Reaction Pathway for Partial Hydrogenation of 1,3-Butadiene over Pt/SiO_2

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Supporting information

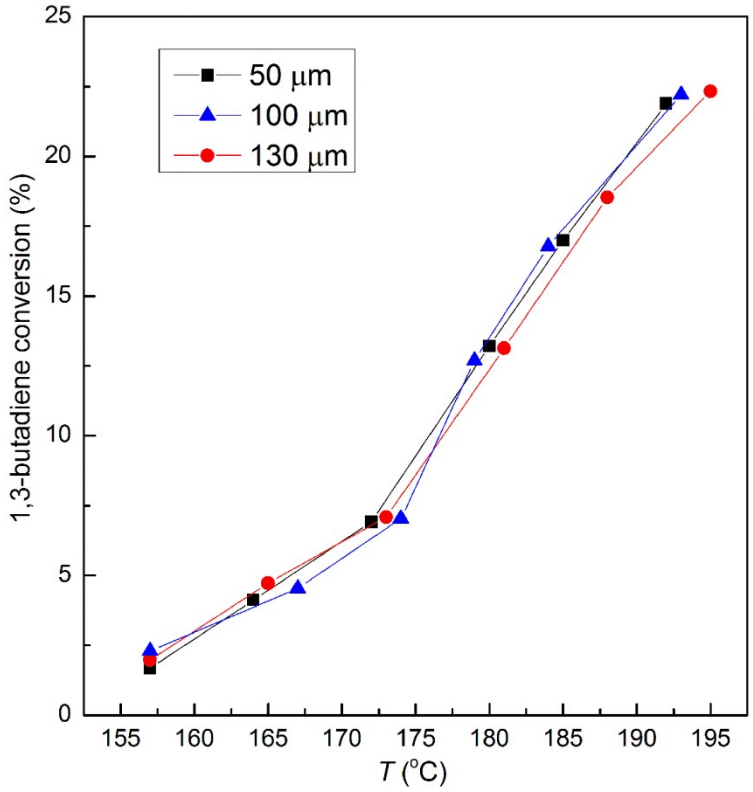

Figure S1. Light-off curves for 1,3-butadiene (0.25%) hydrogenation in 15% H_2/Ar over the Pt/SiO_2 catalyst with different particle size.

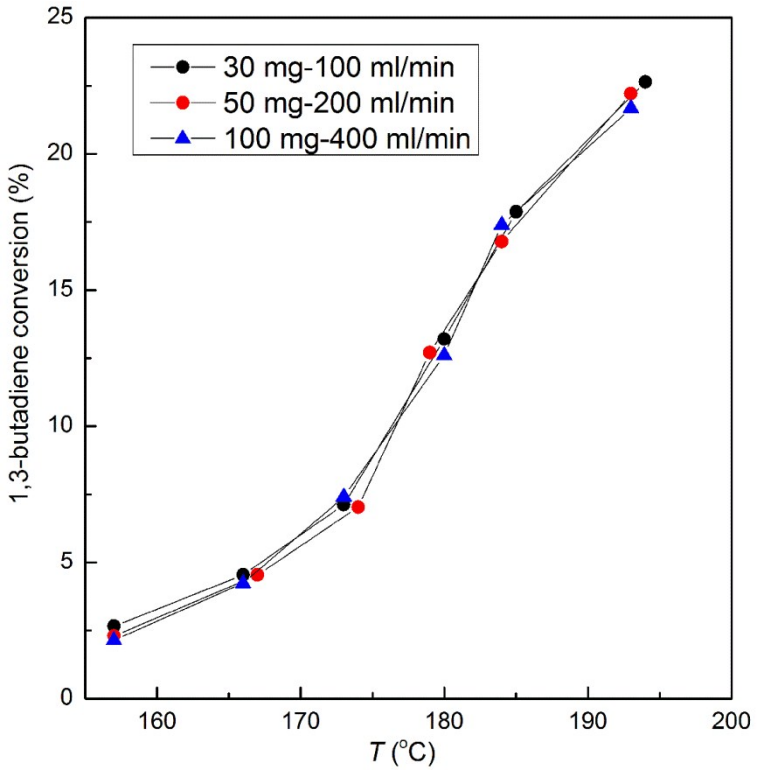

Figure S2. Light-off curves for hydrogenation of 1,3-butadiene (0.25%) in 15% H_2/Ar over the Pt/SiO_2 catalyst with different amounts of catalyst and gas flow rates (STP).

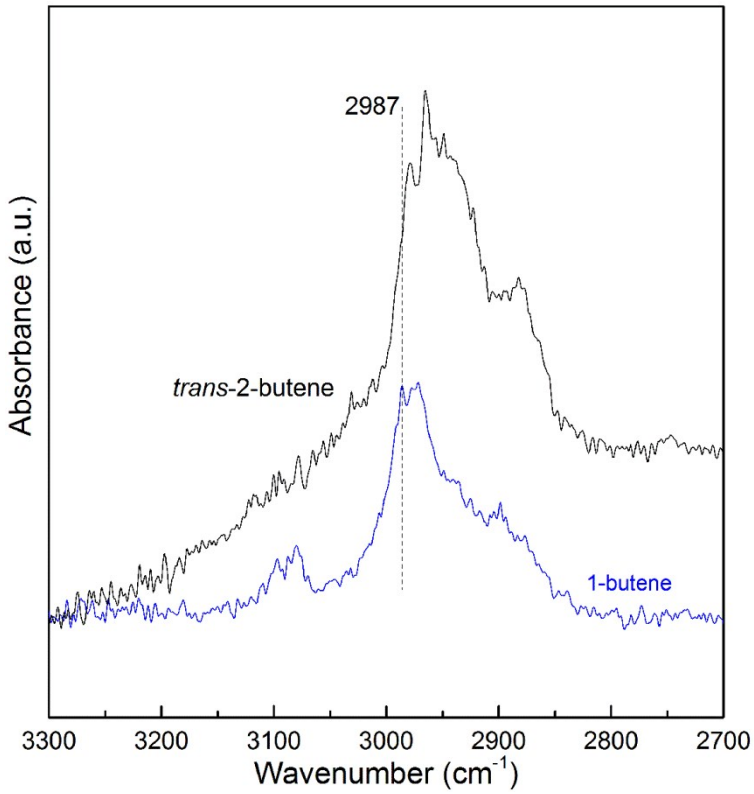

Figure S3.DRIFT spectra for uptake of 1-butene and *trans*-2-butene on the Pt/SiO_2 catalyst at room temperature.

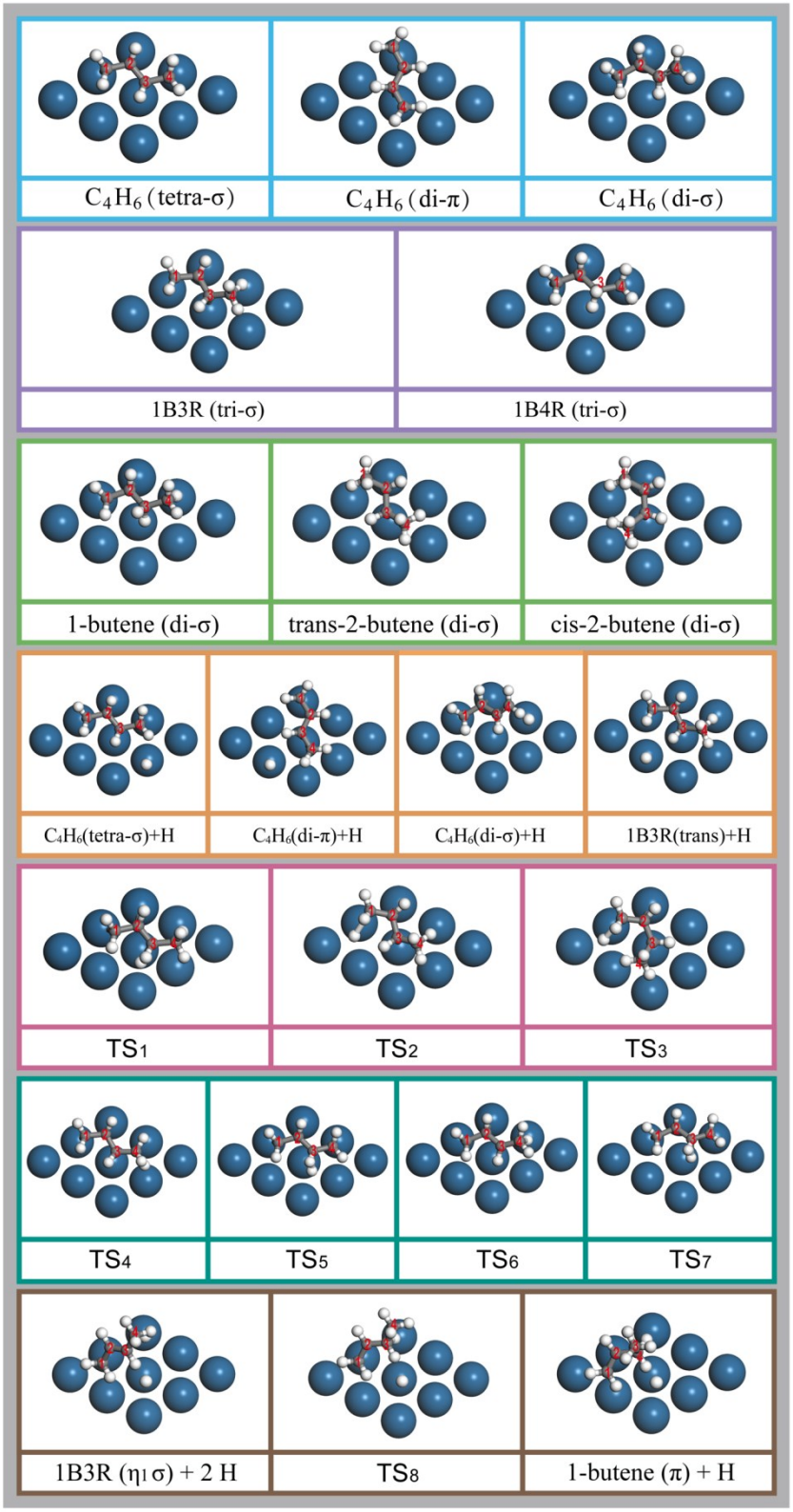

Figure S4. Top view of the carbonaceous species with labeling the number of the carbon atoms.

Table S1. Geometrical parameters (expressed in Å) of C_4H_x and transition states for partial hydrogenation of 1,3-butadiene on the Pt(111) surface. Pt-C represents the distance between the carbon and its coordinating Pt.

Species	Pt-C_1	Pt-C_2	Pt-C_3	Pt-C_4	C_1-C_2	C_2-C_3	C_3-C_4	C-H forming
C_4H_6(tetra-σ)	2.123	2.204	2.201	2.126	1.475	1.477	1.475	
C_4H_6(di-π)	2.204	2.228	2.249	2.185	1.413	1.458	1.414	
C_4H_6(di-σ)	2.129	2.179	-	-	1.485	1.463	1.348	
C_4H_7(1B3R)(tri-σ)	2.120	2.247	2.150	-	1.472	1.478	1.507	
C_4H_7(1B4R)(tri-σ)	2.143	2.145	-	2.108	1.486	1.520	1.516	
1-butene(di-σ)	2.122	2.172	-	-	1.486	1.517	1.517	
tran-2-butene(di-σ)	-	2.144	2.147	-	1.515	1.500	1.515	
cis-2-butene(di-σ)	-	2.160	2.161	-	1.510	1.499	1.512	-
C_4H_6 (tetra-σ) + H(top)	2.125	2.203	2.218	2.121	1.473	1.474	1.475	
C_4H_6 (di-π)+ H(top)	2.204	2.229	2.244	2.188	1.414	1.458	1.414	
C_4H_6 (di-σ)+ H(top)	2.124	2.189	-	-	1.485	1.464	1.345	
C_4H_7 (1B3R) (tri-σ) + H(top)	2.123	2.244	2.149	-	1.473	1.478	1.507	
cis-C_4H_7 (1B3R) (tri-σ) + H(top)	2.128	2.218	2.148	-	1.472	1.487	1.515	
TS_1	2.113	2.240	-	-	1.481	1.431	1.489	1.929
TS_2	-	2.222	2.143	-	1.470	1.488	1.503	2.064
TS_3	-	2.266	2.144	-	1.450	1.488	1.511	2.069
TS_4	2.123	2.215	2.213	-	1.476	1.484	1.457	1.494
TS_5	2.132	2.152	-	2.130	1.484	1.474	1.458	1.786
TS_6	2.122	2.251	-	-	1.474	1.439	1.382	1.643
TS_7	2.137	2.160	-	-	1.489	1.480	1.381	1.776
C_4H_7 (1B3R) (η_1 σ) + 2H(top)	2.141	-	-	-	1.457	1.353	1.486	-
TS_8	2.178	-	-	-	1.431	1.414	1.511	1.469
1-butene (π)+ H(top)	2.211	2.269	-	-	1.407	1.503	1.534	-
TS_9	2.178	2.292	2.235	-	1.428	1.460	1.438	1.699
TS_{10}	2.236	2.213	-	2.146	1.392	1.473	1.441	1.652
C_4H_7(1B3R)(π-σ)	2.179	2.348	2.145	-	1.415	1.466	1.514	-
C_4H_7(1B4R)(π-σ)	2.235	2.233	-	2.096	1.404	1.502	1.515	-

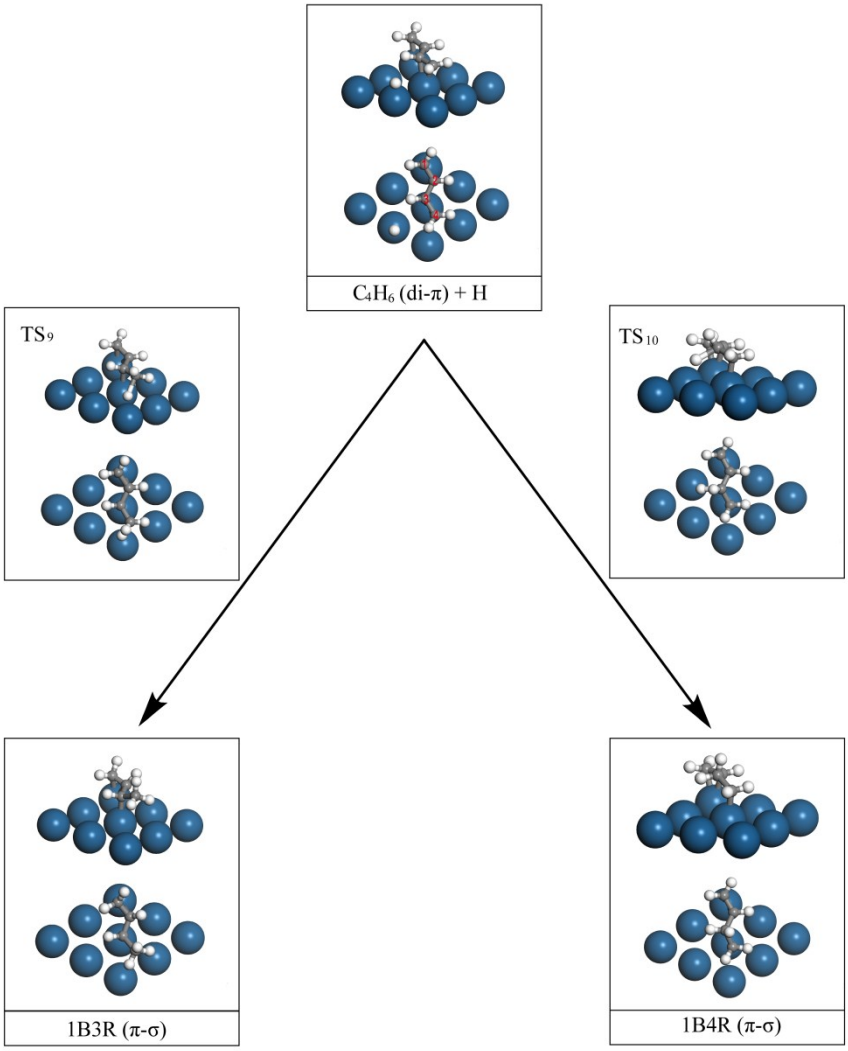

Figure S5. Optimized structures (side and top views) of reactant, transition states, and the products for hydrogenation of C_4H_6 with the di-π configuration to C_4H_7 on the Pt(111) surface.