Supporting Information

In Silico Studies on the Origin of Selective Uptake of Carbon dioxide with Cucurbit[7]uril Amorphous Material

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Contents:

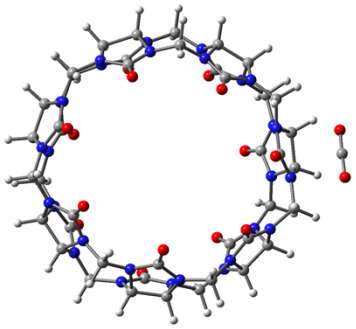
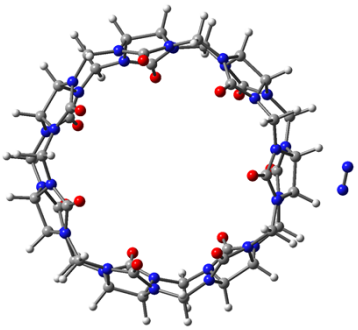
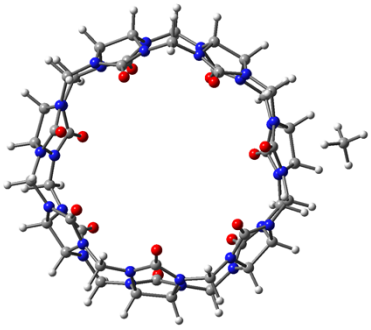
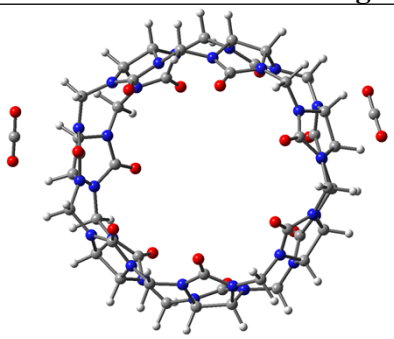
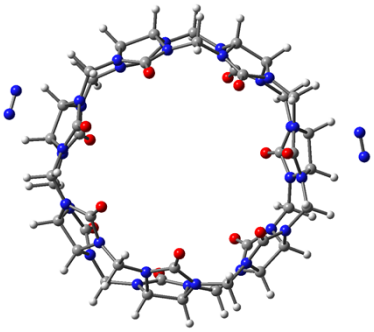
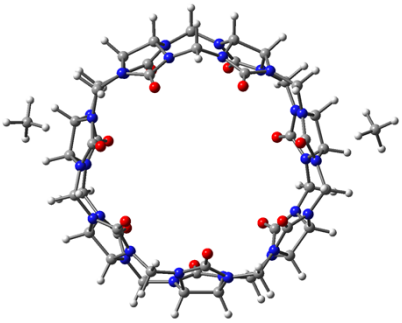
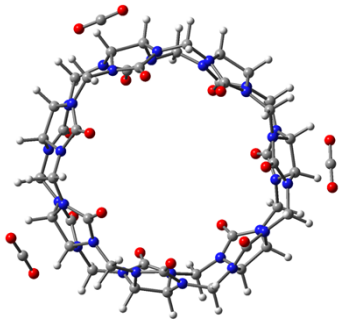
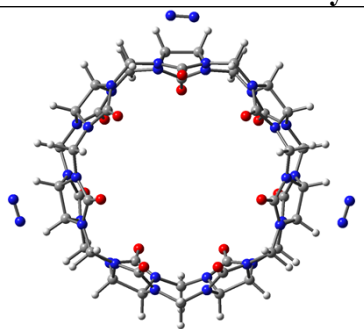
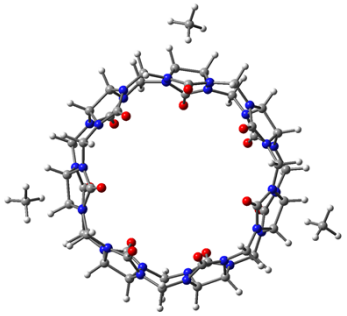
1 gas molecule outside the cavity of CB[7]		
		
ΔH= -6.1 CB[7]+1CO_2	ΔH= -3.2 CB[7]+1N_2	ΔH= -2.7 CB[7]+1CH_4
2 gas molecule outside the cavity of CB[7]		
		
ΔH= -12.0, H_b= -6.0 CB[7]+2CO_2	ΔH= -6.1, H_b= -3.0 CB[7]+2N_2	ΔH= -5.2, H_b= -2.6 CB[7]+2CH_4
3 gas molecule outside the cavity of CB[7]		
		
CB[7]+3CO_2 ΔH= -13.6, H_b=-4.5	CB[7]+3N_2 ΔH= -9.2, H_b=-3.1	CB[7]+3CH_4 ΔH= -8.0, H_b=-2.7

Figure S1: M06-2X/6-31G(d) calculated binding enthalpies (kcal/mol) of CO_2, N_2 and CH_4 towards CB[7]uril and their corresponding average binding enthalpies (H_b) (kcal/mol).

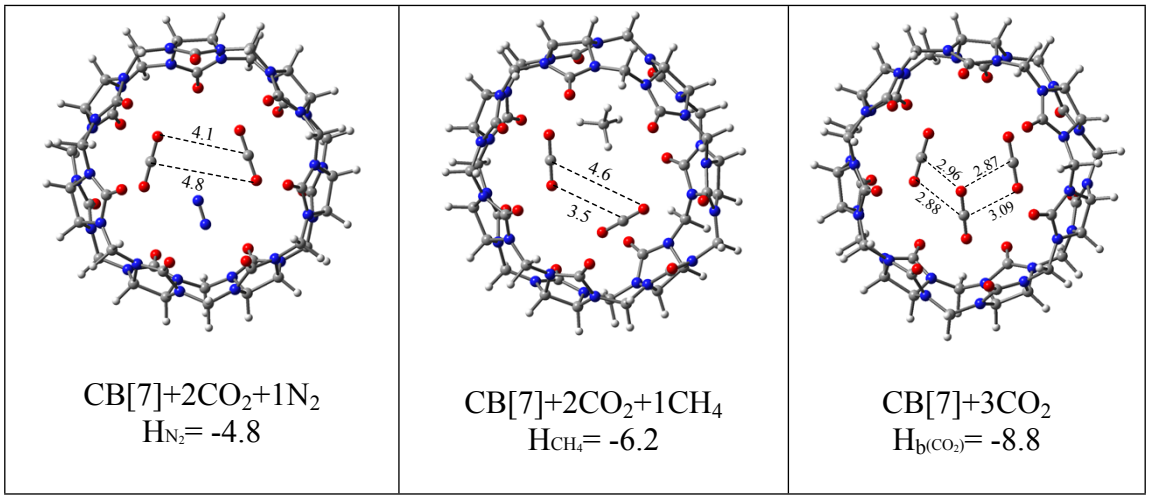


Figure S2: M06-2X/6-31G(d) calculated binding enthalpies (kcal/mol) of N_2 and CH_4 in presence of CO_2 inside the CB[7] cavity. The energies are in kcal/mol.

Table S1: M06-2X/6-31G(d) calculated free energies, **ΔG** (kcal/mol) of single and double gas molecule(s) (CO_2, N_2 and CH_4) inside the CB[7] cavity at 273 K and 298 K.

	ΔG (273K)	**ΔG (298K)**
1 CO_2 inside CB[7]	0.8	1.6
1 N_2 inside CB[7]	3.6	4.0
1 CH_4 inside CB[7]	2.3	2.9
2 CO_2 inside CB[7]	1.6	3.4
2 N_2 inside CB[7]	4.3	5.6
2 CH_4 inside CB[7]	5.8	7.3

Table S2: Calculated adsorption enthalpies (ΔH, kcal/mol) of single and double gas molecules (CO_2, N_2 and CH_4) inside the CB[7] cavity at PBEPBE/6-31G(d) and M06-2X-D3/6-31G(d) levels of theory.

	ΔH [PBEPBE/6-31G(d)]	**ΔH [M06-2X-D3/6-31G(d)]**
1 CO_2 inside CB[7]	-3.1	-10.0
1 N_2 inside CB[7]	-1.3	-5.7
1 CH_4 inside CB[7]	-1.7	-6.6
2 CO_2 inside CB[7]	-6.3	-20.2
2 N_2 inside CB[7]	-2.8	-11.8
2 CH_4 inside CB[7]	-2.7	-13.1