487E-4	3276	0.01548
0.04258	4.18694E-4	2939.2	0.0154
0.06228	6.29339E-4	2591.6	0.01534

0.08395	8.39743E-4	2240	0.01526
0.1063	0.00105	1886.2	0.01515
0.13	0.00127	1533	0.015
0.1562	0.00148	1182.6	0.01475
0.1827	0.00169	838.52	0.01436
0.2173	0.0019	702.54	0.0141
0.2479	0.0021	570.24	0.01377
0.2857	0.00231	443.74	0.01333
0.3254	0.00252	322.63	0.01265
0.3725	0.00272	215.66	0.0117
0.4225	0.00293	169.33	0.01104
0.4772	0.00313	127.13	0.0103
0.5347	0.00334	89.845	0.00947
0.5996	0.00355	82.411	0.00925
0.6766	0.00376	74.584	0.00903
0.7798	0.00396	67.082	0.00881
0.8735	0.00416	59.751	0.00859
1.0059	0.00437	52.638	0.00836
1.1651	0.00457	45.746	0.00812
1.3596	0.00477	39.121	0.00789
1.6136	0.00498	32.723	0.00765
1.9099	0.00518	26.603	0.0074
2.3159	0.00537	18.962	0.00706
2.8471	0.00557	14.023	0.0068
3.5624	0.00575	10.759	0.0066
4.5312	0.00594	8.5573	0.00644
5.7442	0.00611		
7.2749	0.00627		
9.1369	0.00642		
11.245	0.00657		
13.575	0.00671		
16.046	0.00685		
18.607	0.00698		
21.367	0.00711		
24.158	0.00723		
26.993	0.00735		
29.937	0.00748		
32.946	0.00759		
35.92	0.00771		
38.936	0.00782		
42.059	0.00793		
45.042	0.00804		
48.304	0.00815		
51.583	0.00826		
54.79	0.00836		
57.951	0.00846		

61.183	0.00856
64.481	0.00866
67.756	0.00876
71.059	0.00885
74.434	0.00895
77.732	0.00904
80.931	0.00913
84.289	0.00922
87.64	0.0093
90.927	0.00939
94.314	0.00947
97.525	0.00955
100.8	0.00963
118.28	0.01
136.7	0.01036
155.19	0.01069
174.79	0.011
195.67	0.01129
216.01	0.01155
237.7	0.01179
257.08	0.01199
283.21	0.01222
310.07	0.01243
366.93	0.01279
425.59	0.0131
486.68	0.01336
548.18	0.01357
610.18	0.01375
673.42	0.01391
737.42	0.01405
802.27	0.01417
867.1	0.01428
931.01	0.01437
996.67	0.01445
1060.8	0.01453
1298.4	0.01474
1527.4	0.01489
1743.8	0.01501
1949.9	0.01508
2144.3	0.01515
2357.5	0.01523
2569.6	0.01528
2781.3	0.0153
2992.1	0.01536
3199.5	0.01544
3406.6	0.0155

3609.2

0.01567

Table S19. High pressure sorption isotherm data for CO₂ on CPO-27-Mg at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.06908	2.14612E-4	4764.8	0.01385
0.1276	4.2404E-4	4421.6	0.01408
0.2014	6.34086E-4	4073.7	0.01429
0.269	8.40613E-4	3721.5	0.01443
0.3443	0.00105	3366.5	0.01447
0.4266	0.00125	3004.8	0.01448
0.5165	0.00146	2645.2	0.01444
0.6026	0.00168	2427.2	0.01439
0.7102	0.00189	2207	0.01433
0.8203	0.00209	1986.8	0.01423
0.9488	0.00231	1769.7	0.01411
1.0868	0.00252	1553.9	0.01395
1.2382	0.00272	1339	0.01374
1.3956	0.00293	1126.8	0.01349
1.5815	0.00313	919.63	0.01314
1.7893	0.00333	816.75	0.01291
2.0192	0.00353	716.12	0.01265
2.2787	0.00373	617.54	0.01234
2.5747	0.00393	521.88	0.01197
2.915	0.00413	430.27	0.01152
3.3302	0.00434	338.3	0.01094
3.8121	0.00454	254.21	0.01023
4.3848	0.00473	213.34	0.00983
5.0489	0.00493	174.75	0.00939
5.8496	0.00511	138.57	0.00892
6.8469	0.0053	104.75	0.00842
8.0055	0.00547	69.922	0.00782
9.4489	0.00564	60.95	0.00763
11.131	0.0058	52.163	0.00745
13.136	0.00596	43.79	0.00726
15.424	0.0061	35.835	0.00705
18.059	0.00624	28.45	0.00684
20.883	0.00636	19.26	0.0065
23.944	0.00648	14.261	0.00624
27.313	0.0066	11.314	0.00603
30.73	0.0067	9.3986	0.00584
34.278	0.0068		
37.876	0.0069		
41.528	0.00699		
45.384	0.00708		
49.39	0.00718		

53.402	0.00726
57.269	0.00735
61.347	0.00743
65.212	0.00751
69.452	0.00759
73.448	0.00766
77.627	0.00774
81.473	0.00781
85.369	0.00788
89.376	0.00794
93.28	0.00801
97.332	0.00808
101.12	0.00814
121.93	0.00845
143.46	0.00875
164.7	0.00903
185.82	0.00928
207.7	0.00953
229.65	0.00976
250.66	0.00996
276.98	0.01019
304.1	0.01042
360.19	0.01082
417.42	0.01117
476.24	0.01149
536.58	0.01176
597.94	0.01201
660.91	0.01222
724.08	0.01242
787.08	0.01258
850.92	0.01274
914.86	0.01288
978.94	0.01299
1045.7	0.01311
1180.9	0.01331
1316.4	0.01347
1452	0.01362
1588.1	0.01374
1725.1	0.01384
1990.8	0.01398
2245.6	0.0141
2491	0.01417
2719.4	0.01424
2927.8	0.01427
3137	0.01428
3332.3	0.0143

3552	0.01427
3771	0.01425
3991	0.01421
4211	0.01414
4432.9	0.01401
4655.9	0.01387
4875.2	0.01372
5102.3	0.01358

Table S20. High pressure sorption isotherm data for CO₂ on CPO-27-Mg at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
0.5455	2.02485E-4	4854.6	0.01181
1.1567	4.00361E-4	4643.2	0.01188
1.8058	6.01276E-4	4432.1	0.01193
2.4818	7.96422E-4	4218.4	0.01196
3.2079	9.93174E-4	4002.6	0.01198
3.9605	0.00119	3785.2	0.01197
4.7548	0.00138	3565	0.01194
5.5892	0.00157	3344	0.0119
6.4889	0.00176	3120.9	0.01186
7.4429	0.00195	2898.2	0.01176
8.4529	0.00214	2671.9	0.01168
9.5391	0.00232	2449.7	0.01156
10.73	0.00251	2224.9	0.01144
11.987	0.00269	2002.2	0.01126
13.312	0.00287	1778.7	0.01106
14.747	0.00304	1558.5	0.01082
16.319	0.00322	1339.5	0.01052
17.984	0.00338	1126.7	0.01018
19.794	0.00355	916.35	0.00976
21.664	0.00371	811.23	0.00952
23.719	0.00386	707.78	0.00924
25.908	0.00401	605.88	0.00894
28.326	0.00417	506.47	0.00862
30.801	0.00431	409.71	0.00824
33.345	0.00444	310.65	0.0078
36.176	0.00457	217.94	0.00729
39.125	0.0047	173.1	0.00698
42.302	0.00482	131.32	0.00662
45.589	0.00494	93.568	0.00619
49.073	0.00505	83.35	0.00603
52.702	0.00515	73.675	0.00586
56.658	0.00526	64.51	0.00567
60.643	0.00536	56.086	0.00548
64.769	0.00545	48.437	0.00526

68.933	0.00554	41.538	0.00503
73.168	0.00562	35.39	0.00477
77.331	0.0057	29.98	0.0045
81.602	0.00577	23.141	0.00407
85.865	0.00584	18.77	0.0037
90.481	0.0059	15.734	0.0034
94.924	0.00597	13.485	0.00313
99.453	0.00603	11.751	0.0029
103.88	0.00608	10.369	0.0027
127.33	0.00634	9.2441	0.00251
152.74	0.00657		
177.79	0.00677		
202.14	0.00694		
227.83	0.00711		
253.14	0.00726		
283.1	0.00742		
313.58	0.00758		
375.28	0.00786		
438.08	0.00812		
501.06	0.00836		
564.59	0.00858		
628.43	0.00879		
693.11	0.00898		
757.6	0.00915		
822.68	0.00932		
888.39	0.00948		
953.92	0.00962		
1019.1	0.00976		
1155.3	0.01001		
1293.5	0.01024		
1432.2	0.01044		
1571.2	0.01061		
1835.5	0.0109		
2077.6	0.01109		
2323.7	0.01127		
2555.9	0.0114		
2780.7	0.01152		
2986.9	0.01163		
3184.7	0.01167		
3389.6	0.01173		
3597.8	0.01176		
3799.2	0.01183		
4030.9	0.01186		
4263.8	0.01188		
4497.3	0.01189		
4735.7	0.01185		

4972.1	0.01157
5208.9	0.01156

Table S21. High pressure sorption isotherm data for CO₂ on CPO-27-Mg at 393 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
1.7792	1.66891E-4	4466.4	0.0092
3.6632	3.28786E-4	3897.3	0.00937
5.6612	4.89739E-4	3330	0.00936
7.6867	6.4549E-4	2764.2	0.00923
9.7821	7.99367E-4	2384.6	0.00906
11.944	9.51459E-4	2012.3	0.00881
14.197	0.0011	1641.4	0.00849
16.488	0.00125	1277.2	0.00807
18.97	0.00139	920.47	0.00752
21.511	0.00154	777.93	0.00724
24.135	0.00168	638.5	0.00692
26.813	0.00181	502.37	0.00654
29.648	0.00195	371.46	0.00607
32.529	0.00208	246.03	0.00542
35.49	0.00221	187.54	0.00498
38.376	0.00234	135.71	0.00441
41.563	0.00246	91.21	0.00371
44.761	0.00258	82.611	0.00351
47.996	0.00269	73.792	0.00332
51.362	0.0028	65.547	0.00311
54.738	0.00291	57.883	0.00289
58.212	0.00301	50.764	0.00266
61.746	0.00312	44.025	0.00242
65.341	0.00321	37.653	0.00217
68.877	0.00331	31.8	0.00191
72.501	0.0034	26.291	0.00164
76.24	0.00349	19.593	0.00127
80.283	0.00358	15.023	9.90988E-4
84.097	0.00366	11.747	7.68002E-4
87.687	0.00374	9.3078	5.90925E-4
91.691	0.00382		
95.769	0.00389		
99.848	0.00396		
104.04	0.00404		
125.29	0.00436		
147.22	0.00463		
170.33	0.00488		
194.09	0.0051		
218.15	0.00529		
242.73	0.00546		

262.54	0.00559
292.36	0.00576
322.8	0.00592
386.03	0.00619
450.23	0.00643
515.41	0.00664
582.04	0.00683
648.43	0.00701
714.86	0.00716
781.9	0.00731
848.03	0.00744
915.23	0.00757
982.62	0.00769
1050.6	0.0078
1261.9	0.0081
1572.3	0.00847
1851.8	0.00875
2118.3	0.00896
2376.8	0.00912
2613.8	0.00924
2840.2	0.00935
3056.7	0.00943
3442.1	0.0095
3833.2	0.00947
4225.9	0.00942
4624.4	0.0092
5029.7	0.00885

Table S22. High pressure sorption isotherm data for CO₂ on CPO-27-Mg at 473 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
5.6836	7.11074E-5	4737.5	0.00599
11.268	1.35054E-4	4278.9	0.00616
16.977	1.97453E-4	3822.2	0.00615
22.717	2.5866E-4	3518.5	0.00614
28.502	3.19015E-4	3211.1	0.0061
34.064	3.76359E-4	2905.1	0.00603
39.562	4.32034E-4	2595.2	0.0059
45.008	4.85099E-4	2288.7	0.00573
50.587	5.39618E-4	1981.8	0.00548
55.973	5.91193E-4	1680.4	0.00518
61.323	6.41474E-4	1384.1	0.00481
66.583	6.89837E-4	1091.3	0.00436
71.958	7.38467E-4	806.7	0.00376
77.425	7.87811E-4	666.67	0.00338
82.686	8.34657E-4	530.91	0.00293

87.948	8.79183E-4	399.3	0.0024
93.404	9.26029E-4	270.61	0.00176
98.296	9.67253E-4	207.29	0.00136
103.2	0.00101	147.61	9.39725E-4
129.5	0.00122	91.105	4.85411E-4
155.95	0.00141	79.245	3.78799E-4
182.32	0.00159	67.239	2.66467E-4
208.48	0.00176	55.398	1.50352E-4
235.04	0.00193	43.737	3.42777E-5
258.39	0.00206		
288.99	0.00223		
319.47	0.0024		
382.43	0.0027		
445.86	0.00297		
509.83	0.00323		
575.16	0.00345		
641.11	0.00367		
707.69	0.00387		
774.08	0.00405		
841.81	0.00423		
908.15	0.00438		
975.25	0.00452		
1043.3	0.00466		
1183.9	0.00491		
1324.3	0.00513		
1467.6	0.00534		
1733.4	0.00564		
1984	0.00589		
2221.2	0.00608		
2450.2	0.00624		
2670.6	0.00636		
2878.5	0.00647		
3078.6	0.00655		
3289.5	0.00662		
3502.4	0.00665		
3737.8	0.00668		
3974.2	0.0067		
4214.3	0.00665		
4453.4	0.00648		
4696	0.00632		
4943.6	0.00587		
5186.7	0.00566		

Table S23. High pressure sorption isotherm data for CH₄ on CPO-27-Mg at 283 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹

9.3821	1.54689E-4	9603.8	0.00854
23.275	3.81123E-4	8960.5	0.0086
37.304	6.05336E-4	8324	0.00879
50.94	8.1864E-4	7710.2	0.0089
64.43	0.00103	7110	0.009
77.789	0.00122	6513.1	0.00906
91.317	0.00142	5951.9	0.00913
102.82	0.00159	5392.2	0.00917
123.76	0.00188	4860.6	0.00915
143.89	0.00213	4621.9	0.00916
164.52	0.00239	4378.8	0.00912
183.85	0.00262	4145.6	0.00909
202.65	0.00283	3915.2	0.00907
220.89	0.00303	3697	0.00902
239.59	0.00322	3231	0.0089
255.1	0.00337	2767	0.00872
280.7	0.00361	2312.2	0.00847
306.38	0.00383	1864.7	0.00812
415.69	0.00463	1440.3	0.00764
530.68	0.00526	1029.3	0.00692
650.36	0.00579	639.97	0.00578
772.08	0.00621	291	0.00373
894.13	0.00657	253.26	0.00338
1017.9	0.00687	223.63	0.00308
1376.1	0.00751	195.29	0.00277
1736.5	0.00796	168	0.00245
2102.5	0.00829	142.52	0.00213
2470.8	0.00853	118.02	0.0018
2841.9	0.00872	94.31	0.00147
3213.8	0.00887	78.906	0.00124
3581.5	0.00896	63.764	0.00101
3951.6	0.00903	49.03	7.81074E-4
4323.5	0.00907		
4688.9	0.00908		
5058.7	0.00909		
5640.6	0.00908		
6225	0.00905		
6804.2	0.009		
7385.5	0.00889		
7964.9	0.00879		
8544.9	0.00867		
9124.4	0.00846		
9698.4	0.00834		
10277	0.0082		

Table S24. High pressure sorption isotherm data for CH₄ on CPO-27-Mg at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
16.046	1.77737E-4	9567.4	0.00802
31.924	3.51049E-4	9209	0.00815
47.955	5.22754E-4	8847.3	0.0082
63.35	6.85108E-4	8548.7	0.00826
78.563	8.42554E-4	8263.6	0.00835
93.302	9.92728E-4	7974.9	0.00835
106.49	0.00113	7677.5	0.00845
129.91	0.00135	7410.2	0.00845
151.56	0.00156	7133.8	0.00851
172.17	0.00175	6882	0.00856
194.67	0.00195	6631	0.00859
214.74	0.00212	6399.3	0.0086
233.32	0.00228	6181.9	0.00858
250.73	0.00242	5945.5	0.00861
277.38	0.00262	5732.2	0.00862
304.21	0.00283	5514.6	0.00861
417.08	0.00356	5302.5	0.00862
533.47	0.00418	5110.3	0.00861
652.06	0.00471	4928.3	0.00861
773.92	0.00515	4745.7	0.00859
896.23	0.00553	4565	0.00857
1020.9	0.00586	4403.2	0.00855
1382	0.00657	4232.1	0.00852
1749.7	0.00708	4079.5	0.0085
2116.3	0.00745	3932.7	0.00849
2483.6	0.00773	3783.9	0.00845
2855	0.00795	3387.9	0.00832
3226.7	0.00811	2994.5	0.00819
3600.3	0.00824	2604.9	0.00798
3973.6	0.00834	2220.1	0.00772
4349	0.00841	1844	0.00736
4722.5	0.00847	1624.3	0.0071
5090.9	0.00848	1407.5	0.00679
5829.2	0.00851	1194.1	0.00641
6568.2	0.00847	987.76	0.00595
7298.6	0.00843	787.77	0.00537
8035.6	0.00834	596.45	0.00465
8771.9	0.00818	397.76	0.00361
9510.2	0.00801	227.81	0.0024
10247	0.00783	196.68	0.00213
		166.58	0.00186
		138.34	0.00159
		110.92	0.00133
		84.591	0.00106

67.447	8.81414E-4
50.65	7.02954E-4
34.108	5.23869E-4

Table S25. High pressure sorption isotherm data for CH₄ on CPO-27-Mg at 313 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
12.052	8.71732E-5	9666.5	0.00768
29.637	2.18752E-4	9300.9	0.00778
47.105	3.49906E-4	8935.4	0.00784
64.181	4.76533E-4	8621.9	0.00789
80.733	5.98332E-4	8336.1	0.00786
95.7	7.10761E-4	8039.4	0.0079
110.33	8.17257E-4	7739.6	0.00797
135.26	9.93531E-4	7487.5	0.00798
159.59	0.00116	7205.1	0.008
182.11	0.00131	6948.3	0.008
204.94	0.00147	6686.8	0.00802
226.66	0.0016	6465.2	0.00803
246.11	0.00173	6219	0.00801
262.02	0.00182	5997.5	0.00802
290.56	0.002	5780.5	0.00802
319.39	0.00216	5565.5	0.00801
436.89	0.00279	5366.1	0.008
557.12	0.00335	5184.6	0.00799
678.65	0.00383	4988.1	0.00796
801.42	0.00426	4795.8	0.00792
926.17	0.00464	4610.3	0.0079
1051.5	0.00497	4424.8	0.00784
1414.6	0.00571	4256.3	0.00781
1781.2	0.00625	4099.3	0.00775
2152.3	0.00666	3949.6	0.00772
2523.2	0.00698	3803.6	0.00769
2896.2	0.00722	3658.1	0.00765
3271.3	0.00743	3256.8	0.00748
3649.4	0.00758	2867.4	0.00729
4026.6	0.00771	2479.7	0.00703
4397.7	0.0078	2102.6	0.00671
4773.8	0.00788	1727.1	0.00627
5148	0.00794	1495.4	0.00594
5894.8	0.00803	1280.8	0.00555
6641.9	0.00803	1069.7	0.0051
7388.5	0.00803	865.45	0.00455
8134.6	0.00797	668.69	0.00389
8878.4	0.00794	480.01	0.0031
9622.4	0.00776	294.51	0.00211

10371	0.00756	259.33	0.00189
		219.93	0.00164
		186.77	0.00142
		154.86	0.0012
		124.5	9.84474E-4
		95.18	7.72464E-4
		76.136	6.3032E-4
		57.594	4.90096E-4
		39.42	3.50308E-4

Table S26. High pressure sorption isotherm data for CH₄ on CPO-27-Mg at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
13.313	5.61256E-5	9390	0.00668
32.948	1.38489E-4	8702.4	0.00678
52.208	2.18854E-4	8040.5	0.00683
70.854	2.95811E-4	7404.5	0.00684
89.035	3.70237E-4	6790.4	0.00681
105.15	4.33783E-4	6189.8	0.00676
133.51	5.45106E-4	5595.4	0.00673
160.37	6.52628E-4	5034.5	0.00662
186.69	7.55778E-4	4494.5	0.00648
211.67	8.53574E-4	4257.9	0.0064
233.81	9.39368E-4	4013.3	0.00631
254.42	0.00101	3786.3	0.00621
285.99	0.00113	3315.5	0.00598
317.1	0.00124	2843.3	0.00567
445.32	0.00168	2380.4	0.00528
572.17	0.00208	1924.4	0.00478
698.87	0.00245	1479.6	0.00416
826.25	0.00279	1057.1	0.00337
954.74	0.0031	650.01	0.00235
1082.9	0.00339	257.4	0.00106
1451.3	0.00408	219.22	9.12733E-4
1822.8	0.00462	182.77	7.72375E-4
2196.8	0.00507	147.29	6.31882E-4
2570.5	0.00542	113.78	4.91434E-4
2948	0.00571	81.144	3.56737E-4
3326.2	0.00595	60.331	2.69515E-4
3704	0.00614	39.852	1.8314E-4
4086.3	0.00632		
4464.5	0.00644		
4840.7	0.00654		
5222.1	0.00661		
5826.8	0.00671		
6436	0.0068		

7040.8	0.00683
7649.7	0.00681
8258.3	0.00679
8864.8	0.00675
9472.4	0.00671
10083	0.00658

Table S27. High pressure sorption isotherm data for CO₂ on CPO-27-Ni at 278 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.04246	7.95813E-5	3339.3	0.01224
0.06825	1.5696E-4	2994	0.0123
0.09582	2.34333E-4	2642.7	0.01234
0.1251	3.11744E-4	2283	0.01236
0.1505	3.90959E-4	1927.4	0.01234
0.1801	4.70046E-4	1572.4	0.01227
0.2096	5.50719E-4	1224.3	0.01214
0.2374	6.31071E-4	888.12	0.01189
0.2665	7.11442E-4	755.87	0.01175
0.3004	7.91062E-4	629.37	0.01156
0.3255	8.70681E-4	510.71	0.0113
0.3576	9.48375E-4	399.87	0.01098
0.3939	0.00103	299.01	0.01055
0.4254	0.00111	254.06	0.01026
0.4557	0.00118	213.61	0.00995
0.4888	0.00126	177.89	0.0096
0.515	0.00134	146.96	0.00922
0.5529	0.00142	120.13	0.00881
0.5888	0.0015	95.778	0.00838
0.6229	0.00158	91.135	0.00826
0.6598	0.00165	85.877	0.00815
0.6946	0.00173	80.797	0.00804
0.7327	0.00181	75.917	0.00793
0.77	0.00189	71.094	0.00782
0.8092	0.00197	66.422	0.00771
0.8517	0.00204	61.88	0.00759
0.8878	0.00212	57.483	0.00748
0.9311	0.0022	53.2	0.00736
0.9754	0.00227	49.071	0.00725
1.0219	0.00235	45.038	0.00713
1.0697	0.00243	41.145	0.00701
1.1159	0.00251	37.388	0.00689
1.1645	0.00259	33.775	0.00677
1.2154	0.00267	30.296	0.00665
1.2727	0.00275	26.976	0.00653
1.3271	0.00282	22.767	0.00637

1.3835	0.0029	19.502	0.00622
1.4474	0.00298	16.937	0.0061
1.5096	0.00306		
1.5752	0.00314		
1.6466	0.00322		
1.7172	0.00329		
1.788	0.00337		
1.8729	0.00345		
1.9503	0.00353		
2.0456	0.0036		
2.1384	0.00368		
2.2377	0.00376		
2.3414	0.00383		
2.4527	0.00391		
2.5704	0.00399		
2.689	0.00407		
2.8275	0.00414		
2.972	0.00422		
3.1233	0.0043		
3.2963	0.00437		
3.4818	0.00445		
3.6741	0.00453		
3.8949	0.0046		
4.1315	0.00468		
4.381	0.00476		
4.6614	0.00483		
4.9666	0.00491		
5.3049	0.00498		
5.6667	0.00505		
6.087	0.00513		
6.5337	0.0052		
7.02	0.00527		
7.5626	0.00535		
8.1712	0.00542		
8.8402	0.00549		
9.5702	0.00556		
10.354	0.00563		
11.2	0.0057		
12.124	0.00577		
13.125	0.00583		
14.199	0.0059		
15.345	0.00597		
16.512	0.00603		
17.759	0.0061		
19.085	0.00616		
20.427	0.00622		

21.854	0.00628
23.328	0.00635
24.889	0.00641
26.453	0.00647
28.063	0.00653
29.668	0.00659
31.322	0.00665
32.976	0.00671
34.695	0.00676
36.452	0.00682
38.313	0.00688
40.139	0.00694
42.001	0.007
43.797	0.00705
45.645	0.0071
47.564	0.00716
49.527	0.00722
51.461	0.00727
53.376	0.00732
55.387	0.00738
57.326	0.00743
59.329	0.00748
61.382	0.00753
63.363	0.00758
65.382	0.00764
67.384	0.00768
69.507	0.00773
71.583	0.00778
73.757	0.00783
75.806	0.00788
77.856	0.00793
79.952	0.00797
82.114	0.00802
84.165	0.00807
86.188	0.00811
88.302	0.00815
90.369	0.0082
92.481	0.00824
94.63	0.00828
96.929	0.00833
99.218	0.00837
101.35	0.00841
112.64	0.00861
124.44	0.00881
137.03	0.00899
149.99	0.00917

163.04	0.00934
176.74	0.0095
191.02	0.00965
206.36	0.0098
222.7	0.00994
239.07	0.01007
253.92	0.01018
274.78	0.01032
296.59	0.01045
319.25	0.01057
368.17	0.01078
419.1	0.01097
472.74	0.01113
528.61	0.01128
585.45	0.0114
644.37	0.01151
704.05	0.01161
765.12	0.01169
826.09	0.01177
887.96	0.01183
950.42	0.01189
1012.1	0.01195
1282.2	0.01211
1540.6	0.01221
1786.2	0.01227
2018.2	0.0123
2239	0.01232
2447.4	0.01232
2646.6	0.01231
2834.8	0.01229
3048.6	0.01227
3261.2	0.01224
3472.5	0.01222
3674.9	0.01229

Table S28. High pressure sorption isotherm data for CO₂ on CPO-27-Ni at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.08561	7.92924E-5	4799.1	0.01104
0.1748	1.5757E-4	4266.8	0.01121
0.2626	2.37928E-4	3730.6	0.01133
0.3513	3.16161E-4	3189.4	0.01141
0.4463	3.96038E-4	2648.5	0.01141
0.5369	4.73815E-4	2289.3	0.01136
0.6291	5.52953E-4	1928.3	0.01127
0.7255	6.30679E-4	1573.7	0.01112

0.8149	7.06947E-4	1228.2	0.0109
0.908	7.83356E-4	897.2	0.01054
1.0054	8.6105E-4	768.96	0.01034
1.1014	9.38743E-4	647.38	0.01008
1.2027	0.00102	532.1	0.00978
1.2992	0.00109	425.84	0.00941
1.3997	0.00117	327.83	0.00893
1.5023	0.00125	241.42	0.00837
1.6076	0.00133	202.05	0.00805
1.712	0.0014	165.84	0.0077
1.8187	0.00148	133.33	0.00733
1.9315	0.00156	102.78	0.00695
2.0442	0.00163	76.421	0.00656
2.1594	0.00171	70.538	0.00646
2.2726	0.00179	64.776	0.00636
2.3936	0.00186	59.274	0.00625
2.5137	0.00194	54.04	0.00615
2.6381	0.00201	49.013	0.00604
2.765	0.00209	44.255	0.00593
2.8937	0.00217	39.796	0.00582
3.0363	0.00224	35.651	0.00571
3.1824	0.00232	31.831	0.00559
3.3278	0.0024	28.372	0.00547
3.4691	0.00248	24.041	0.00529
3.6163	0.00255	20.914	0.00514
3.7812	0.00263	18.563	0.005
3.9393	0.0027	16.731	0.00487
4.1123	0.00278	15.281	0.00476
4.2854	0.00286	14.081	0.00465
4.4683	0.00293	13.096	0.00455
4.6545	0.00301	12.247	0.00446
4.851	0.00309	11.537	0.00437
5.0586	0.00316	10.897	0.00429
5.2687	0.00324	10.343	0.00421
5.4899	0.00331	9.8623	0.00413
5.7224	0.00339		
5.9714	0.00346		
6.2178	0.00354		
6.4891	0.00361		
6.7602	0.00369		
7.0546	0.00376		
7.3722	0.00384		
7.6863	0.00391		
8.0354	0.00399		
8.3995	0.00406		
8.7972	0.00414		

9.2085	0.00421
9.6511	0.00428
10.118	0.00436
10.607	0.00443
11.14	0.0045
11.684	0.00457
12.293	0.00464
12.915	0.00471
13.619	0.00479
14.358	0.00486
15.14	0.00492
15.956	0.00499
16.838	0.00506
17.809	0.00513
18.831	0.00519
19.91	0.00526
21.103	0.00532
22.31	0.00539
23.592	0.00545
25.001	0.00551
26.502	0.00557
28.14	0.00564
29.727	0.0057
31.476	0.00575
33.254	0.00581
35.173	0.00587
37.118	0.00593
39.03	0.00598
41.089	0.00603
43.192	0.00608
45.357	0.00613
47.499	0.00618
49.695	0.00623
52.033	0.00628
54.405	0.00633
56.78	0.00638
59.277	0.00643
61.862	0.00647
64.373	0.00652
66.994	0.00657
69.591	0.00661
72.225	0.00666
74.794	0.0067
77.47	0.00674
79.933	0.00678
82.648	0.00682

85.335	0.00687
87.947	0.0069
90.552	0.00694
93.081	0.00698
95.81	0.00702
98.32	0.00705
101.03	0.00709
114.85	0.00727
129.21	0.00745
143.75	0.00761
159.03	0.00778
174.48	0.00793
189.74	0.00808
205.38	0.00822
221.5	0.00836
238.06	0.00849
253.17	0.0086
273.64	0.00875
294.54	0.00889
316.2	0.00902
362.23	0.00926
410.05	0.00948
460.42	0.00969
512.8	0.00987
567.19	0.01003
622.89	0.01018
679.89	0.01031
738.58	0.01043
797.89	0.01053
858.37	0.01063
919.52	0.01071
980.04	0.01079
1042.9	0.01087
1289	0.01108
1527.5	0.01123
1757	0.01134
1977	0.01142
2186	0.01147
2387.4	0.01152
2580.8	0.01154
2801.4	0.01156
3023.5	0.01157
3397.4	0.01154
3772.5	0.0115
4152.7	0.0114
4533.8	0.0113

4922.3	0.01107
5315.3	0.01075

Table S29. High pressure sorption isotherm data for CO₂ on CPO-27-Ni at 343 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.6266	7.31282E-5	4596.2	0.00951
1.2605	1.45646E-4	4029.9	0.0096
1.9014	2.18627E-4	3463.5	0.00962
2.5628	2.92911E-4	2906.9	0.00955
3.2165	3.65583E-4	2533.9	0.00945
3.8743	4.38127E-4	2165.3	0.0093
4.5424	5.10768E-4	1802.5	0.0091
5.2158	5.83389E-4	1451.5	0.00882
5.895	6.56221E-4	1113.3	0.00843
6.5706	7.26852E-4	793.77	0.0079
7.2764	7.99409E-4	671.67	0.00763
7.9753	8.71323E-4	554.56	0.00733
8.6665	9.41312E-4	443.07	0.00698
9.3849	0.00101	334.48	0.00656
10.11	0.00108	238.87	0.00607
10.873	0.00116	195.18	0.00578
11.616	0.00123	156.03	0.00546
12.356	0.0013	122.7	0.00509
13.127	0.00137	95.197	0.00468
13.897	0.00144	89.435	0.00458
14.668	0.00151	84.015	0.00447
15.483	0.00158	78.888	0.00436
16.299	0.00165	74.019	0.00424
17.129	0.00172	69.441	0.00413
17.97	0.00179	65.123	0.00401
18.846	0.00186	61.031	0.00389
19.708	0.00193	57.192	0.00377
20.593	0.00199	53.58	0.00365
21.479	0.00206	50.183	0.00352
22.375	0.00213	46.989	0.0034
23.293	0.00219	43.969	0.00327
24.249	0.00226	41.116	0.00314
25.218	0.00233	38.418	0.00301
26.183	0.00239	35.858	0.00288
27.246	0.00246	33.424	0.00275
28.265	0.00253	31.105	0.00261
29.344	0.0026	28.909	0.00248
30.419	0.00266	25.9	0.00229
31.512	0.00273	23.367	0.00211
32.626	0.00279	21.2	0.00195

33.746	0.00285	19.322	0.0018
34.946	0.00292	17.676	0.00167
36.191	0.00298	16.221	0.00155
37.422	0.00305	14.924	0.00143
38.655	0.00311	13.765	0.00133
39.931	0.00317	12.723	0.00123
41.266	0.00323	11.766	0.00114
42.635	0.00329	10.908	0.00106
44.024	0.00335	10.123	9.8369E-4
45.483	0.00342	9.4071	9.12418E-4
46.946	0.00348		
48.451	0.00354		
50.025	0.0036		
51.598	0.00365		
53.191	0.00371		
54.854	0.00377		
56.531	0.00383		
58.235	0.00388		
60.049	0.00394		
61.872	0.00399		
63.618	0.00405		
65.482	0.0041		
67.409	0.00415		
69.333	0.0042		
71.381	0.00425		
73.504	0.0043		
75.569	0.00435		
77.571	0.0044		
79.726	0.00445		
81.978	0.00449		
84.263	0.00454		
86.538	0.00459		
88.879	0.00463		
91.35	0.00468		
93.776	0.00472		
96.059	0.00476		
98.56	0.0048		
101.09	0.00484		
113.99	0.00503		
128.06	0.00521		
143.33	0.00538		
159.33	0.00554		
175.78	0.00568		
193.5	0.00582		
211.57	0.00595		
229.81	0.00607		

248.73	0.00618
262.92	0.00626
286.19	0.00638
310.14	0.0065
360.21	0.00671
411.81	0.00691
465.42	0.0071
520.02	0.00727
575.85	0.00743
632.56	0.00758
690.4	0.00772
748.62	0.00785
807.9	0.00797
867.61	0.00808
928.5	0.00819
989.91	0.00829
1052	0.00839
1323.4	0.00873
1583.8	0.00897
1837.8	0.00916
2080.5	0.00931
2315.6	0.00942
2542	0.0095
2758.9	0.00956
2967.5	0.00962
3163	0.00965
3550.6	0.00968
3940.2	0.00967
4336.7	0.00963
4740.2	0.00953
5156	0.00933

Table S30. High pressure sorption isotherm data for CO₂ on CPO-27-Ni at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
2.1861	5.83241E-5	4617.6	0.00827
4.2179	1.19462E-4	4057.6	0.00829
6.1102	1.77527E-4	3495.6	0.00823
8.0974	2.37466E-4	2939.9	0.00811
10.122	2.98074E-4	2569.4	0.00797
12.133	3.58283E-4	2202.6	0.00778
14.186	4.18081E-4	1839.9	0.00754
16.219	4.77873E-4	1487.3	0.00724
18.241	5.37158E-4	1145.5	0.00684
20.26	5.94465E-4	821.8	0.00632
22.144	6.52369E-4	697.1	0.00605

24.129	7.09515E-4	578.79	0.00574
26.1	7.65378E-4	467.55	0.00537
27.935	8.19314E-4	362.05	0.00493
29.949	8.7325E-4	269.98	0.00438
31.877	9.29112E-4	228.62	0.00406
33.939	9.8369E-4	191.27	0.0037
35.833	0.00104	158.02	0.00332
37.883	0.00109	128.72	0.00292
39.827	0.00114	102.44	0.0025
41.908	0.0012	79.62	0.00206
43.909	0.00125	74.351	0.00195
45.994	0.0013	69.304	0.00184
48.14	0.00136	64.408	0.00173
50.144	0.00141	59.609	0.00162
52.282	0.00146	54.96	0.00151
54.364	0.00151	50.383	0.00139
56.497	0.00156	45.903	0.00128
58.582	0.00161	41.482	0.00117
60.597	0.00166	37.303	0.00105
62.813	0.00171	33.129	9.35533E-4
64.899	0.00176	29.02	8.19956E-4
67.129	0.00181	23.228	6.51085E-4
69.22	0.00185	18.721	5.15044E-4
71.465	0.0019	15.161	4.04873E-4
73.683	0.00195	12.312	3.15378E-4
75.658	0.00199	10.021	2.42526E-4
77.953	0.00204	8.1824	1.83036E-4
80.096	0.00208		
82.196	0.00213		
84.343	0.00217		
86.426	0.00222		
88.93	0.00226		
91.229	0.00231		
93.437	0.00235		
95.723	0.00239		
97.783	0.00243		
99.975	0.00247		
102.32	0.00251		
114.13	0.00271		
126.66	0.0029		
139.85	0.00308		
153.03	0.00326		
167.43	0.00343		
182.79	0.0036		
197.57	0.00376		
213.23	0.00391		

228.88	0.00405
245.11	0.00418
258.45	0.00429
279.14	0.00443
300.59	0.00458
345.69	0.00484
393.7	0.00507
443.98	0.00529
496.51	0.00548
550.68	0.00567
606.06	0.00583
663.08	0.00598
720.99	0.00612
779.93	0.00625
840.22	0.00637
900.4	0.00649
960.35	0.00659
1022.5	0.00669
1243.7	0.00699
1460.4	0.00723
1667.4	0.00743
1870.7	0.0076
2063.2	0.00774
2284.3	0.00786
2507.7	0.00798
2731.9	0.00808
2960.2	0.00815
3187.5	0.00822
3574.7	0.0083
3966.7	0.00836
4363.8	0.00831
4767.8	0.00826
5177	0.00807

Table S31. High pressure sorption isotherm data for CO₂ on CPO-27-Ni at 473 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
5.331	2.92962E-5	4530.6	0.00584
10.54	5.71837E-5	3962.4	0.00584
15.838	8.48786E-5	3395.7	0.0057
21.096	1.12315E-4	2833.7	0.00545
26.116	1.38712E-4	2462	0.00522
31.385	1.65609E-4	2097.2	0.00495
36.453	1.91794E-4	1740.2	0.0046
41.513	2.17818E-4	1394.9	0.00415
46.542	2.43335E-4	1063.2	0.00361

51.598	2.69147E-4	751.33	0.00293
56.423	2.93855E-4	631.91	0.00261
61.474	3.19038E-4	516.08	0.00226
66.229	3.42988E-4	404.56	0.00189
71.045	3.6699E-4	294.88	0.00147
75.702	3.90079E-4	240.42	0.00124
80.388	4.13009E-4	188.01	0.00101
85.094	4.36323E-4	137.29	7.8143E-4
89.714	4.58263E-4	88.239	5.44407E-4
94.387	4.80737E-4	77.512	4.88654E-4
98.589	5.01258E-4	66.807	4.34089E-4
102.93	5.21902E-4	56.083	3.78612E-4
126.32	6.31597E-4	45.562	3.23167E-4
149.81	7.40336E-4	35.146	2.68036E-4
172.47	8.41145E-4	24.796	2.12379E-4
195.14	9.41312E-4	12.05	1.43502E-4
216.93	0.00104	5.9416	1.09529E-4
238.38	0.00113		
258.29	0.00121		
284.22	0.00131		
310.13	0.00142		
363.63	0.00162		
417.59	0.00181		
472.38	0.002		
528.03	0.00218		
584.47	0.00235		
641.29	0.00251		
698.59	0.00267		
756.71	0.00282		
816.19	0.00297		
876.19	0.0031		
936.68	0.00323		
997.3	0.00336		
1057.4	0.00348		
1251.5	0.00381		
1449.5	0.0041		
1727.5	0.00444		
1989	0.00471		
2236	0.00492		
2468.5	0.0051		
2689.2	0.00524		
2896.5	0.00536		
3095.6	0.00546		
3482.5	0.00562		
3876.8	0.00571		
4278.4	0.00577		

4681.6	0.0058
5097.8	0.00573

Table S32. High pressure sorption isotherm data for CH₄ on CPO-27-Ni at 283 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
2.476	5.25472E-5	9406.2	0.0072
9.8356	2.08411E-4	8730.8	0.00734
17.183	3.62611E-4	8064.2	0.0075
24.48	5.14421E-4	7411.7	0.00764
31.737	6.63927E-4	6796	0.00774
39.025	8.12893E-4	6192	0.00782
46.241	9.56723E-4	5606.1	0.00787
53.461	0.0011	5041.4	0.0079
60.605	0.00124	4492.1	0.00792
68.008	0.00138	4378.1	0.00791
75.41	0.00151	4262.6	0.00791
82.838	0.00165	4145	0.00791
89.309	0.00176	4040.7	0.0079
95.754	0.00187	3933	0.0079
102.1	0.00198	3836.6	0.00789
113.17	0.00216	3741.4	0.00788
124.64	0.00234	3657.4	0.00787
136.06	0.00251	3567	0.00786
148.44	0.00268	3480.8	0.00784
160.47	0.00284	3163.3	0.0078
172.62	0.003	2844.8	0.00773
185.15	0.00314	2534.5	0.00764
197.96	0.00329	2227.1	0.00752
210.41	0.00343	1925.3	0.00737
222.92	0.00355	1630.9	0.00718
235.24	0.00367	1354.1	0.00693
247.15	0.00378	1088.9	0.00662
257.06	0.00387	836.75	0.00621
275.19	0.00402	605.02	0.00565
294.35	0.00417	398.56	0.00484
314	0.00431	235.11	0.00371
399.92	0.00481	214.99	0.00351
494.97	0.00524	196.54	0.00331
597.58	0.00559	179.05	0.00311
705.23	0.00589	162.27	0.0029
815.4	0.00614	146.56	0.00269
931.36	0.00636	131.81	0.00248
1048.8	0.00654	117.7	0.00226
1379.9	0.00694	104.26	0.00205
1724.6	0.00722	89.576	0.0018

2074.2	0.00743	80.896	0.00164
2431	0.00758	72.426	0.00149
2789.9	0.0077	64.158	0.00133
3151.6	0.00778	56.083	0.00118
3515.6	0.00785	48.168	0.00102
3882.3	0.00789	40.388	8.63619E-4
4249.3	0.00791	32.715	7.0759E-4
4615.1	0.00792	24.453	5.36317E-4
4985.5	0.00791		
5354.6	0.00788		
5943.7	0.00783		
6533.1	0.00776		
7123	0.00768		
7712.7	0.00758		
8306.1	0.00746		
8897.6	0.0073		
9491.7	0.00717		
10087	0.00701		

Table S33. High pressure sorption isotherm data for CH₄ on CPO-27-Ni at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
9.6517	1.3353E-4	9437.7	0.00687
19.241	2.65121E-4	9078.5	0.00693
28.853	3.9582E-4	8743.6	0.00699
38.375	5.24124E-4	8431.9	0.00705
47.717	6.48517E-4	8111.7	0.0071
57.222	7.73083E-4	7820.2	0.00714
66.609	8.94439E-4	7521	0.00719
76.003	0.00101	7251.6	0.00722
85.202	0.00113	6973.1	0.00726
92.866	0.00123	6695	0.00729
100.63	0.00132	6443.6	0.00731
114.57	0.00149	6187.5	0.00734
128.49	0.00165	5939.3	0.00736
142.23	0.0018	5703.4	0.00737
155.67	0.00195	5480.5	0.00739
169.17	0.00209	5253.4	0.00739
183.29	0.00223	5035.2	0.0074
197.51	0.00237	4836.6	0.0074
211.05	0.0025	4776.3	0.0074
225.06	0.00262	4723.6	0.0074
238.23	0.00274	4672	0.0074
250.05	0.00283	4626	0.00739
268.84	0.00299	4570.4	0.00739
288.07	0.00313	4516.5	0.00739

307.83	0.00328	4468.9	0.00738
392.73	0.00381	4424.1	0.00738
485.21	0.00427	4381.6	0.00738
583.9	0.00466	4343.7	0.00738
687.28	0.00499	4315.9	0.00738
796.45	0.00529	4279	0.00738
909.06	0.00553	4250.7	0.00738
1022.8	0.00575	4224.5	0.00738
1350.3	0.0062	4200	0.00737
1692.1	0.00653	4176.3	0.00737
2043	0.00677	4156.9	0.00737
2400.2	0.00696	4135.8	0.00736
2762.5	0.0071	4090.3	0.00736
3126.5	0.0072	4064.4	0.00736
3491.5	0.00728	4035.6	0.00736
3859.6	0.00733	4001.4	0.00736
4230.4	0.00737	3969.3	0.00735
4599.7	0.00739	3935.9	0.00735
4971	0.0074	3911.9	0.00734
5341.8	0.00739	3883.9	0.00734
5939	0.00735	3862.9	0.00734
6534.3	0.0073	3837	0.00733
7134.9	0.00723	3820.5	0.00733
7731.2	0.00715	3801.6	0.00733
8332.4	0.00705	3775.4	0.00733
8929.7	0.00694	3758.8	0.00733
9528.2	0.00682	3737.1	0.00732
10131	0.00669	3714.1	0.00732
		3692.9	0.00732
		3677.7	0.00732
		3656.6	0.00731
		3644.9	0.00731
		3632.2	0.00731
		3605.9	0.00731
		3587.4	0.00731
		3570.3	0.00731
		3549	0.0073
		3533	0.0073
		3520.3	0.00729
		3510.5	0.00729
		3495.1	0.00728
		3483.1	0.00728
		3237.3	0.00724
		2983.4	0.00718
		2735.8	0.0071
		2496.1	0.00701

2255.6	0.0069
2020.1	0.00677
1788.9	0.00662
1565.2	0.00644
1356.3	0.00622
1154.9	0.00597
962.71	0.00565
780.82	0.00527
611.82	0.00478
458.71	0.00417
321.13	0.0034
205.24	0.00248
185.66	0.00228
167	0.0021
148.97	0.0019
131.91	0.00171
115.06	0.00151
99.149	0.00132
88.273	0.00118
77.72	0.00105
67.309	9.14987E-4
57.068	7.80788E-4
47	6.45948E-4

Table S34. High pressure sorption isotherm data for CH₄ on CPO-27-Ni at 343 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
5.1572	2.58309E-5	9823.4	0.00607
20.373	1.01907E-4	9106.9	0.00611
35.541	1.77077E-4	8403.3	0.00614
50.402	2.50263E-4	7721	0.00616
65.12	3.22191E-4	7069	0.00618
79.547	3.91974E-4	6430.5	0.00617
93.742	4.60113E-4	5815	0.00613
106.25	5.18852E-4	5218.7	0.00607
127.11	6.16566E-4	4655.7	0.00599
147.4	7.11442E-4	4382.7	0.00592
167.02	8.00051E-4	4124	0.00587
186.05	8.8545E-4	3882.3	0.00581
205.43	9.73417E-4	3645.2	0.00573
223.97	0.00105	3174.6	0.00555
240.96	0.00113	2718.6	0.00532
255.28	0.00119	2267.8	0.00502
279.92	0.00129	1830.8	0.00463
304.72	0.00139	1422.9	0.00413
406.94	0.00179	1040.5	0.00348

512.32	0.00216	684.15	0.00263
619.38	0.0025	357	0.00154
727.03	0.00281	176.61	7.83999E-4
838.62	0.00309	150.57	6.60074E-4
952.09	0.00336	124.59	5.36535E-4
1066.5	0.00359	99.673	4.16733E-4
1390.9	0.00414	83.104	3.3493E-4
1728.4	0.00457	66.828	2.54771E-4
2075.6	0.00492	50.858	1.75478E-4
2430.6	0.0052	35.121	9.61538E-5
2791.2	0.00543		
3155	0.0056		
3523.6	0.00575		
3894.1	0.00587		
4268.1	0.00598		
4644.1	0.00605		
5021	0.00612		
5626.7	0.0062		
6234	0.00623		
6843.4	0.00626		
7456.5	0.00626		
8069.2	0.00623		
8683.4	0.00621		
9301.8	0.00617		
9921.7	0.00607		
10544	0.006		

Table S35. High pressure sorption isotherm data for N₂ on CPO-27-Ni at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
3.521	4.04836E-5	9818.3	0.00656
14.347	1.62813E-4	9108.1	0.00658
25.221	2.82243E-4	8423.3	0.00659
36.115	3.98586E-4	7760.5	0.00659
47.208	5.13608E-4	7113	0.00658
58.321	6.25502E-4	6471.5	0.00655
69.472	7.34407E-4	5847.4	0.00651
80.832	8.42465E-4	5250.9	0.00645
90.518	9.32765E-4	4672.3	0.00637
100.27	0.00102	4111.3	0.00627
120.74	0.0012	3566.6	0.00614
141.42	0.00136	2831.6	0.00591
162.07	0.00153	2110.8	0.00555
183.1	0.00168	1428.6	0.00502
203.87	0.00182	1100	0.00462
224.86	0.00196	790.39	0.00407

244.97	0.00209	495.38	0.00326
271.02	0.00224	255.06	0.00216
297.78	0.00239	209.91	0.00188
325.21	0.00253	167.94	0.00158
421.37	0.00296	128.69	0.00127
523.09	0.00334	91.566	9.51058E-4
629.99	0.00367	71.376	7.60819E-4
741.66	0.00395	51.855	5.6661E-4
856.58	0.00419	32.185	3.60792E-4
974.9	0.00441	20.246	2.30392E-4
1093.2	0.00459	12.893	1.46864E-4
1421.9	0.005	8.2512	9.34059E-5
1760.6	0.0053		
2106.8	0.00554		
2457.9	0.00574		
2813.3	0.00589		
3171.3	0.00602		
3532.8	0.00613		
3895.6	0.00623		
4259.3	0.0063		
4624	0.00637		
4989.9	0.00642		
5356.1	0.00646		
6089.3	0.00653		
6825.7	0.00657		
7564	0.00659		
8302.1	0.0066		
9044.8	0.00658		
9788.1	0.00655		
10536	0.00653		

Table S36. High pressure sorption isotherm data for N₂ on CPO-27-Ni at 313 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
4.5314	3.21228E-5	9806.2	0.00615
13.63	9.64264E-5	9426.9	0.00614
22.632	1.59325E-4	9056.1	0.00615
31.626	2.21201E-4	8692.8	0.00615
40.508	2.81409E-4	8349.2	0.00615
49.434	3.41059E-4	8031.6	0.00616
58.367	3.99889E-4	7739.1	0.00616
67.07	4.56367E-4	7443.3	0.00614
75.592	5.10886E-4	7145.1	0.00614
84.234	5.65406E-4	6853	0.00612
92.741	6.18498E-4	6566.2	0.00611
100.18	6.6338E-4	6305.8	0.00609

120.51	7.86518E-4	5932.8	0.00605
140.25	9.01401E-4	5686.2	0.00602
160.03	0.00101	5448.2	0.006
179.44	0.00112	5201.8	0.00596
198.84	0.00122	4967.3	0.00593
218.52	0.00132	4743.4	0.00589
236.68	0.00141	4515.2	0.00585
253.18	0.00149	4144.3	0.00577
277.09	0.0016	3940.7	0.00572
301.05	0.00171	3744.6	0.00566
401.37	0.00211	3550.2	0.00561
506.1	0.00248	3365.8	0.00554
613.66	0.0028	3186.6	0.00548
725.53	0.00309	2802.9	0.00532
839.45	0.00335	2427.4	0.00513
956.02	0.00358	2069.6	0.00489
1073.8	0.00378	1721.1	0.00461
1398.2	0.00422	1513.7	0.0044
1734.9	0.00458	1310.9	0.00416
2077.8	0.00485	1114	0.00388
2427.7	0.00508	924.57	0.00355
2782.2	0.00527	742.49	0.00317
3139.2	0.00542	570.16	0.00271
3499.7	0.00554	403.13	0.00216
3861.8	0.00566	251.73	0.00152
4226.3	0.00574	224.54	0.00138
4592.6	0.00582	199.17	0.00125
4961	0.00589	173.78	0.00112
5329.7	0.00595	149.77	9.8385E-4
6066.2	0.00604	126.54	8.47819E-4
6808.4	0.0061	104.06	7.13661E-4
7550.1	0.00613	79.652	5.61167E-4
8295.8	0.00615	65.172	4.67476E-4
9042.5	0.00616	50.958	3.7332E-4
9786.4	0.00614	36.983	2.78531E-4
10535	0.00612	20.002	1.60449E-4
		10.922	9.56411E-5
		6.0144	5.98153E-5

Table S37. High pressure sorption isotherm data for N₂ on CPO-27-Ni at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
6.0441	1.96306E-5	9796.9	0.00541
17.759	5.78433E-5	9413.8	0.00537
29.363	9.53333E-5	9031.2	0.00535
40.685	1.31726E-4	8657.5	0.00534

52.113	1.68145E-4	8295.7	0.00532
63.352	2.03547E-4	7978.2	0.00529
74.387	2.38204E-4	7689	0.00527
85.118	2.71589E-4	7392.6	0.00523
96.013	3.05104E-4	7099.2	0.0052
105.59	3.34514E-4	6810.4	0.00518
130.67	4.10239E-4	6527	0.00514
155.86	4.84742E-4	6267.4	0.00511
179.86	5.55992E-4	5895.8	0.00505
203.26	6.22111E-4	5650.4	0.005
226.27	6.85822E-4	5398.5	0.00495
249.81	7.49487E-4	5154.7	0.00489
277.96	8.25957E-4	4924.9	0.00484
306.14	9.00375E-4	4703.1	0.00479
421.19	0.00119	4476.4	0.00472
538.61	0.00145	4266.4	0.00466
657.01	0.0017	4062.2	0.00459
775.77	0.00193	3857.7	0.00452
896.32	0.00214	3657.5	0.00444
1017.6	0.00234	3289.3	0.00428
1345.7	0.00279	3113.4	0.00419
1680.6	0.00317	2735	0.00399
2024	0.0035	2363.3	0.00374
2372.4	0.00377	2009.1	0.00347
2726.3	0.004	1659.6	0.00313
3083.1	0.0042	1452.2	0.0029
3443.7	0.00437	1247.9	0.00265
3806.5	0.00451	1049.7	0.00237
4171.6	0.00465	857.22	0.00205
4538.6	0.00476	669.54	0.0017
4906.7	0.00485	487.7	0.00132
5276.5	0.00493	308.71	8.81458E-4
6016	0.00508	133.54	3.90653E-4
6761.3	0.00519	104.94	3.03119E-4
7505.7	0.00527	74.513	2.06973E-4
8256.3	0.00534	56.401	1.48639E-4
9009.5	0.00538	38.502	9.06175E-5
9762.7	0.00541	15.763	1.60391E-5
10522	0.00542		

Table S38. High pressure sorption isotherm data for N₂ on CPO-27-Ni at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.0531	1.11448E-5	9620.7	0.00436
20.629	3.25288E-5	9231.5	0.00431
34.032	5.35246E-5	8849.7	0.00429

47.102	7.36593E-5	8488.4	0.00425
60.15	9.37316E-5	8131.3	0.0042
73.27	1.13996E-4	7800.5	0.00416
85.82	1.33256E-4	7502.9	0.00412
97.992	1.51994E-4	7210.4	0.00408
109.16	1.69314E-4	6908	0.00402
138.93	2.14076E-4	6634	0.00398
167.67	2.57228E-4	6363.4	0.00391
195.41	2.98247E-4	6109.3	0.00386
222.98	3.37673E-4	5841.6	0.00381
248.89	3.74873E-4	5590.8	0.00375
267.19	4.02989E-4	5347.4	0.00368
299.22	4.47711E-4	5109.2	0.00362
331.09	4.91702E-4	4880.2	0.00355
460.8	6.66369E-4	4652.1	0.00348
589.65	8.32783E-4	4429.9	0.00341
718.77	9.90631E-4	4223.4	0.00334
848.39	0.00114	4020.4	0.00326
978.63	0.00128	3821	0.00318
1108.1	0.00142	3627.1	0.0031
1453.5	0.00175	3439.3	0.00302
1804.2	0.00204	3253.7	0.00294
2158.4	0.0023	2871.3	0.00274
2514.5	0.00254	2488.7	0.00252
2874	0.00274	2124.7	0.00228
3236.5	0.00294	1766.7	0.00201
3601.6	0.00311	1550.1	0.00183
3969.2	0.00325	1335.4	0.00164
4336.7	0.00339	1125.7	0.00144
4705.4	0.00351	918.92	0.00122
5076.2	0.00362	715.32	9.85233E-4
5817.3	0.00382	514.93	7.37307E-4
6566.8	0.00397	312.81	4.64754E-4
7315.9	0.00409	118.01	1.81271E-4
8065.6	0.00418	85.051	1.30133E-4
8818.3	0.00428	64.173	9.6761E-5
9577.5	0.00436	43.433	6.40939E-5
10340	0.0044	22.919	3.14491E-5
		7.3346	6.21041E-6

Table S39. High pressure sorption isotherm data for N₂ on CPO-27-Ni at 473 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.7675	4.25538E-6	9806.9	0.00259
22.913	1.26439E-5	9416.6	0.00255
37.794	2.08307E-5	9022.9	0.00251

52.293	2.87544E-5	8648	0.00246
66.601	3.66601E-5	8295.6	0.00242
80.609	4.42134E-5	7969.4	0.00237
94.278	5.17712E-5	7657.7	0.00233
107.26	5.88115E-5	7362.6	0.00228
140.58	7.74873E-5	7064.7	0.00224
173.1	9.52887E-5	6772	0.00218
203.97	1.11252E-4	6485	0.00213
234.43	1.28E-4	6216.2	0.00208
261.28	1.42594E-4	5950.9	0.00203
297.03	1.61283E-4	5685.6	0.00198
332.48	1.79946E-4	5426.3	0.00193
476.36	2.54198E-4	5175.9	0.00188
619.62	3.2577E-4	4935.8	0.00183
762.42	3.96547E-4	4706.9	0.00177
902.34	4.64174E-4	4472	0.00171
1043.3	5.30784E-4	4254.3	0.00165
1415.4	6.96128E-4	4043.8	0.00159
1788.9	8.51522E-4	3835.1	0.00154
2163.7	9.96788E-4	3628.9	0.00147
2539.6	0.00114	3426.7	0.00142
2914.9	0.00126	3236.7	0.00136
3292.3	0.00138	2841	0.00124
3670.8	0.0015	2445.7	0.0011
4049.3	0.0016	2052.7	9.54314E-4
4427.8	0.0017	1674.8	8.04007E-4
4808.6	0.0018	1443.6	7.06389E-4
5188.3	0.00188	1217.3	6.08771E-4
5950.2	0.00203	992.04	5.03435E-4
6709	0.00217	768.76	3.96792E-4
7472.9	0.0023	547.48	2.88329E-4
8236.9	0.00242	322.58	1.71478E-4
9004.9	0.00251	104.16	5.57197E-5
9775.9	0.00258	65.521	3.42777E-5
10547	0.00265	42.471	2.11653E-5
		19.605	8.169E-6

Table S40. High pressure sorption isotherm data for CO₂ on CPO-27-Mn at 278 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
0.3472	1.967E-4	3238.3	0.01185
0.7367	3.9822E-4	2891.1	0.01199
1.1562	5.9768E-4	2538.8	0.01205
1.5958	7.9768E-4	2182.4	0.01209
2.051	9.9716E-4	1825.1	0.01206
2.5461	0.0012	1469.3	0.012

3.0372	0.00139	1115.5	0.01184
3.566	0.00158	769.15	0.01152
4.1422	0.00177	632.43	0.01129
4.7441	0.00196	500.13	0.01098
5.393	0.00215	373.73	0.01054
6.0921	0.00235	257.21	0.00983
6.8579	0.00254	202.25	0.00935
7.6531	0.00272	155.09	0.00872
8.4784	0.0029	112.55	0.00801
9.3949	0.00308	75.792	0.00718
10.41	0.00326	69.351	0.00694
11.488	0.00344	62.213	0.00671
12.698	0.00361	55.464	0.00648
13.974	0.00379	49.018	0.00624
15.361	0.00396	43.035	0.00599
16.866	0.00412	37.433	0.00573
18.454	0.00429	32.287	0.00546
20.218	0.00445	27.639	0.00518
22.056	0.00461	21.988	0.00477
23.978	0.00475	18.135	0.00442
26.119	0.00491	15.414	0.00413
28.303	0.00505	13.358	0.00387
30.558	0.00519	11.773	0.00364
33.05	0.00533	10.513	0.00343
35.562	0.00546	9.4645	0.00325
38.181	0.00559		
40.852	0.00572		
43.677	0.00584		
46.616	0.00596		
49.647	0.00608		
52.704	0.0062		
55.967	0.00631		
59.195	0.00642		
62.434	0.00653		
65.561	0.00663		
68.946	0.00673		
72.325	0.00683		
75.757	0.00692		
79.161	0.00701		
82.54	0.0071		
85.823	0.00719		
89.212	0.00727		
92.701	0.00735		
96.131	0.00743		
99.533	0.00751		
103.05	0.00758		

121.98	0.00792
141.37	0.00826
162.13	0.00857
183.08	0.00884
204.91	0.00909
226.67	0.00931
249.84	0.00951
277.3	0.00972
305.19	0.0099
364.18	0.01021
425.05	0.01046
487.25	0.01068
550.77	0.01085
614.9	0.011
679.75	0.01112
744.56	0.01123
810.35	0.01133
876.14	0.01141
942.59	0.01148
1007.4	0.01155
1215.6	0.01168
1423.3	0.01178
1631.3	0.01184
1968.2	0.01188
2282.9	0.01188
2577.6	0.01187
2848	0.01182
3106.4	0.01176
3341.9	0.01171
3580.8	0.01169

Table S41. High pressure sorption isotherm data for CO₂ on CPO-27-Mn at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
0.7522	1.9037E-4	4583	0.01085
1.5517	3.8236E-4	4059.1	0.01122
2.3713	5.7068E-4	3530.2	0.01146
3.209	7.5735E-4	2992.7	0.01161
4.102	9.4608E-4	2626.7	0.01164
5.0017	0.00113	2264.8	0.01166
5.9596	0.00132	1901.5	0.0116
6.9462	0.0015	1541.4	0.01145
7.9886	0.00168	1187	0.0112
9.0594	0.00186	840.59	0.01076
10.208	0.00204	704.28	0.01047
11.416	0.00222	572.48	0.0101

12.611	0.00239	446.25	0.00962
13.897	0.00256	325.18	0.00892
15.305	0.00273	216.33	0.00802
16.728	0.0029	166.48	0.00744
18.258	0.00306	122.11	0.00676
19.825	0.00322	82.588	0.00598
21.533	0.00339	75.408	0.00576
23.338	0.00354	67.848	0.00555
25.194	0.0037	60.65	0.00532
27.233	0.00385	53.927	0.00509
29.304	0.004	47.709	0.00484
31.508	0.00415	41.955	0.00459
33.845	0.00429	36.707	0.00432
36.228	0.00442	31.95	0.00403
38.704	0.00456	27.645	0.00374
41.266	0.00469	22.428	0.00332
43.996	0.00481	18.723	0.00296
46.787	0.00493	15.965	0.00265
49.781	0.00506	13.824	0.00239
53.011	0.00518	12.104	0.00215
56.117	0.00529	10.702	0.00194
59.31	0.0054	9.527	0.00176
62.769	0.00551		
66.045	0.00561		
69.396	0.00571		
73.009	0.0058		
76.658	0.0059		
80.401	0.00599		
84.17	0.00608		
87.906	0.00617		
91.775	0.00625		
95.431	0.00633		
99.073	0.0064		
102.7	0.00647		
122.26	0.00681		
142.74	0.00713		
163.13	0.00742		
185	0.00769		
206.68	0.00794		
228.86	0.00817		
250.48	0.00837		
277.16	0.0086		
304.6	0.00882		
362	0.00918		
420.68	0.00951		
480.87	0.00979		

542.59	0.01003
604.81	0.01023
668.27	0.01041
732.81	0.01057
797.2	0.01071
861.91	0.01083
927.49	0.01094
993.88	0.01104
1059.7	0.01112
1270.5	0.01133
1480.6	0.01148
1818.2	0.01163
2135.6	0.01169
2432.8	0.01173
2711.7	0.01174
2970.9	0.01173
3218.1	0.01168
3588.1	0.0116
3963.4	0.01135
4337.9	0.01113
4720.2	0.01072
5103.7	0.01012

Table S42. High pressure sorption isotherm data for CO₂ on CPO-27-Mn at 313 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
1.3354	1.3354	4610.3	0.01066
2.662	2.662	4063.9	0.01096
4.0084	4.0084	3518.3	0.0112
5.4333	5.4333	2967.3	0.01128
6.8852	6.8852	2602.2	0.01127
8.3929	8.3929	2235.4	0.01122
9.9168	9.9168	1872.3	0.0111
11.494	11.494	1511.6	0.01088
13.11	13.11	1155.8	0.01052
14.818	14.818	811.81	0.00995
16.547	16.547	678.05	0.00958
18.359	18.359	548.32	0.00914
20.237	20.237	424.03	0.00859
22.171	22.171	304.43	0.00784
24.205	24.205	196.7	0.0069
26.306	26.306	148.64	0.00629
28.471	28.471	105.43	0.00558
30.671	30.671	70.773	0.00474
32.928	32.928	63.623	0.00451
35.359	35.359	56.909	0.00427

37.805	37.805	50.592	0.00402
40.22	40.22	44.766	0.00376
42.741	42.741	39.321	0.0035
45.309	45.309	34.302	0.00322
48.156	48.156	29.643	0.00294
50.951	50.951	23.356	0.0025
53.906	53.906	18.881	0.00214
57.031	57.031	15.545	0.00185
60.036	60.036	12.953	0.0016
63.112	63.112	10.905	0.00139
66.338	66.338	9.2562	0.00122
69.6	69.6		
72.967	72.967		
76.538	76.538		
79.926	79.926		
83.508	83.508		
87.009	87.009		
90.337	90.337		
94.094	94.094		
97.529	97.529		
101.19	101.19		
120.64	120.64		
140.53	140.53		
161.87	161.87		
183.43	183.43		
205.85	205.85		
228.4	228.4		
251.61	251.61		
278.67	278.67		
306.48	306.48		
363.83	363.83		
422.7	422.7		
482.59	482.59		
544.07	544.07		
606.49	606.49		
669.98	669.98		
733.83	733.83		
798.46	798.46		
863.96	863.96		
928.64	928.64		
994.12	994.12		
1060.2	1060.2		
1346	1346		
1621.2	1621.2		
1879.8	1879.8		
2126.4	2126.4		

2358.3	2358.3
2580.3	2580.3
2792.8	2792.8
2991.2	2991.2
3215.6	3215.6
3593.9	3593.9
3974.6	3974.6
4358.9	4358.9
4748	4748
5147.4	5147.4

Table S43. High pressure sorption isotherm data for CO₂ on CPO-27-Mn at 343 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
2.8139	1.3537E-4	4497	0.00938
5.663	2.6734E-4	3938.3	0.00965
8.6289	3.9973E-4	3378.9	0.00976
11.659	5.3123E-4	2818.9	0.00972
14.591	6.5476E-4	2443	0.00961
17.576	7.7751E-4	2069.8	0.00944
20.705	9.0197E-4	1703.9	0.00917
23.904	0.00103	1342	0.00878
27.18	0.00115	990.39	0.0082
30.463	0.00127	851.65	0.00788
33.858	0.00139	715.58	0.00751
37.231	0.0015	583.44	0.00707
40.62	0.00162	456.65	0.00653
43.9	0.00172	333.24	0.00582
47.183	0.00182	221.28	0.00492
50.596	0.00193	170.65	0.00433
54.046	0.00203	125.09	0.00365
57.51	0.00213	84.875	0.00287
61.035	0.00223	77.174	0.00266
64.622	0.00232	69.115	0.00245
68.341	0.00242	61.278	0.00224
72.056	0.00251	53.774	0.00202
75.654	0.0026	46.542	0.0018
79.3	0.00269	39.549	0.00157
82.948	0.00278	32.819	0.00134
86.621	0.00286	26.332	0.0011
90.365	0.00294	18.125	7.7923E-4
94.201	0.00302	12.715	5.5279E-4
98.074	0.0031	9.0286	3.9149E-4
101.87	0.00318		
120.8	0.00352		
140.83	0.00385		

161.62	0.00415
182.45	0.00441
204.35	0.00467
226.49	0.00489
249.34	0.00511
276.82	0.00534
304.55	0.00555
362.21	0.00593
421.44	0.00626
482.07	0.00656
544.14	0.00683
606.47	0.00707
669.5	0.00729
733.33	0.00749
797.96	0.00767
862.62	0.00783
928.12	0.00799
993.26	0.00812
1059.1	0.00826
1355.7	0.00871
1641.7	0.00903
1912.7	0.00926
2170.3	0.00942
2413.1	0.00953
2649.1	0.00961
2873.5	0.00966
3081.3	0.0097
3467	0.00965
3854.7	0.00967
4248	0.00953
4649.2	0.00934
5056	0.0089

Table S44. High pressure sorption isotherm data for CO₂ on CPO-27-Mn at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
4.9215	8.5202E-5	4493.9	0.00779
9.8961	1.6645E-4	3923.8	0.00793
14.891	2.4477E-4	3357.9	0.00798
19.78	3.2183E-4	2795.3	0.00786
24.793	3.9818E-4	2423.6	0.00768
29.845	4.7347E-4	2051.1	0.00742
34.755	5.4782E-4	1683.6	0.00707
39.79	6.1948E-4	1321.1	0.00658
44.653	6.9078E-4	969.9	0.00591
49.529	7.6034E-4	831.15	0.00555

54.568	8.2896E-4	694.8	0.00513
59.485	8.9567E-4	563.59	0.00464
64.103	9.5733E-4	437.47	0.00407
68.756	0.00102	313.65	0.00333
73.54	0.00108	200.18	0.00245
78.045	0.00114	147.07	0.00192
82.698	0.0012	96.868	0.00135
87.344	0.00126	86.105	0.00121
92.053	0.00132	75.359	0.00107
96.711	0.00137	64.714	9.2487E-4
101.13	0.00143	54.281	7.7957E-4
124.88	0.0017	44.209	6.3041E-4
148.86	0.00195	34.144	4.8087E-4
172.55	0.00219	24.289	3.2862E-4
196.67	0.00241	12.531	1.4015E-4
219.67	0.00261	6.5978	4.0481E-5
243.87	0.0028		
262.47	0.00295		
291.07	0.00316		
319.41	0.00335		
378.52	0.00372		
438.87	0.00405		
499.81	0.00435		
562.37	0.00461		
625.2	0.00486		
688.63	0.00508		
752.93	0.00529		
817.53	0.00548		
882.13	0.00566		
947.66	0.00582		
1013.5	0.00597		
1316.5	0.00653		
1602.3	0.00694		
1875.2	0.00724		
2135.5	0.00746		
2383.1	0.00764		
2619.1	0.00779		
2842.9	0.00789		
3055.4	0.00795		
3444.4	0.008		
3838.6	0.00798		
4237.4	0.00789		
4641.9	0.00766		
5052.9	0.00722		

Table S45. High pressure sorption isotherm data for CO₂ on CPO-27-Mn at 473 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
7.2054	2.6745E-5	4718.4	0.00451
14.476	5.2463E-5	4144.3	0.00472
21.674	7.7469E-5	3564.8	0.00473
28.584	1.0116E-4	2987.7	0.00456
35.69	1.2521E-4	2603.4	0.00436
42.331	1.4816E-4	2222.8	0.00407
49.266	1.7177E-4	1844.1	0.0037
56.261	1.9517E-4	1472.3	0.00326
62.814	2.1708E-4	1108.2	0.00271
69.486	2.3952E-4	750.65	0.00205
75.964	2.6118E-4	609.31	0.00173
82.152	2.8118E-4	470.33	0.00138
88.421	3.0248E-4	327.9	0.001
94.737	3.2294E-4	190.81	5.9683E-4
100.96	3.4348E-4	123.11	3.7475E-4
132.31	4.427E-4	56.804	1.5317E-4
163.49	5.4239E-4	43.758	1.0146E-4
194.68	6.3669E-4	29.969	4.8177E-5
223.34	7.2612E-4		
252.02	8.0648E-4		
286.05	9.1061E-4		
319.97	0.001		
388.04	0.0012		
455.85	0.00137		
524.07	0.00155		
592.58	0.00171		
661.22	0.00187		
730.24	0.00202		
799.04	0.00217		
867.06	0.00231		
935.73	0.00245		
1004.4	0.00257		
1217.3	0.00293		
1435.2	0.00325		
1652.1	0.00353		
2014.7	0.0039		
2352.9	0.00418		
2665.8	0.00438		
2966	0.00452		
3245.3	0.00466		
3642.5	0.00475		
4043.7	0.00475		
4450.2	0.00468		
4862.7	0.00445		

5284.8	0.00392
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Table S46. High pressure sorption isotherm data for CH₄ on CPO-27-Mn at 278 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
8.7915	1.6656E-4	9067.5	0.00744
21.882	4.1109E-4	8384.9	0.0076
35.14	6.5351E-4	7716.9	0.00776
48.191	8.8585E-4	7072.3	0.00791
61.019	0.00111	6435.5	0.008
73.605	0.00132	5815.1	0.0081
86.478	0.00153	5197.3	0.00815
98.03	0.00171	4611.2	0.00819
108.82	0.00187	4202	0.00817
128.58	0.00215	3803.9	0.00815
148.26	0.00241	3431.2	0.0081
168.1	0.00267	3069.4	0.00803
187.07	0.00289	2509.2	0.00786
206.13	0.0031	1956.5	0.00756
225.45	0.0033	1425.2	0.00709
244.92	0.00348	912.18	0.00628
258.64	0.0036	712.24	0.00578
284.75	0.00383	522.06	0.00511
311.23	0.00404	335.38	0.00409
423.89	0.00475	178.44	0.00267
541.16	0.0053	141.65	0.00221
662.83	0.00574	106.94	0.00171
786.87	0.0061	70.776	0.00114
912.11	0.0064	56.507	9.003E-4
1037.8	0.00665	42.632	6.5495E-4
1385.9	0.00715		
1739	0.00751		
2096	0.00777		
2455.1	0.00796		
2816.8	0.00809		
3178	0.0082		
3541.9	0.00826		
3904.5	0.00829		
4266.8	0.0083		
4630.1	0.00831		
4993.4	0.0083		
5353.9	0.00831		
5935.2	0.00825		
6512.8	0.00812		
7092.9	0.00797		
7669.2	0.00786		

8248.4	0.00768
8827.3	0.00746
9411.6	0.00723
9760	0.00718

Table S47. High pressure sorption isotherm data for CH₄ on CPO-27-Mn at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
15.959	1.7642E-4	9018.7	0.0069
31.804	3.4857E-4	8322.1	0.00705
47.4	5.1503E-4	7644	0.00716
63.054	6.7859E-4	6968.4	0.00723
78.275	8.3433E-4	6311.3	0.00732
93.223	9.8428E-4	5678.1	0.00738
106.01	0.00111	5063.6	0.00739
129.54	0.00133	4469.2	0.00738
151.73	0.00154	4075.7	0.00735
174.51	0.00174	3685.6	0.00728
196.16	0.00192	3306.1	0.00722
216.31	0.00209	2739.1	0.00703
237.49	0.00225	2180.9	0.00671
255.96	0.00239	1631.3	0.00624
283.09	0.00259	1107.6	0.0055
310.76	0.00277	614.15	0.0042
425.98	0.00345	428.64	0.00338
544.67	0.00401	253.24	0.00229
665.63	0.00447	208	0.00193
788.74	0.00485	165.05	0.00157
911.55	0.00517	124.49	0.00119
1038	0.00545	85.37	8.145E-4
1385.6	0.00603	68.306	6.3506E-4
1741.7	0.00644	51.552	4.5838E-4
2102.1	0.00675	35.07	2.7994E-4
2464.3	0.00697		
2828.7	0.00714		
3195.6	0.00725		
3562.9	0.00736		
3930.8	0.00743		
4300.1	0.00747		
4667.3	0.00743		
5035.4	0.00743		
5626.6	0.0074		
6215.9	0.00732		
6805.3	0.00725		
7398.1	0.0072		
7994.2	0.00707		

8589.1	0.00694
9184.2	0.00682
9728.3	0.00666

Table S48. High pressure sorption isotherm data for CH₄ on CPO-27-Mn at 313 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
11.762	9.0712E-5	9199.7	0.0064
29.125	2.2384E-4	8636.7	0.00653
46.104	3.522E-4	8085.8	0.00658
63.116	4.7865E-4	7541	0.00663
79.682	6.0007E-4	6997.7	0.00669
95.763	7.1627E-4	6460.1	0.0067
109.92	8.1859E-4	5963.3	0.00675
135.9	0.001	5470.9	0.00675
160.27	0.00117	4986	0.00673
183.99	0.00132	4559.8	0.0067
207.49	0.00147	4151.2	0.00663
231.33	0.00162	3755.3	0.00656
252.43	0.00174	3374.2	0.00643
281.34	0.00191	2800.6	0.0062
310.05	0.00207	2234.2	0.00586
428.9	0.00267	1681.2	0.00535
550.58	0.00319	1154.3	0.00457
674.16	0.00363	654.65	0.00331
799.57	0.00402	252.48	0.00148
924.89	0.00434	191.15	0.0011
1050.3	0.00462	132.65	6.9935E-4
1399.9	0.00523	76.237	2.9829E-4
1758.5	0.0057	57.765	1.5602E-4
2119.8	0.00603	39.691	1.5267E-5
2483.3	0.00629		
2847.2	0.00649		
3215.4	0.00663		
3585.4	0.00676		
3958.1	0.00684		
4327.9	0.00692		
4702	0.00695		
5075.6	0.00697		
5672.5	0.00696		
6272.2	0.00693		
6871.2	0.00681		
7471.3	0.00675		
8073.2	0.00664		
8670.1	0.00652		
9271.2	0.00627		

9796	0.00621
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Table S49. High pressure sorption isotherm data for CH₄ on CPO-27-Mn at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
13.234	5.5569E-5	9029.3	0.00607
32.87	1.3798E-4	8309.2	0.00611
52.248	2.1883E-4	7586	0.00618
71.039	2.9602E-4	6897.2	0.00618
89.431	3.7119E-4	6240.7	0.00617
105.68	4.3767E-4	5579.8	0.00611
133.46	5.429E-4	4947.7	0.00602
160.83	6.5416E-4	4518.5	0.00593
187.8	7.5588E-4	4093.6	0.00583
213.29	8.5492E-4	3687.5	0.00569
237.94	9.4899E-4	3307.5	0.00553
259.21	0.00103	2731.9	0.00521
290.81	0.00114	2163.7	0.00476
322.27	0.00125	1618	0.00416
450.14	0.00168	1086.7	0.00331
578.3	0.00206	578.8	0.0021
706.59	0.00242	373.63	0.00146
834.81	0.00273	179.54	7.5602E-4
964.42	0.00302	129.65	5.554E-4
1093.1	0.00328		
1448.2	0.00387		
1808.4	0.00433		
2173.7	0.00471		
2541.2	0.00503		
2911.2	0.00528		
3282.9	0.00547		
3655.3	0.00564		
4029.5	0.00578		
4406.2	0.00587		
4783	0.00595		
5159.8	0.00599		
5767.1	0.00607		
6377.3	0.00611		
6982.7	0.00608		
7592.8	0.00606		
8203.5	0.00598		
8820.2	0.00594		
9439.8	0.00591		
9774.2	0.00582		

Table S50. High pressure sorption isotherm data for CH₄ on CPO-27-Mn at 393 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
14.319	3.3199E-5	8809.7	0.00498
35.329	8.125E-5	8076.6	0.00499
55.946	1.2826E-4	7369.3	0.00501
75.955	1.7365E-4	6679.1	0.00497
95.526	2.1729E-4	6013.5	0.0049
112.74	2.5645E-4	5366.2	0.00482
142.58	3.2123E-4	4737.2	0.00468
171.01	3.8263E-4	4300.3	0.00453
198.28	4.3909E-4	3884.6	0.00438
225.2	4.9522E-4	3493	0.00421
250.89	5.4771E-4	3110.3	0.00402
285.07	6.1839E-4	2525.7	0.00363
319.01	6.8965E-4	1955.5	0.00316
455.91	9.5823E-4	1405	0.00255
590.89	0.00121	868.06	0.00178
725.4	0.00145	654.21	0.00142
859.85	0.00167	443.99	0.00103
992.5	0.00188	232.48	5.9328E-4
1126.5	0.00208	176.63	4.72E-4
1491.1	0.00255	122.92	3.517E-4
1859.5	0.00295	71.015	2.3772E-4
2229.6	0.00329	42.04	1.6794E-4
2602.2	0.00359		
2978.7	0.00383		
3354.1	0.00405		
3732.8	0.00423		
4111.4	0.00438		
4490.3	0.00451		
4870.2	0.00462		
5251	0.00473		
5862.1	0.00482		
6475.8	0.00488		
7090	0.00494		
7704.8	0.005		
8321.7	0.00503		
8941.6	0.00494		
9564.5	0.00488		

Table S51. High pressure sorption isotherm data for CH₄ on CPO-27-Mn at 473 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
15.209	1.3205E-5	8893.8	0.00301
37.909	3.315E-5	8136.4	0.00303
59.861	5.2219E-5	7404.9	0.00297

81.234	7.0611E-5	6695.6	0.00294
100.51	8.9106E-5	6007.9	0.00286
132.65	1.1453E-4	5344.8	0.00274
163.46	1.4069E-4	4716.9	0.00259
193.61	1.6758E-4	4274.2	0.00247
221.2	1.9237E-4	3848	0.00235
247.39	2.1229E-4	3438.7	0.00221
265.23	2.2411E-4	3044.7	0.00204
301.14	2.5744E-4	2447.5	0.00176
446.61	3.7541E-4	1858.5	0.00144
590.49	4.9613E-4	1286.4	0.00108
732.88	6.0487E-4	724.62	6.7615E-4
872.67	7.1039E-4	500.34	4.9973E-4
1013.6	8.148E-4	271.51	3.0489E-4
1395.8	0.00108	210.21	2.4605E-4
1778.5	0.00132	151.65	1.9067E-4
2162.7	0.00153	94.768	1.3789E-4
2546.6	0.00175	63.111	1.0941E-4
2933.4	0.00193	32.068	8.0022E-5
3319.2	0.0021	7.383	5.5773E-5
3706.4	0.00224		
4093	0.00235		
4478.8	0.00246		
4867.6	0.00257		
5256.4	0.00267		
5877.2	0.00282		
6503.2	0.00291		
7126.3	0.00301		
7752.8	0.00308		
8382.4	0.003		
9008.4	0.003		
9643.9	0.00295		

Table S52. High pressure sorption isotherm data for N₂ on CPO-27-Mn at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
6.6673	2.882E-5	9627.9	0.00588
19.615	8.4576E-5	8935.8	0.00593
32.452	1.3916E-4	8244.6	0.00594
45.267	1.93E-4	7577.7	0.00593
57.87	2.4521E-4	6946.6	0.00587
70.067	2.9512E-4	6315.6	0.00582
82.503	3.4552E-4	5711.5	0.00576
94.406	3.9304E-4	5122.4	0.00565
105.12	4.3506E-4	4542.7	0.00553
133.61	5.4565E-4	4156.3	0.00541

161.43	6.5128E-4	3781.2	0.00528
188.7	7.5371E-4	3410.6	0.00513
215.07	8.529E-4	2845.7	0.00484
242.34	9.4826E-4	2302	0.00448
264.33	0.00102	1762.8	0.004
295.55	0.00113	1236.4	0.00333
327.18	0.00123	725.93	0.0024
455.35	0.00161	525.71	0.00191
583.84	0.00195	325.06	0.00133
713.23	0.00226	134.18	6.5923E-4
842.9	0.00254	86.898	4.7005E-4
972.92	0.00278	53.486	3.3124E-4
1103.4	0.00301	18.176	1.7927E-4
1451.8	0.00352	6.3405	1.2399E-4
1805.1	0.00393		
2160.7	0.00425		
2519.2	0.00452		
2878.5	0.00475		
3239.1	0.00494		
3601.1	0.0051		
3964.7	0.00525		
4329.1	0.00535		
4694	0.00546		
5061.1	0.00554		
5643.7	0.00564		
6227.2	0.0057		
6810.3	0.00577		
7396.5	0.00583		
7983.6	0.00587		
8569.9	0.00591		
9158.2	0.00592		
9748.3	0.00587		
10341	0.00585		

Table S53. High pressure sorption isotherm data for N₂ on CPO-27-Mn at 313 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
6.9136	2.1559E-5	9556.5	0.00544
20.534	6.4088E-5	9180.8	0.00546
34.025	1.0584E-4	8805.6	0.00545
47.434	1.4687E-4	8430.6	0.00545
60.286	1.86E-4	8112.6	0.00543
73.224	2.2502E-4	7815.4	0.00539
86.245	2.6398E-4	7526.4	0.00538
98.521	3.0002E-4	7235.7	0.00536
109.48	3.3382E-4	6961	0.00532

139.64	4.1925E-4	6687.9	0.00528
168.89	5.0564E-4	6421.5	0.00526
196.94	5.8434E-4	6165.8	0.00522
224.85	6.6033E-4	5902.5	0.00519
251.67	7.3286E-4	5649.7	0.00514
284.29	8.1877E-4	5408.7	0.00509
316.86	9.0395E-4	5171.3	0.00503
448.47	0.00122	4941.7	0.00499
580.47	0.00151	4719.9	0.00493
712.7	0.00177	4499.6	0.00486
844.82	0.00201	4278.4	0.00479
977.2	0.00223	4061.4	0.00472
1108.3	0.00244	3862.1	0.00465
1460.5	0.00291	3492.1	0.00449
1815.3	0.0033	3303.8	0.00439
2173.4	0.00362	3117.6	0.0043
2533.5	0.00389	2731.6	0.00409
2896.7	0.00413	2364	0.00383
3260.5	0.00432	1984.1	0.00352
3625.2	0.00449	1755.1	0.0033
3991.5	0.00465	1534.1	0.00306
4358.6	0.00477	1317	0.00279
4725.8	0.00486	1102.4	0.00249
5093.9	0.00495	891.19	0.00216
5828.8	0.00506	684.29	0.00178
6562.2	0.00518	480.52	0.00135
7300.6	0.00528	276.8	8.5987E-4
8038.8	0.00533	238.98	7.5634E-4
8777.8	0.00536	201.81	6.5432E-4
9521.7	0.00539	165.71	5.5601E-4
10265	0.00537	130.97	4.5107E-4
		97.528	3.5391E-4
		75.877	2.8803E-4
		54.784	2.2321E-4
		33.97	1.5756E-4
		10.585	8.2853E-5
		3.3792	5.8041E-5

Table S54. High pressure sorption isotherm data for N₂ on CPO-27-Mn at 343 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.4303	1.3373E-5	9694.5	0.00457
21.784	3.9365E-5	8969.7	0.00452
35.876	6.4636E-5	8279.4	0.00445
49.797	8.9701E-5	7607.6	0.00439
63.589	1.1425E-4	6961.3	0.0043

77.136	1.3835E-4	6320	0.0042
90.519	1.6207E-4	5687.9	0.00406
102.64	1.8347E-4	5075.9	0.00391
133.99	2.3895E-4	4480.6	0.00373
164.69	2.8989E-4	4083	0.00359
194.96	3.4432E-4	3703.2	0.00343
224.52	3.9344E-4	3330.4	0.00326
253.11	4.4345E-4	2755.4	0.00295
287.14	4.9746E-4	2188.3	0.00258
321.44	5.5291E-4	1639.4	0.00214
459.39	7.6397E-4	1098.2	0.00159
597.13	9.6672E-4	566.47	9.0814E-4
734.11	0.00115	348.75	5.8012E-4
871.37	0.00133	139.66	2.3323E-4
1008.1	0.0015	86.982	1.4001E-4
1369	0.00189	64.575	9.8444E-5
1732.4	0.00223	42.519	5.7208E-5
2097.3	0.00253	20.633	1.5899E-5
2463.9	0.00279		
2831	0.00302		
3200.3	0.00323		
3568.7	0.0034		
3939.8	0.00354		
4310.1	0.00368		
4681.7	0.00379		
5054.7	0.00392		
5648.4	0.00406		
6244.6	0.00416		
6840.9	0.00425		
7436.9	0.00436		
8036	0.00447		
8636.2	0.00452		
9236.4	0.00456		
9841.1	0.00455		
10442	0.0046		

Table S55. High pressure sorption isotherm data for N₂ on CPO-27-Mn at 393 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
7.7142	7.9932E-6	9852.9	0.00353
22.767	2.3581E-5	9133	0.00349
37.463	3.8747E-5	8438.1	0.00342
52.045	5.3369E-5	7743.9	0.00335
65.927	6.7817E-5	7071	0.00326
79.852	8.2125E-5	6430.8	0.00317
93.638	9.6255E-5	5788.3	0.00306

105.55	1.0664E-4	5170	0.00291
138.35	1.3647E-4	4572.9	0.00274
170.31	1.7147E-4	4168.2	0.00263
200.59	2.0355E-4	3779.7	0.00249
230.6	2.3179E-4	3394.9	0.00233
260.75	2.586E-4	2809.8	0.00208
296.56	2.925E-4	2234.1	0.0018
331.92	3.2699E-4	1674.2	0.00147
475.63	4.5713E-4	1119.7	0.00109
617.4	5.8464E-4	572.31	6.493E-4
757.77	7.0031E-4	348.57	4.4562E-4
898.32	8.1417E-4	131.02	2.3296E-4
1038.4	9.267E-4	76.239	1.7778E-4
1408.6	0.00119	53.112	1.5373E-4
1779.5	0.00144	30.338	1.2902E-4
2150.2	0.00165	7.4542	1.0352E-4
2522.7	0.00185		
2897	0.00202		
3270.5	0.00219		
3645.3	0.00233		
4020	0.00246		
4394.4	0.00259		
4770.5	0.0027		
5147	0.0028		
5749.7	0.00294		
6352.2	0.00305		
6955.6	0.00317		
7559.6	0.00326		
8165.2	0.00332		
8772.6	0.00342		
9377.5	0.00347		
9985.6	0.00351		
10590	0.00356		

Table S56. High pressure sorption isotherm data for N₂ on CPO-27-Mn at 473 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
8.0178	3.447E-6	9459.5	0.00203
23.567	1.0352E-5	8742	0.002
38.812	1.6968E-5	8046.3	0.00193
53.751	2.3421E-5	7353.6	0.00188
68.452	2.9934E-5	6678.5	0.00181
82.642	3.6024E-5	6025.8	0.0017
96.941	4.2293E-5	5382.4	0.0016
109.7	4.9863E-5	4764.3	0.00148
144.76	6.1803E-5	4342	0.00141

177.19	7.6166E-5	3936.3	0.00132
208.83	8.773E-5	3539	0.00123
239.31	1.0262E-4	3161.8	0.00113
266.15	1.1581E-4	2568.7	9.7163E-4
302.91	1.3255E-4	1988	7.9322E-4
451.95	1.9336E-4	1410.8	5.9435E-4
599.52	2.5514E-4	839.21	3.8735E-4
746.17	3.1207E-4	610.25	2.9832E-4
890.97	3.6672E-4	383	2.0246E-4
1035	4.2286E-4	155.86	1.0305E-4
1417.3	5.56E-4	98.234	7.6625E-5
1801.7	6.8983E-4	58.546	5.6584E-5
2185.2	8.1455E-4	12.524	3.4942E-5
2568.3	9.368E-4	2.7515	2.9155E-5
2951.8	0.00104		
3336	0.00114		
3719.6	0.00123		
4105.5	0.00132		
4490.8	0.00141		
4877.2	0.00149		
5262.2	0.00157		
5876.2	0.00166		
6492.2	0.00175		
7108.9	0.00187		
7727.3	0.00194		
8346.8	0.00201		
8961.5	0.00205		
9580.6	0.00207		
10202	0.00211		

Table S57. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mg at 278 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
9.7395E-5	1.3061E-6	97.184	0.01054
0.00333	4.772E-5	87.8	0.0103
0.00672	9.3691E-5	78.123	0.01003
0.01034	1.4162E-4	68.426	0.00974
0.01776	2.3779E-4	58.721	0.00942
0.02144	2.8537E-4	49.024	0.00908
0.02513	3.3283E-4	39.559	0.00873
0.03287	4.3096E-4	29.647	0.00832
0.03697	4.8019E-4	19.373	0.00784
0.04098	5.2824E-4	10.517	0.0073
0.04904	6.2394E-4	9.6676	0.00723
0.05309	6.7212E-4	6.8378	0.00697
0.05731	7.2102E-4	3.9511	0.00653

0.06168	7.7126E-4	1.9995	0.00582
0.06625	8.2136E-4	1.3733	0.00532
0.07075	8.7182E-4	1.015	0.00483
0.07998	9.6997E-4	0.9884	0.00478
0.08928	0.00107	0.7434	0.00429
0.09414	0.00112	0.6852	0.00414
0.099	0.00117	0.529	0.00368
0.1041	0.00122	0.4095	0.00321
0.1265	0.00143	0.3898	0.00312
0.1524	0.00166	0.2976	0.00264
0.1796	0.00188	0.2251	0.00219
0.2015	0.00205	0.1623	0.00171
0.2329	0.00227	0.1121	0.00127
0.2577	0.00244	0.09705	0.00112
0.2886	0.00263		
0.3297	0.00285		
0.372	0.00306		
0.4178	0.00327		
0.4655	0.00346		
0.5094	0.00362		
0.546	0.00375		
0.6156	0.00396		
0.6855	0.00416		
0.7559	0.00433		
0.7989	0.00442		
0.8588	0.00455		
0.9172	0.00466		
0.993	0.00479		
1.0389	0.00486		
1.3002	0.00523		
1.7596	0.00563		
1.9995	0.00579		
2.5687	0.00607		
2.8208	0.00617		
3.0769	0.00625		
3.329	0.00633		
3.6868	0.00642		
4.2316	0.00653		
4.5691	0.0066		
5.9352	0.00681		
6.3214	0.00686		
7.1102	0.00694		
7.4232	0.00698		
7.7404	0.00701		
8.2039	0.00706		
8.6511	0.0071		

9.2203	0.00715
9.6676	0.00718
10.509	0.00725
13.054	0.00742
15.185	0.00754
17.612	0.00768
20.397	0.00783
22.89	0.00795
25.553	0.00807
27.634	0.00817
30.135	0.00828
32.765	0.00839
35.282	0.0085
37.791	0.0086
40.291	0.00871
42.788	0.0088
45.304	0.0089
47.805	0.00899
50.305	0.00908
52.818	0.00917
55.322	0.00926
57.843	0.00935
60.34	0.00943
62.84	0.00951
65.345	0.0096
67.849	0.00968
70.085	0.00975
72.85	0.00984
75.371	0.00992
77.875	0.00999
80.384	0.01007
82.892	0.01014
85.393	0.01021
87.889	0.01028
90.41	0.01035
92.907	0.01041
95.411	0.01048
97.907	0.01055
100.43	0.01061

Table S58. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mg at 288 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
1.6844E-4	1.2197E-6	97.145	0.0096
0.00594	4.6288E-5	87.646	0.0094
0.01246	9.4191E-5	77.941	0.00917

0.01965	1.4244E-4	68.219	0.00894
0.02617	1.9045E-4	58.513	0.00868
0.03367	2.4189E-4	49.235	0.00843
0.04112	2.9243E-4	39.123	0.00812
0.04877	3.4415E-4	29.413	0.0078
0.05622	3.9365E-4	19.911	0.00742
0.06383	4.439E-4	10.648	0.00688
0.07148	4.9358E-4	9.7009	0.0068
0.07953	5.4457E-4	6.8913	0.00649
0.08742	5.9454E-4	4.0654	0.00594
0.09551	6.4491E-4	3.8581	0.00587
0.1039	6.9613E-4	2.1585	0.00505
0.1315	8.6004E-4	1.512	0.00444
0.1507	9.7006E-4	1.1628	0.00395
0.1811	0.00114	0.9792	0.00363
0.2027	0.00125	0.7463	0.00312
0.2356	0.00142	0.6871	0.00297
0.258	0.00152	0.5246	0.0025
0.308	0.00175	0.3965	0.00205
0.3563	0.00195	0.2844	0.00159
0.4066	0.00215	0.1915	0.00114
0.4574	0.00233	0.1097	6.7864E-4
0.5075	0.0025	0.09773	6.0511E-4
0.5514	0.00264		
0.6009	0.00279		
0.6454	0.00291		
0.6745	0.00299		
0.7022	0.00306		
0.7756	0.00324		
0.8432	0.00339		
0.8993	0.0035		
0.9294	0.00356		
0.984	0.00367		
1.014	0.00372		
1.3128	0.00421		
1.5892	0.00453		
1.8861	0.00483		
2.0324	0.00495		
2.252	0.00511		
2.7196	0.00538		
2.7847	0.00543		
3.0489	0.00554		
3.2807	0.00564		
3.5409	0.00574		
4.2281	0.00595		
4.594	0.00605		

5.7976	0.00629
6.2367	0.00637
6.4359	0.0064
6.6677	0.00643
7.1393	0.00649
7.4484	0.00654
8.229	0.00662
8.4486	0.00665
8.7942	0.00668
9.1846	0.00672
9.518	0.00675
9.9286	0.00679
10.201	0.00681
13.064	0.00701
15.084	0.00713
17.926	0.00728
20.651	0.0074
22.655	0.00749
25.188	0.00759
27.978	0.00769
30.291	0.00777
32.837	0.00786
35.341	0.00794
38.281	0.00804
40.363	0.00811
42.867	0.00818
45.368	0.00826
47.913	0.00833
50.377	0.00841
52.89	0.00848
55.387	0.00856
57.895	0.00862
60.396	0.00869
63.063	0.00877
65.405	0.00883
67.902	0.0089
70.419	0.00897
72.618	0.00903
75.444	0.00909
77.933	0.00915
80.437	0.00922
82.946	0.00928
85.447	0.00934
87.947	0.0094
90.456	0.00945
92.961	0.00951

95.465	0.00956
97.974	0.00962
100.47	0.00967

Table S59. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mg at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
1.3836E-4	9.8389E-7	97.106	0.00891
0.01006	4.4677E-5	87.523	0.00874
0.0217	9.2219E-5	77.817	0.00856
0.03332	1.3815E-4	68.201	0.00837
0.04497	1.8377E-4	58.381	0.00816
0.05751	2.3183E-4	49.204	0.00795
0.06981	2.7827E-4	39.007	0.00769
0.08194	3.2345E-4	29.76	0.00742
0.09464	3.7026E-4	19.441	0.00702
0.1074	4.1662E-4	10.638	0.00643
0.1358	5.1762E-4	9.7393	0.00634
0.151	5.708E-4	6.8686	0.00593
0.183	6.8011E-4	4.2217	0.00524
0.2139	7.8174E-4	3.937	0.00513
0.2304	8.3546E-4	2.3228	0.00422
0.2635	9.3995E-4	1.6153	0.00353
0.281	9.9398E-4	1.1948	0.00297
0.3373	0.00116	0.9819	0.00262
0.3879	0.0013	0.7311	0.00214
0.4563	0.00149	0.6864	0.00204
0.5237	0.00166	0.4684	0.00153
0.5715	0.00177	0.3888	0.00131
0.6284	0.0019	0.2331	8.5255E-4
0.6899	0.00204	0.1011	4.0235E-4
0.7492	0.00216	0.09666	3.8545E-4
0.8228	0.00231		
0.8882	0.00243		
0.92	0.00249		
0.978	0.00259		
1.0285	0.00268		
1.2738	0.00307		
1.5625	0.00343		
1.8674	0.00375		
2.0097	0.00389		
2.3757	0.0042		
2.7904	0.00448		
3.0222	0.00461		
3.3597	0.00479		
3.5508	0.00489		

4.0875	0.00511
4.6079	0.0053
5.3398	0.00551
5.783	0.00562
6.4011	0.00576
6.8402	0.00585
7.1329	0.0059
7.6859	0.00599
7.9258	0.00603
8.2104	0.00607
8.4341	0.0061
8.6699	0.00614
9.2676	0.00621
9.662	0.00626
10.134	0.00631
13.049	0.00657
15.582	0.00674
17.599	0.00685
20.12	0.00698
22.629	0.00709
25.272	0.00719
27.687	0.00728
30.2	0.00736
32.843	0.00745
35.368	0.00752
37.872	0.00759
40.373	0.00767
42.898	0.00773
45.39	0.0078
47.899	0.00786
50.416	0.00793
52.921	0.00798
55.417	0.00804
57.926	0.0081
60.431	0.00816
62.935	0.00822
65.436	0.00827
67.953	0.00833
70.457	0.00839
72.938	0.00845
75.459	0.00849
77.972	0.00854
80.468	0.00858
82.615	0.00863
85.481	0.00868
87.982	0.00873

90.491	0.00878
92.987	0.00883
95.492	0.00887
98.009	0.00892
100.51	0.00896

Table S60. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mg at 308 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
2.2303E-4	1.3379E-6	97.059	0.0084
0.01636	4.3864E-5	87.427	0.00826
0.03444	8.7762E-5	77.71	0.0081
0.05361	1.325E-4	67.992	0.00793
0.07245	1.7602E-4	58.287	0.00774
0.09279	2.2175E-4	48.594	0.00753
0.113	2.6699E-4	38.97	0.0073
0.1354	3.1624E-4	29.306	0.007
0.1594	3.6829E-4	19.405	0.00657
0.1837	4.2011E-4	10.9	0.00586
0.2089	4.7314E-4	9.8384	0.00571
0.2341	5.257E-4	7.0655	0.00521
0.2592	5.7714E-4	6.7687	0.00514
0.3697	7.9111E-4	4.8822	0.00458
0.4793	9.8983E-4	3.8494	0.00415
0.5809	0.00116	2.3369	0.0032
0.6774	0.00132	1.597	0.00251
0.77	0.00146	1.1573	0.00199
0.8288	0.00155	0.9732	0.00174
0.8664	0.00161	0.6955	0.00132
0.9359	0.00171	0.4275	8.5844E-4
1.0034	0.0018	0.3805	7.6912E-4
1.3001	0.00218	0.1554	3.1727E-4
1.5156	0.00243	0.09796	1.9071E-4
1.8572	0.00278		
2.1946	0.00307		
2.2597	0.00313		
2.6744	0.00343		
2.7557	0.00349		
3.0119	0.00365		
3.3412	0.00385		
3.5323	0.00395		
3.7519	0.00406		
4.0202	0.00419		
4.3211	0.00432		
5.1749	0.00464		
6.0857	0.00492		

6.5939	0.00505
6.8907	0.00512
7.2526	0.0052
7.5941	0.00527
7.8746	0.00533
8.517	0.00545
9.131	0.00555
9.4319	0.00559
9.6717	0.00563
9.9238	0.00567
10.432	0.00574
12.628	0.00599
15.201	0.00621
17.555	0.00638
20.048	0.00653
22.796	0.00667
25.224	0.00678
27.586	0.00687
30.099	0.00696
32.733	0.00705
35.238	0.00713
37.751	0.0072
40.231	0.00727
42.764	0.00733
45.24	0.00739
47.728	0.00746
50.225	0.00752
52.697	0.00757
55.181	0.00762
57.669	0.00768
60.17	0.00773
62.63	0.00778
65.175	0.00783
67.696	0.00788
70.119	0.00792
72.595	0.00797
75.051	0.00802
77.641	0.00807
80.117	0.00811
82.601	0.00815
85.073	0.0082
87.574	0.00824
90.017	0.00828
92.53	0.00832
94.929	0.00836
98.019	0.00841

100.53	0.00845
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Table S61. Standard pressure sorption isotherm data for CO₂ on CPO-27-Ni at 278 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
2.6147E-4	5.4305E-7	96.862	0.00805
0.0156	4.3261E-5	87.301	0.00788
0.03124	8.5879E-5	77.633	0.00769
0.04753	1.2972E-4	67.949	0.00748
0.06378	1.7304E-4	58.273	0.00725
0.07985	2.16E-4	48.597	0.00701
0.09677	2.6004E-4	38.95	0.00674
0.1135	3.041E-4	29.331	0.00643
0.1316	3.5077E-4	19.296	0.00604
0.1718	4.5445E-4	9.9177	0.00547
0.2249	5.8736E-4	6.9503	0.00515
0.2776	7.1638E-4	4.3328	0.00463
0.3289	8.4001E-4	3.7874	0.00446
0.3791	9.5784E-4	2.5214	0.00385
0.4265	0.00107	1.8986	0.00337
0.474	0.00117	1.4223	0.00285
0.5201	0.00128	1.0921	0.00238
0.564	0.00137	0.9957	0.00222
0.6072	0.00146	0.7416	0.00177
0.6469	0.00154	0.6938	0.00167
0.6746	0.0016	0.4745	0.00121
0.8004	0.00184	0.3922	0.00102
0.8435	0.00192	0.2015	5.4577E-4
0.883	0.00199	0.09392	2.6118E-4
0.9432	0.00209		
0.9782	0.00215		
1.0092	0.0022		
1.2645	0.00258		
1.5241	0.00292		
1.7887	0.00321		
2.0451	0.00344		
2.3382	0.00365		
2.5133	0.00377		
2.9163	0.004		
3.018	0.00405		
3.5716	0.00429		
3.8118	0.00438		
4.5079	0.0046		
5.3993	0.0048		
6.0262	0.00492		
6.8037	0.00504		

7.3492	0.00512
7.7277	0.00517
8.375	0.00525
8.9082	0.0053
9.5595	0.00536
10.02	0.00541
13.036	0.00563
15.092	0.00575
17.733	0.00589
20.168	0.006
22.704	0.00611
25.447	0.00622
27.763	0.0063
30.491	0.0064
33.023	0.00649
35.652	0.00657
38.331	0.00665
40.578	0.00672
43.085	0.00679
45.589	0.00686
48.096	0.00694
50.608	0.007
53.128	0.00707
55.627	0.00714
58.13	0.0072
60.638	0.00726
63.145	0.00732
65.653	0.00738
68.16	0.00744
70.664	0.0075
73.179	0.00756
75.679	0.00761
78.182	0.00767
80.69	0.00772
83.197	0.00777
85.709	0.00782
88.212	0.00787
90.712	0.00792
93.223	0.00797
95.723	0.00802
98.238	0.00807
100.74	0.00811

Table S62. Standard pressure sorption isotherm data for CO₂ on CPO-27-Ni at 288 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹

4.2946E-4	4.9924E-7	96.823	0.00737
0.02599	4.198E-5	87.155	0.00723
0.05362	8.471E-5	77.504	0.00706
0.08181	1.2775E-4	67.771	0.00688
0.1099	1.7021E-4	58.083	0.00669
0.2094	3.1468E-4	48.407	0.00649
0.304	4.4865E-4	38.775	0.00625
0.3943	5.7446E-4	29.62	0.00599
0.4793	6.9019E-4	19.289	0.00559
0.5589	7.9566E-4	11.07	0.00504
0.633	8.9288E-4	9.7269	0.00489
0.7022	9.814E-4	6.8448	0.00445
0.7651	0.00106	4.5245	0.00384
0.8239	0.00113	3.9262	0.00361
0.8713	0.00119	2.7009	0.00295
0.908	0.00124	2.0251	0.00244
0.9486	0.00129	1.443	0.00188
0.9859	0.00133	1.0128	0.00138
1.0424	0.0014	0.9781	0.00134
1.2761	0.00166	0.6748	9.5614E-4
1.5692	0.00197	0.3843	5.6215E-4
1.8012	0.0022	0.09322	1.2971E-4
2.0536	0.00242		
2.3264	0.00263		
2.5584	0.00279		
2.8108	0.00296		
3.0102	0.00308		
3.5191	0.00336		
3.9669	0.00356		
4.321	0.00371		
4.895	0.00391		
5.298	0.00403		
5.587	0.00411		
5.8719	0.00418		
6.1447	0.00425		
6.7064	0.00437		
7.0891	0.00445		
7.4392	0.00451		
7.7241	0.00456		
7.9846	0.00461		
8.4935	0.00468		
9.1366	0.00477		
9.5356	0.00482		
10.354	0.00491		
12.747	0.00514		
15.426	0.00532		

17.6	0.00545
20.123	0.00557
22.761	0.00569
25.456	0.00579
27.78	0.00587
30.797	0.00597
33.068	0.00604
36.007	0.00612
38.108	0.00618
40.994	0.00625
43.135	0.00631
45.85	0.00637
48.158	0.00643
50.654	0.00649
53.173	0.00654
55.685	0.0066
58.176	0.00665
60.692	0.00671
63.199	0.00675
65.711	0.00681
68.21	0.00686
70.722	0.00691
73.384	0.00696
75.733	0.007
78.237	0.00704
80.736	0.00709
83.248	0.00713
85.751	0.00718
88.234	0.00722
90.754	0.00727
93.27	0.00731
95.769	0.00735
98.289	0.00739
100.78	0.00743

Table S63. Standard pressure sorption isotherm data for CO₂ on CPO-27-Ni at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
6.3871E-4	5.0009E-7	96.777	0.00682
0.04074	3.7649E-5	87.044	0.00669
0.08359	7.6077E-5	77.36	0.00655
0.1276	1.1503E-4	67.663	0.00639
0.267	2.35E-4	58.337	0.00623
0.4106	3.5488E-4	48.47	0.00604
0.5418	4.6172E-4	38.741	0.0058
0.61	5.178E-4	29.211	0.00552

0.704	5.9186E-4	19.678	0.0051
0.7875	6.5762E-4	11.711	0.00445
0.8625	7.1513E-4	9.9159	0.0042
0.9289	7.6577E-4	7.213	0.0037
0.9869	8.1007E-4	6.8303	0.0036
1.0439	8.5348E-4	4.6443	0.00293
1.3389	0.00108	3.8383	0.00259
1.6239	0.00128	2.6008	0.00195
1.7826	0.00139	1.864	0.00148
2.1001	0.00161	1.1476	9.4753E-4
2.2833	0.00172	0.9554	7.9548E-4
2.6212	0.00192	0.6594	5.5662E-4
2.8044	0.00202	0.3572	3.0341E-4
3.0201	0.00214	0.07984	4.7974E-5
3.3702	0.00232		
3.7732	0.00251		
4.339	0.00276		
5.0026	0.00301		
5.5684	0.00319		
6.0569	0.00334		
6.3459	0.00343		
6.6227	0.0035		
6.8914	0.00357		
7.156	0.00363		
7.4206	0.00369		
7.7015	0.00375		
7.9701	0.00381		
8.2388	0.00387		
8.4708	0.00391		
8.7151	0.00396		
9.1221	0.00403		
9.4559	0.00408		
9.7327	0.00413		
9.9892	0.00417		
10.335	0.00422		
12.68	0.00451		
15.236	0.00475		
18.086	0.00495		
20.264	0.00508		
22.617	0.0052		
25.169	0.00532		
27.876	0.00542		
30.274	0.00551		
33.034	0.0056		
35.574	0.00567		
38.098	0.00574		

40.621	0.00581
43.137	0.00587
45.649	0.00592
48.164	0.00598
50.684	0.00604
53.184	0.00609
55.699	0.00614
58.207	0.00619
60.718	0.00623
63.226	0.00628
65.738	0.00633
68.233	0.00637
70.737	0.00641
73.244	0.00645
75.752	0.00649
78.271	0.00653
80.767	0.00658
83.266	0.00662
85.778	0.00665
88.281	0.00669
90.793	0.00673
93.288	0.00676
95.804	0.0068
98.316	0.00683
100.8	0.00686

Table S64. Standard pressure sorption isotherm data for CO₂ on CPO-27-Ni at 308 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
8.7502E-4	4.8224E-7	96.738	0.00637
0.05947	3.4376E-5	86.998	0.00625
0.1214	6.8926E-5	77.302	0.00611
0.188	1.0519E-4	67.615	0.00597
0.3856	2.0954E-4	57.96	0.0058
0.5599	2.9824E-4	48.358	0.0056
0.7085	3.7135E-4	38.805	0.00536
0.8351	4.3342E-4	29.418	0.00503
0.9396	4.8483E-4	19.674	0.00449
1.0263	5.2677E-4	12.188	0.00374
1.2839	6.5419E-4	9.9456	0.00339
1.5403	7.7795E-4	7.3691	0.00286
1.9799	9.8037E-4	6.73	0.00269
2.0654	0.00102	4.5442	0.00204
2.3096	0.00113	3.8889	0.0018
2.566	0.00124	2.4439	0.00121
3.0341	0.00143	1.3161	6.7868E-4

3.4086	0.00158	0.9539	4.9567E-4
3.6162	0.00166	0.6414	3.3377E-4
3.8319	0.00175	0.3736	1.9138E-4
4.0802	0.00184	0.06982	6.0351E-6
4.3285	0.00193		
4.589	0.00201		
4.8373	0.0021		
5.0937	0.00218		
5.3542	0.00226		
5.6147	0.00234		
5.8671	0.00242		
6.1235	0.00249		
6.4288	0.00257		
6.6608	0.00264		
6.9132	0.0027		
7.1615	0.00276		
7.4301	0.00283		
7.6743	0.00289		
7.9348	0.00295		
8.1994	0.003		
8.4477	0.00306		
8.7082	0.00311		
8.9565	0.00316		
9.2211	0.00321		
9.4734	0.00326		
9.7258	0.00331		
10.023	0.00336		
12.758	0.00378		
15.225	0.00406		
17.533	0.00428		
20.28	0.00449		
22.718	0.00465		
25.181	0.00479		
27.652	0.00491		
30.188	0.00502		
32.976	0.00513		
35.52	0.00522		
38.052	0.0053		
40.657	0.00537		
43.115	0.00544		
45.626	0.0055		
48.15	0.00556		
50.824	0.00562		
53.181	0.00567		
55.697	0.00573		
58.208	0.00578		

60.719	0.00582
63.223	0.00587
65.742	0.00591
68.25	0.00596
70.749	0.006
73.252	0.00604
75.772	0.00608
78.263	0.00611
80.778	0.00615
83.286	0.00619
85.793	0.00622
88.292	0.00626
90.804	0.00629
93.315	0.00632
95.814	0.00635
98.326	0.00638
100.83	0.00641

Table S65. Standard pressure sorption isotherm data for CO₂ on CPO-27-Co at 278 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
-1.2326E-35	8.1355E-7	95.874	0.00823
0.03719	3.2318E-5	84.947	0.008
0.0743	6.5379E-5	75.591	0.00779
0.1114	9.8546E-5	65.83	0.00754
0.1566	1.3684E-4	56.161	0.00728
0.2019	1.7868E-4	46.643	0.00698
0.2513	2.2244E-4	36.89	0.00663
0.4653	4.1657E-4	27.453	0.00621
0.6669	5.8316E-4	18.561	0.00566
0.7739	6.7824E-4	9.8675	0.00466
0.8933	7.7983E-4	7.3732	0.00412
0.9426	8.2181E-4	6.9589	0.00401
0.9879	8.6334E-4	4.9318	0.00332
1.0332	9.0586E-4	3.8837	0.00283
1.422	0.00122	2.9535	0.00231
1.7713	0.00149	1.8648	0.00154
2.1857	0.00179	1.1648	9.8684E-4
2.2629	0.00185	0.9714	8.1578E-4
2.7138	0.00214	0.6381	5.3132E-4
2.7869	0.00219	0.3501	2.6941E-4
3.2581	0.00248	0.05781	1.3239E-5
3.6116	0.00267		
3.7984	0.00277		
4.3834	0.00306		
4.8831	0.00327		

5.7889	0.00361
6.3902	0.00381
6.8005	0.00393
7.1051	0.00402
7.621	0.00415
8.0598	0.00426
8.3848	0.00433
8.6691	0.00439
8.925	0.00445
9.181	0.0045
9.4409	0.00455
9.7009	0.0046
9.9569	0.00464
10.201	0.00469
13.04	0.00509
15.514	0.00536
18.276	0.0056
20.645	0.00578
23.062	0.00593
25.633	0.00608
28.176	0.00621
30.719	0.00634
33.404	0.00645
35.891	0.00656
38.413	0.00665
40.932	0.00675
43.43	0.00684
45.961	0.00693
48.463	0.00701
50.97	0.00709
53.488	0.00717
55.987	0.00725
58.501	0.00732
61.008	0.00739
63.526	0.00746
66.021	0.00753
68.527	0.00759
71.042	0.00765
73.536	0.00772
76.054	0.00778
78.549	0.00784
81.063	0.0079
83.57	0.00796
86.08	0.00801
88.574	0.00807
91.077	0.00812

93.575	0.00817
96.11	0.00822
98.592	0.00828
101.11	0.00833

Table S66. Standard pressure sorption isotherm data for CO₂ on CPO-27-Co at 288 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.00496	1.4171E-7	95.811	0.00749
0.05814	3.2045E-5	84.827	0.00728
0.1203	6.3108E-5	75.516	0.00709
0.1783	9.7372E-5	65.869	0.00687
0.2487	1.3814E-4	56.051	0.00662
0.3191	1.7051E-4	47.642	0.00637
0.5469	2.9072E-4	36.67	0.00598
0.7167	3.809E-4	27.591	0.00554
0.845	4.5208E-4	18.926	0.00492
0.9444	5.0607E-4	10.343	0.00377
1.0314	5.4711E-4	9.8799	0.00368
1.6296	8.4447E-4	7.4872	0.00311
1.7718	9.1902E-4	6.8576	0.00293
2.3689	0.00121	4.8387	0.00226
2.5233	0.00128	3.9369	0.00192
3.1366	0.00156	2.8117	0.00142
3.3479	0.00165	1.5037	7.8384E-4
3.5754	0.00175	0.9278	4.8166E-4
3.8272	0.00185	0.6297	3.2528E-4
4.0709	0.00195	0.3357	1.698E-4
4.53	0.00213	0.05814	1.7763E-5
5.0702	0.00234		
5.3343	0.00243		
5.5943	0.00252		
6.0655	0.00267		
6.3498	0.00276		
6.6098	0.00284		
6.8738	0.00292		
7.1338	0.00299		
7.3857	0.00306		
7.6375	0.00313		
7.8975	0.0032		
8.1453	0.00326		
8.4093	0.00333		
8.8196	0.00343		
9.4493	0.00357		
9.6808	0.00362		
9.9489	0.00367		

10.294	0.00374
12.687	0.00415
15.063	0.00448
17.724	0.00477
20.377	0.00501
22.988	0.00522
25.572	0.00539
28.119	0.00554
30.662	0.00567
33.38	0.0058
35.886	0.00591
38.4	0.00601
40.927	0.00611
43.442	0.0062
45.956	0.00628
48.483	0.00636
50.993	0.00644
53.508	0.00652
56.002	0.00659
58.528	0.00666
61.039	0.00672
63.541	0.00678
66.056	0.00685
68.562	0.00691
71.072	0.00697
73.567	0.00703
76.093	0.00708
78.579	0.00714
81.098	0.00719
83.6	0.00724
86.102	0.0073
88.617	0.00735
91.107	0.0074
93.626	0.00744
96.124	0.00749
98.642	0.00754
101.12	0.00758

Table S67. Standard pressure sorption isotherm data for CO₂ on CPO-27-Co at 298 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
0.0025	4.0907E-7	95.769	0.00684
0.07054	2.6367E-5	84.76	0.00664
0.1533	5.0892E-5	75.485	0.00645
0.2443	8.3921E-5	65.715	0.00623
0.327	1.1174E-4	56.116	0.00598

0.6165	2.0898E-4	46.821	0.00569
1.0259	3.3796E-4	37.185	0.00531
1.3306	4.3304E-4	27.777	0.00479
1.5378	4.9955E-4	19.262	0.00408
1.7734	5.7767E-4	10.508	0.00285
2.0253	6.5508E-4	9.9104	0.00273
2.2731	7.3427E-4	7.3592	0.00218
2.525	8.1293E-4	6.8148	0.00205
2.785	8.8806E-4	4.5561	0.00146
3.0328	9.6221E-4	3.9509	0.00129
3.3618	0.00106	1.6637	5.7959E-4
3.634	0.00114	0.9184	3.3273E-4
3.8859	0.00121	0.6206	2.3319E-4
4.1377	0.00128	0.3435	1.3978E-4
4.3937	0.00135	0.06226	4.4985E-5
4.8933	0.00149		
5.5067	0.00166		
5.8683	0.00175		
6.1405	0.00182		
6.4045	0.00188		
6.6605	0.00195		
6.9123	0.00201		
7.1601	0.00207		
7.4526	0.00214		
7.7451	0.00221		
8.1676	0.0023		
8.4235	0.00236		
8.8582	0.00245		
9.1669	0.00251		
9.4391	0.00257		
9.6829	0.00262		
9.9429	0.00267		
10.187	0.00272		
12.657	0.00316		
15.533	0.00358		
17.645	0.00384		
20.237	0.00411		
22.853	0.00435		
25.441	0.00456		
28.02	0.00473		
30.779	0.00491		
33.302	0.00505		
35.812	0.00518		
38.404	0.0053		
41.004	0.00541		
43.376	0.0055		

45.948	0.0056
48.454	0.00568
50.977	0.00577
53.479	0.00584
56.002	0.00592
58.521	0.00599
61.019	0.00606
63.546	0.00613
66.044	0.00619
68.555	0.00625
71.057	0.00631
73.576	0.00637
76.078	0.00642
78.597	0.00648
81.083	0.00653
83.606	0.00659
86.112	0.00664
88.615	0.00669
91.121	0.00673
93.624	0.00678
96.122	0.00683
98.641	0.00688
101.14	0.00692

Table S68. Standard pressure sorption isotherm data for CO₂ on CPO-27-Co at 308 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.00506	3.0426E-8	95.754	0.00622
0.1035	2.1388E-5	84.757	0.00601
0.2149	4.8496E-5	75.499	0.00581
0.3263	7.1848E-5	65.749	0.00557
0.9206	1.9563E-4	56.191	0.00529
1.1599	2.4742E-4	46.652	0.00494
1.3529	2.8564E-4	37.224	0.00451
1.6007	3.3734E-4	27.961	0.00393
1.8404	3.8752E-4	19.028	0.00313
2.1045	4.3724E-4	10.124	0.00196
2.3442	4.8867E-4	9.628	0.00188
2.6001	5.4194E-4	6.9996	0.00143
2.8398	5.92E-4	4.1519	8.9047E-4
3.0998	6.4232E-4	3.7782	8.1003E-4
3.441	7.129E-4	1.2135	2.7317E-4
3.705	7.639E-4	0.9412	2.1046E-4
3.9488	8.161E-4	0.6441	1.4635E-4
4.2007	8.6602E-4	0.3098	7.2348E-5
4.4688	9.1528E-4	0.04983	1.5588E-5

4.7125	9.5994E-4
5.4965	0.00111
6.244	0.00125
6.6828	0.00133
6.9549	0.00138
7.2068	0.00143
7.4627	0.00147
7.7105	0.00152
7.9624	0.00156
8.2183	0.0016
8.4702	0.00164
8.7221	0.00168
8.9617	0.00172
9.2624	0.00177
9.7011	0.00184
9.9692	0.00189
10.217	0.00193
12.707	0.0023
15.108	0.00262
17.684	0.00293
20.734	0.00325
22.944	0.00346
25.414	0.00368
27.974	0.00387
30.586	0.00406
33.234	0.00423
35.769	0.00437
38.674	0.00453
41.099	0.00465
43.317	0.00475
45.897	0.00486
48.423	0.00496
51.162	0.00506
53.4	0.00514
55.992	0.00523
58.49	0.00531
61.009	0.00539
63.523	0.00546
66.038	0.00553
68.532	0.0056
71.071	0.00567
73.561	0.00573
76.064	0.00579
78.582	0.00585
81.089	0.00591
83.612	0.00597

86.094	0.00603
88.621	0.00607
91.127	0.00612
93.617	0.00617
96.14	0.00622
98.634	0.00627
101.15	0.00632

Table S69. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mn at 278 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
2.8567E-4	2.5413E-7	96.814	0.0082
0.16	1.0685E-4	87.307	0.00798
0.3423	2.2324E-4	77.689	0.00773
0.5615	3.5872E-4	68.08	0.00745
0.8064	5.0625E-4	58.52	0.00714
1.1365	6.972E-4	49.009	0.00679
2.107	0.00122	39.607	0.00638
3.1005	0.00169	30.393	0.0059
4.2283	0.00217	28.821	0.0058
5.0956	0.00249	19.961	0.00512
6.0687	0.00281	14.33	0.00449
7.1151	0.00311	10.515	0.00388
8.3366	0.00342	9.7129	0.00372
9.3464	0.00364	7.5304	0.00322
10.132	0.0038	6.6469	0.00298
14.481	0.0045	4.8716	0.00241
15.405	0.00462	3.7438	0.00197
20.1	0.00513	2.5019	0.0014
25.462	0.00556	1.5532	9.0042E-4
30.617	0.0059	0.9086	5.2829E-4
35.092	0.00615	0.673	3.8592E-4
40.177	0.0064	0.3828	2.0595E-4
45.356	0.00663	0.09533	1.9569E-5
50.487	0.00683		
55.592	0.00702		
60.694	0.0072		
65.768	0.00736		
70.833	0.00752		
75.878	0.00767		
80.943	0.00781		
85.983	0.00794		
91.036	0.00806		
96.073	0.00818		
101.11	0.0083		

Table S70. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mn at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
8.6773E-4	2.2012E-7	96.697	0.0065
0.209	5.5764E-5	87.034	0.00629
0.4538	1.1769E-4	77.425	0.00605
0.6907	1.7684E-4	67.86	0.00579
0.9583	2.4237E-4	58.348	0.00549
1.2582	3.1442E-4	48.943	0.00514
2.3814	5.8178E-4	39.659	0.00472
3.0776	7.4061E-4	30.615	0.00419
4.3603	0.00102	28.885	0.00407
5.0973	0.00117	21.474	0.00347
6.4125	0.00143	19.532	0.00327
7.3205	0.0016	14.01	0.00263
8.2977	0.00177	10.069	0.00207
9.1487	0.00192	9.4012	0.00196
10.085	0.00207	6.5468	0.00146
14.845	0.00274	4.23	9.9237E-4
15.603	0.00283	3.7006	8.7673E-4
20.244	0.00334	1.4774	3.5822E-4
25.403	0.0038	0.9637	2.2929E-4
30.628	0.00418	0.6384	1.4721E-4
35.778	0.0045	0.3555	7.4681E-5
40.233	0.00473	0.0707	-6.3268E-6
45.315	0.00497		
50.486	0.00519		
55.637	0.00538		
60.759	0.00556		
65.869	0.00572		
70.938	0.00587		
75.67	0.006		
81.069	0.00614		
86.143	0.00626		
91.175	0.00637		
96.22	0.00648		
101.26	0.00659		

Table S71. Standard pressure sorption isotherm data for CO₂ on CPO-27-Mn at 313 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.00127	2.9275E-7	96.689	0.00535
0.3471	5.1664E-5	87.059	0.00513
0.6721	9.6752E-5	77.449	0.00489
1.0202	1.4436E-4	67.913	0.00461
1.5996	2.2337E-4	58.422	0.0043

2.1208	2.9565E-4	49.008	0.00392
2.642	3.6319E-4	39.671	0.00349
3.1509	4.2983E-4	30.469	0.00296
3.9246	5.2851E-4	28.803	0.00285
4.515	6.0458E-4	21.051	0.00228
5.3782	7.1232E-4	19.239	0.00213
6.3473	8.2859E-4	13.119	0.00157
7.3449	9.4508E-4	10.171	0.00126
8.3425	0.00106	9.2505	0.00116
9.3564	0.00117	6.5346	8.4702E-4
10.362	0.00128	4.0101	5.3377E-4
14.41	0.00169	3.4482	4.5953E-4
15.574	0.0018	1.3593	1.7516E-4
19.568	0.00215	0.9889	1.2315E-4
20.668	0.00224	0.5375	5.9017E-5
24.76	0.00256	0.3092	2.4245E-5
25.762	0.00263		
29.948	0.00292		
30.835	0.00298		
35.135	0.00323		
40.152	0.0035		
45.311	0.00375		
50.465	0.00398		
55.6	0.00418		
60.722	0.00437		
65.82	0.00454		
70.906	0.0047		
75.988	0.00484		
81.057	0.00498		
86.13	0.0051		
91.155	0.00522		
96.229	0.00533		
101.27	0.00544		

Table S72. Standard pressure sorption isotherm data for CO₂ on CPO-27-Zn at 278 K.

Adsorption branch		Desorption branch	
<i>p</i> / kPa	<i>n</i> _{ads} / mol g ⁻¹	<i>p</i> / kPa	<i>n</i> _{des} / mol g ⁻¹
9.8095E-21	1.50821E-6	96.142	0.00745
0.07231	1.92826E-5	85.196	0.00721
0.1422	4.45124E-5	76.603	0.007
0.2366	7.62559E-5	66.653	0.00673
0.327	1.06536E-4	56.491	0.00641
0.9223	3.10306E-4	46.825	0.00605
1.2796	4.27345E-4	37.57	0.00563
1.5681	5.31186E-4	27.782	0.00505
1.8362	6.18408E-4	18.543	0.00422

2.0963	7.07237E-4	9.5356	0.00278
2.3319	7.86473E-4	7.0084	0.00219
2.5797	8.63255E-4	6.8662	0.00215
2.8357	9.48782E-4	4.1887	0.00139
3.0917	0.00102	3.8677	0.00129
3.433	0.00113	2.206	7.38423E-4
3.6808	0.00121	0.951	2.964E-4
3.9368	0.00129	0.6472	1.83586E-4
4.1887	0.00137	0.3434	7.67422E-5
4.4325	0.00144	0.05174	-3.33087E-5
4.7047	0.00152		
4.9728	0.00159		
5.241	0.00167		
7.4838	0.00226		
8.5645	0.00252		
9.239	0.00268		
10.413	0.00293		
13.038	0.00339		
15.285	0.00374		
19.079	0.00421		
21.213	0.00444		
23.931	0.00468		
25.471	0.00482		
29.696	0.00512		
30.366	0.00516		
33.434	0.00535		
36.904	0.00554		
38.09	0.0056		
41.767	0.00577		
43.161	0.00582		
47.008	0.00599		
48.833	0.00606		
51.226	0.00616		
53.375	0.00624		
56.544	0.00635		
58.328	0.00641		
62.196	0.00654		
63.098	0.00657		
66.141	0.00666		
69.013	0.00675		
70.838	0.00681		
73.588	0.00689		
76.115	0.00696		
79.26	0.00704		
80.784	0.00708		
83.957	0.00716		

85.903	0.0072
88.593	0.00727
91.595	0.00735
93.387	0.00739
96.365	0.00746
98.892	0.0075
100.99	0.00755

Table S73. Standard pressure sorption isotherm data for CO₂ on CPO-27-Zn at 288 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.00622	2.6661E-8	96.462	0.00661
0.08428	1.4482E-5	84.497	0.00635
0.1664	3.11323E-5	75.591	0.00614
0.2691	5.39261E-5	66.616	0.0059
0.3635	7.31864E-5	56.913	0.00559
1.0615	2.33274E-4	46.947	0.0052
1.3888	3.00477E-4	37.61	0.00475
1.6407	3.55751E-4	27.871	0.00412
2.0145	4.38423E-4	18.494	0.00324
2.4939	5.35335E-4	9.0109	0.00188
2.8758	6.14393E-4	6.6991	0.00147
3.1927	6.79486E-4	3.7372	8.84492E-4
3.4812	7.39895E-4	0.9548	2.78027E-4
3.6925	7.84688E-4	0.6345	2.02681E-4
3.9647	8.38048E-4	0.343	1.33912E-4
4.2247	8.89712E-4	0.06784	6.68466E-5
4.4604	9.37896E-4		
4.7204	9.85456E-4		
4.9764	0.00104		
5.2405	0.00109		
5.4883	0.00114		
6.2237	0.00128		
7.597	0.00153		
8.7671	0.00174		
9.4253	0.00185		
9.986	0.00195		
10.778	0.00207		
13.789	0.00252		
15.313	0.00273		
18.441	0.00311		
20.424	0.00333		
23.479	0.00364		
26.417	0.00389		
27.965	0.00401		
30.707	0.00422		

33.295	0.00439
37.033	0.00462
38.012	0.00467
41.783	0.00487
44.062	0.00498
46.126	0.00508
48.312	0.00517
50.973	0.00528
53.415	0.00538
56.393	0.00549
58.835	0.00557
61.322	0.00566
64.263	0.00575
66.246	0.00581
68.635	0.0059
71.04	0.00597
74.055	0.00605
76.651	0.00612
78.39	0.00617
81.145	0.00624
83.481	0.0063
86.114	0.00636
88.6	0.00642
91.05	0.00648
93.549	0.00653
96.052	0.00659
98.563	0.00664
101.06	0.00669

Table S74. Standard pressure sorption isotherm data for CO₂ on CPO-27-Zn at 298 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
-8.8644E-19	9.09209E-7	95.838	0.0056
0.06468	8.45454E-6	84.621	0.00536
0.1228	1.74222E-5	76.049	0.00515
0.2057	2.52298E-5	65.657	0.00485
0.2928	3.78246E-5	56.776	0.00454
0.3633	4.82511E-5	46.591	0.00413
0.4296	5.77541E-5	37.458	0.00367
1.201	1.6433E-4	27.772	0.00305
1.6452	2.24025E-4	18.14	0.00225
1.8971	2.53244E-4	8.3324	0.0012
2.1612	2.86259E-4	6.6626	9.96119E-4
2.3806	3.17668E-4	3.4328	5.80932E-4
2.6406	3.51468E-4	0.8982	2.28103E-4
2.8884	3.83528E-4	0.6494	1.86473E-4

3.1362	4.17636E-4	0.3633	1.40038E-4
3.445	4.54314E-4	0.05223	8.8708E-5
3.6766	4.85411E-4		
3.9447	5.17623E-4		
4.1722	5.44035E-4		
4.4485	5.76738E-4		
4.7126	6.07701E-4		
7.7514	9.7573E-4		
9.3115	0.00116		
10.429	0.00129		
14.235	0.0017		
16.198	0.00189		
19.578	0.00221		
21.764	0.00241		
23.901	0.00259		
25.822	0.00274		
29.353	0.003		
31.437	0.00315		
33.245	0.00327		
36.462	0.00347		
38.425	0.00358		
41.687	0.00376		
43.771	0.00386		
46.444	0.00399		
48.91	0.0041		
50.962	0.0042		
53.302	0.0043		
56.349	0.00442		
58.291	0.00449		
61.139	0.00459		
63.849	0.00469		
66.018	0.00477		
68.692	0.00486		
71.365	0.00494		
73.299	0.005		
75.964	0.00508		
78.418	0.00515		
81.42	0.00523		
83.277	0.00528		
86.023	0.00535		
88.44	0.00541		
90.967	0.00548		
93.584	0.00554		
96.066	0.0056		
98.564	0.00565		
101.08	0.00571		

Table S75. Standard pressure sorption isotherm data for CO₂ on CPO-27-Zn at 308 K.

Adsorption branch		Desorption branch	
p / kPa	n_{ads} / mol g ⁻¹	p / kPa	n_{des} / mol g ⁻¹
0.00857	-9.24333E-7	95.863	0.00506
0.0862	7.22763E-6	86.059	0.00482
0.1847	1.7266E-5	75.052	0.00451
0.3079	2.7175E-5	66.431	0.00424
0.4516	4.23262E-5	56.322	0.00386
1.3011	1.19872E-4	47.57	0.00348
1.7277	1.6342E-4	37.21	0.00296
2.3616	2.22727E-4	27.426	0.00236
2.8572	2.67427E-4	17.598	0.00166
3.1863	2.96806E-4	7.9034	8.41795E-4
3.4911	3.2469E-4	6.6033	7.12903E-4
3.7389	3.47042E-4	3.1782	3.88628E-4
3.9705	3.66347E-4		
4.2143	3.8877E-4		
4.4865	4.16722E-4		
4.7465	4.42902E-4		
5.3031	4.92371E-4		
5.7623	5.33818E-4		
6.2945	5.83832E-4		
6.7577	6.24922E-4		
7.7653	7.09512E-4		
8.5251	7.77595E-4		
9.1101	8.31891E-4		
9.7196	8.81949E-4		
10.727	9.70331E-4		
13.157	0.00118		
15.692	0.00138		
18.191	0.00158		
20.69	0.00177		
23.851	0.002		
25.553	0.00212		
28.275	0.00231		
30.725	0.00247		
33.362	0.00263		
36.763	0.00283		
38.12	0.00291		
40.944	0.00306		
43.381	0.00319		
46.953	0.00336		
48.472	0.00344		
51.93	0.00359		
53.088	0.00365		

56.411	0.00379
58.556	0.00387
61.262	0.00398
63.383	0.00406
66.39	0.00416
68.328	0.00423
71.473	0.00434
73.333	0.0044
76.49	0.0045
78.335	0.00456
82.028	0.00467
83.162	0.0047
86.989	0.00481
88.176	0.00484
91.783	0.00494
93.258	0.00498
96.557	0.00506
98.365	0.00511
101.14	0.00517

3. Structural characteristics of CO₂ adsorption predicted by different DFT methods

Table S76. Structure characteristics of CO₂ adsorption predicted by different DFT methods. All the angles are in degree, while the distances are in angstrom. d(C-O) is the CO₂ gas phase equilibrium bond length predicted by different methods. M represents the metal atom. M, O_I, C and O_{II} are shown in Figure 3.

Method	MOFs	M-O _I -C angle	O _I -C-O _{II} angle	d(M-O _I)	d(O _I -C)	d(C-O _{II})	d (C-O) Equilibrium m
LDA- VASP	Mg	138.2	175.0	2.15	1.174	1.158	1.165
	Mn	134.6	177.3	2.31	1.174	1.161	
	Fe	118.0	177.4	2.45	1.172	1.162	
	Co	130.0	177.4	2.20	1.174	1.160	
	Ni	132.9	177.1	2.13	1.174	1.159	
	Cu	113.7	178.3	2.60	1.168	1.165	
	Zn	131.7	176.6	2.28	1.173	1.160	
GGA- VASP	Mg	150.4	178.4	2.33	1.176	1.166	1.173
	Mn	142.7	179.3	2.66	1.177	1.169	
	Fe	129.8	179.4	2.93	1.175	1.171	
	Co	140.2	179.3	2.67	1.176	1.170	
	Ni	138.6	179.0	2.49	1.177	1.169	
	Cu	128.1	179.7	3.06	1.174	1.172	
	Zn	143.0	179.3	2.67	1.176	1.170	
LSDA- Gaussian	Mg	130.3	173.7	2.13	1.184	1.162	1.171
	Mn	124.8	177.6	2.27	1.183	1.165	
	Fe	123.4	177.5	2.30	1.178	1.169	
	Co	121.7	177.1	2.18	1.182	1.165	
	Ni	129.7	174.5	2.11	1.180	1.169	
	Cu	113.1	178.1	2.46	1.175	1.171	
	Zn	132.1	174.0	2.17	1.183	1.164	
B3LYP- Gaussian	Mg	145.9	175.7	2.25	1.177	1.160	1.169
	Mn	144.9	176.8	2.52	1.175	1.163	
	Fe	143.5	177.3	2.60	1.173	1.165	
	Co	145.0	176.9	2.46	1.174	1.164	
	Ni	147.1	176.2	2.37	1.174	1.164	
	Cu	125.9	178.3	3.00	1.170	1.169	
	Zn	143.1	176.7	2.43	1.175	1.162	

4. Experimental sorption isotherms

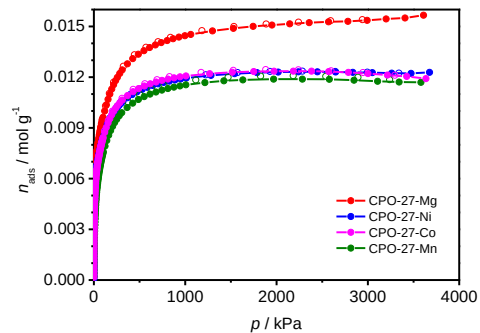


Figure S1. High pressure sorption isotherms of CO₂ on CPO-27-M at 278 K.

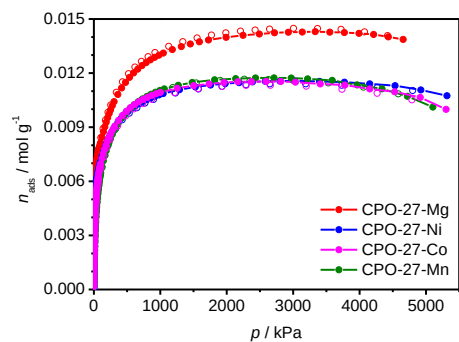


Figure S2. High pressure sorption isotherms of CO₂ on CPO-27-M at 298 K.

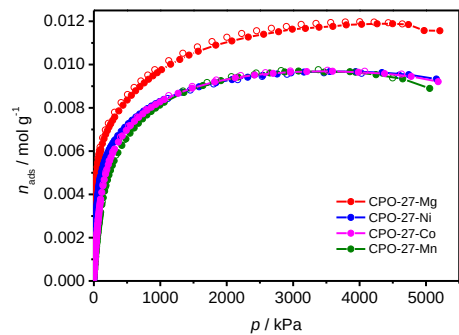


Figure S3. High pressure sorption isotherms of CO₂ on CPO-27-M at 343 K.

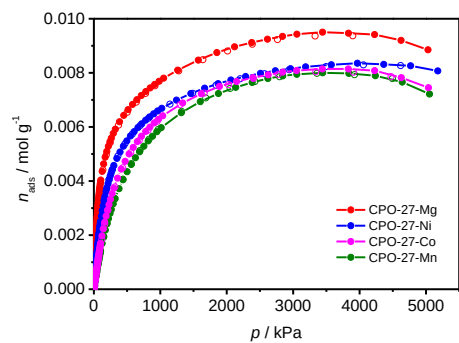


Figure S4. High pressure sorption isotherms of CO₂ on CPO-27-M at 393 K.

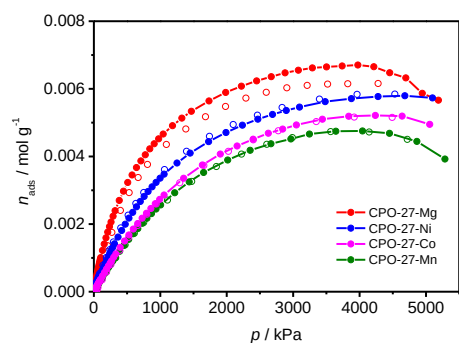


Figure S5. High pressure sorption isotherms of CO₂ on CPO-27-M at 473 K.

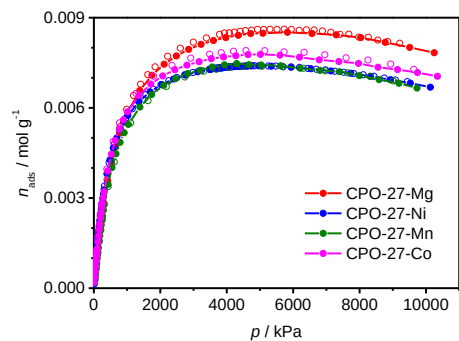


Figure S6. High pressure sorption isotherms of CH₄ on CPO-27-M at 298 K.

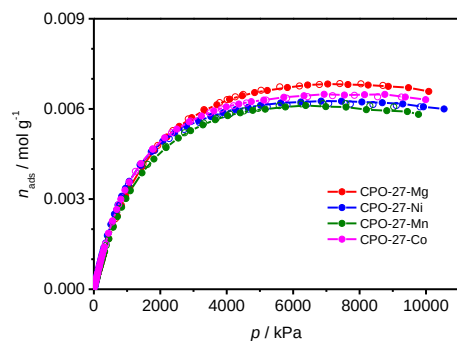


Figure S7. High pressure sorption isotherms of CH₄ on CPO-27-M at 343 K.

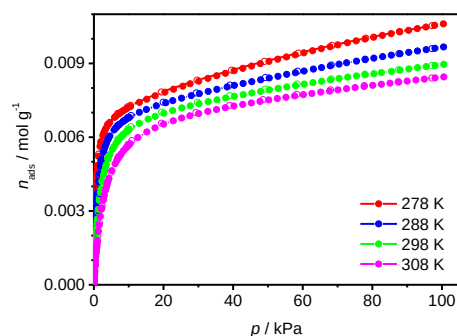


Figure S8. Standard pressure sorption isotherms of CO₂ on CPO-27-Mg in the temperature range 278-308 K.

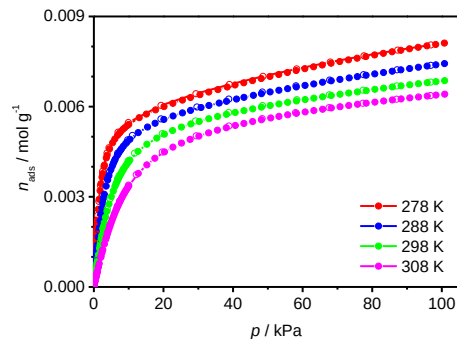


Figure S9. Standard pressure sorption isotherms of CO₂ on CPO-27-Ni in the temperature range 278-308 K.

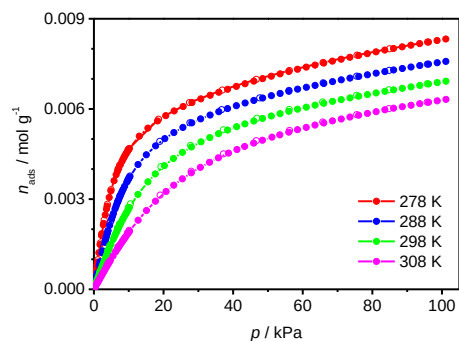


Figure S10. Standard pressure sorption isotherms of CO₂ on CPO-27-Co in the temperature range 278-308 K.

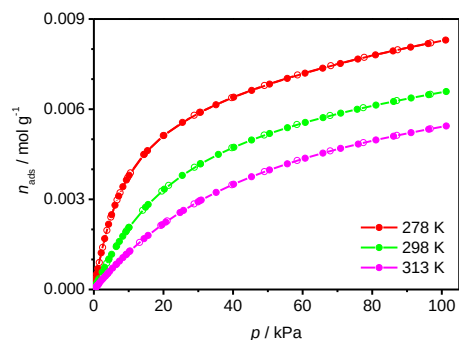


Figure S11. Standard pressure sorption isotherms of CO₂ on CPO-27-Mn in the temperature range 278-313 K.

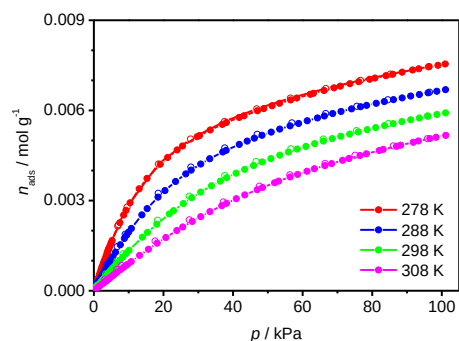


Figure S12. Standard pressure sorption isotherms of CO₂ on CPO-27-Zn in the temperature range 278-308 K.