Supporting information

The Effect of the Zeolite Nanocavity on the Reaction Mechanism of *n*-Hexane Cracking: A Density Functional Theory Study

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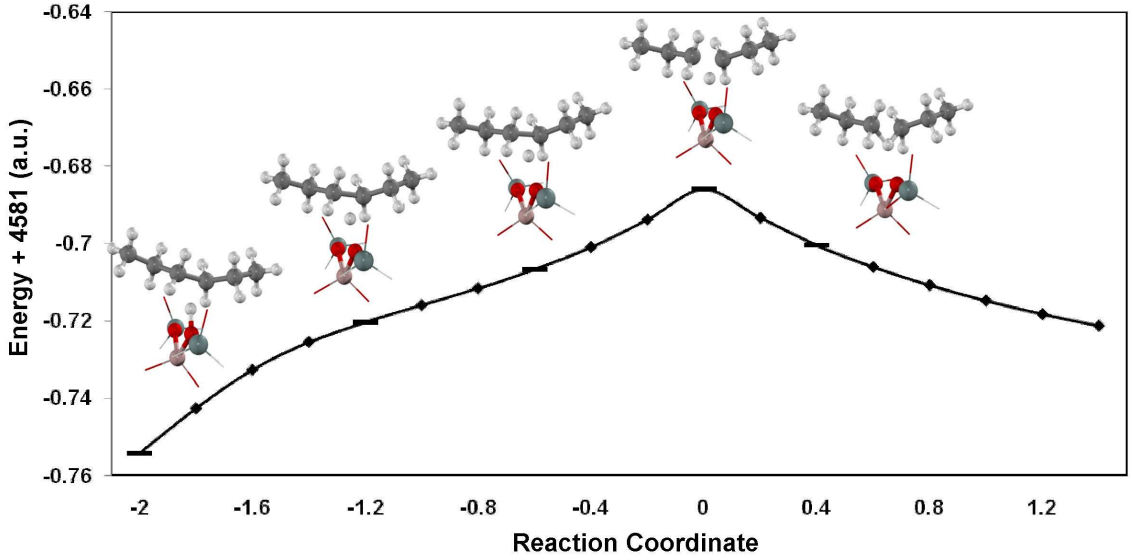
Table S1. Optimized geometrical parameters and adsorption energies of *n*-hexane adsorbed on H-FAU and H-ZSM-5 obtained from M06-2X/6-311+G(2df,2p)//M06-2X/6-31G(d,p) and from B3LYP/6-311+G(2df,2p)//B3LYP/6-31G(d,p) calculations.

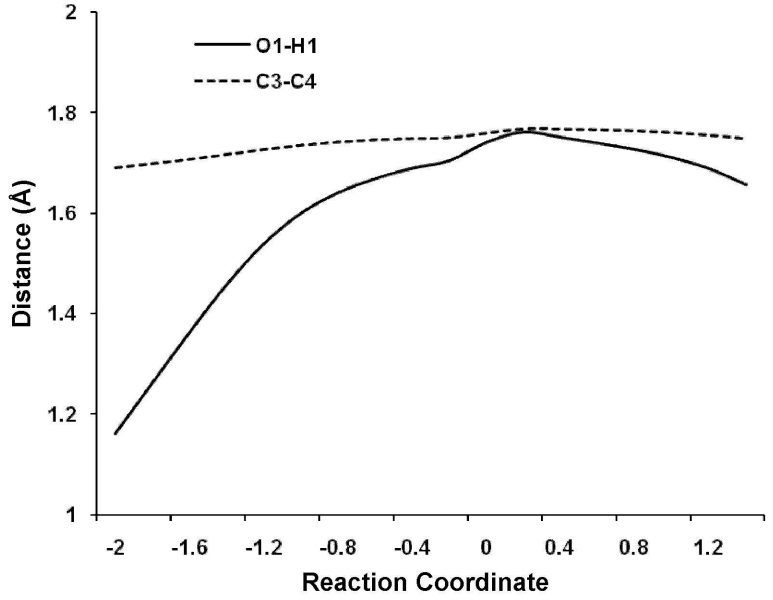
Parameter	Isolated molecule		*n*-Hexane adsorption			
			Ads_FAU		Ads_ZSM-5	
	M06-2X	B3LYP	M06-2X	B3LYP	M06-2X	B3LYP
Distances (Å)						
O1-H1	0.97 (0.97)	0.97 (0.97)	0.98	0.97	0.97	0.97
Al-O1	1.97 (1.82)	1.98 (1.83)	1.96	1.97	1.82	1.82
Al-O2	1.72 (1.68)	1.73 (1.68)	1.72	1.73	1.68	1.68
H1-C3	-	-	2.40	2.87	2.81	2.91
H1-C4	-	-	2.46	3.03	3.04	2.95
C1-C2	1.53	1.53	1.53	1.53	1.52	1.53
C2-C3	1.53	1.53	1.53	1.53	1.53	1.53
C3-C4	1.53	1.53	1.53	1.53	1.53	1.54
C4-C5	1.53	1.53	1.53	1.53	1.53	1.54
C5-C6	1.53	1.53	1.53	1.53	1.53	1.53
Angles (°)						
O2-Al-O1*	106.2 (90.4)	105.1 (90.0)	107.1	105.4	90.5	90.6
Si1-O1-Al*	132.3 (130.5)	132.1 (130.4)	131.5	131.6	130.1	130.6
Energy(kcal/mol)**			–10.8	–1.65	–18.2	1.06

* The parameters in parentheses were obtained from the isolate structure of H-ZSM-5 zeolite

** The experimental adsorption energies of n-hexane on H-FAU and H-ZSM-5 are –12.7 and –19.6 kcal/mol, respectively [39].

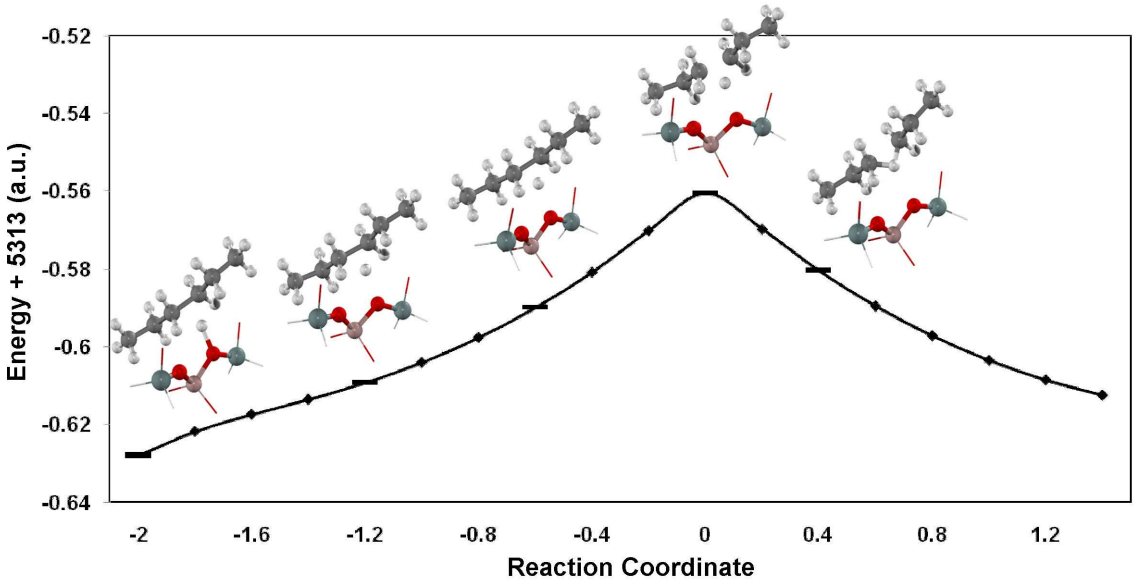


(**a**)

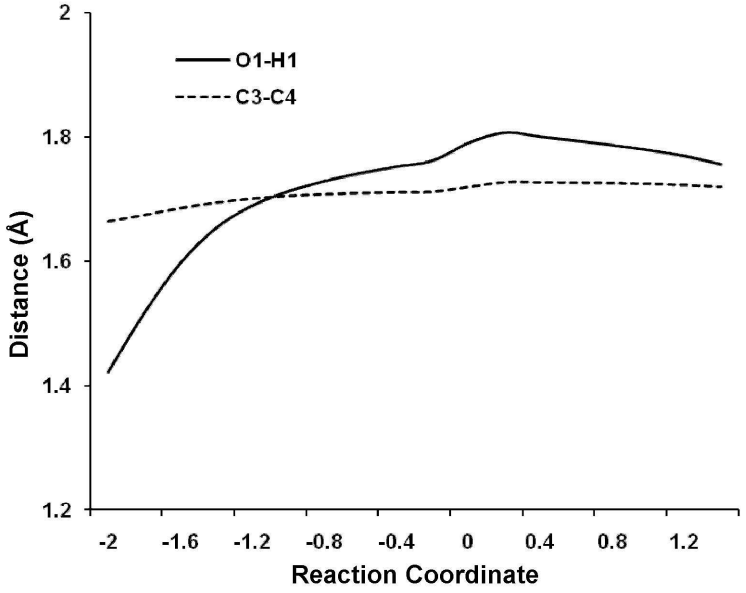


(**b**)

Figure S1 Results from the IRC calculation for the protonation of *n*-Hexane over H-ZSM-5 zeolite. (a) Energy profile and structural changes; (b) Evolution of the O1-H1 and C3-H4 distances along the reaction coordinate.



(**a**)



(**b**)

Figure S2 Results from the IRC calculation for the protonation of *n*-Hexane over H-FAU zeolite. (a) Energy profile and structural changes; (b) Evolution of the O1-H1 and C3-H4 distances along the reaction coordinate.