Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2020

Supporting Information

Insight into the performance and action mechanism of metal-free acetylene hydrochlorination catalyzed by imidazole

Chaoyue Zhao, Xianliang Qiao, Zenghuimin Yi, Qingxin Guan, * Wei Li *

College of Chemistry, State Key Laboratory of Elemento-Organic Chemistry, Nankai University, Tianjin 300071, China.

Contents

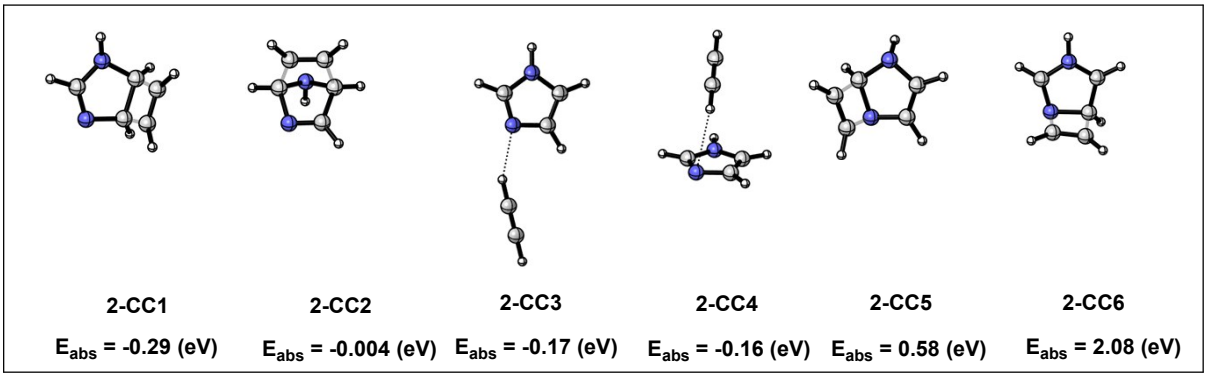

Fig. S1 Optimized geometries of **2-CCn** (n=1-6).

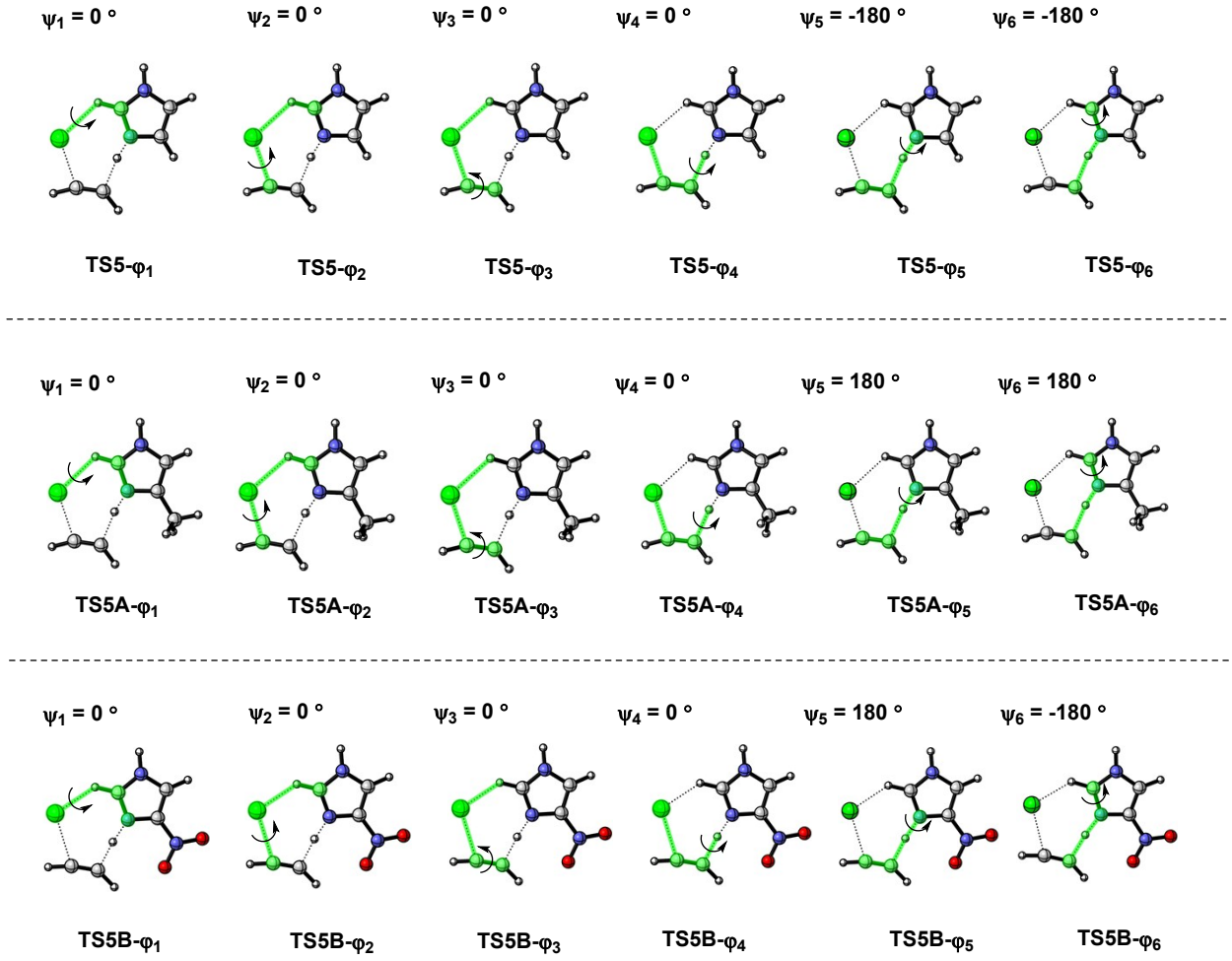

Fig. S2 Gauche conformation (ψ) of transition states **TS5**, **TS5A** and **TS5B**.

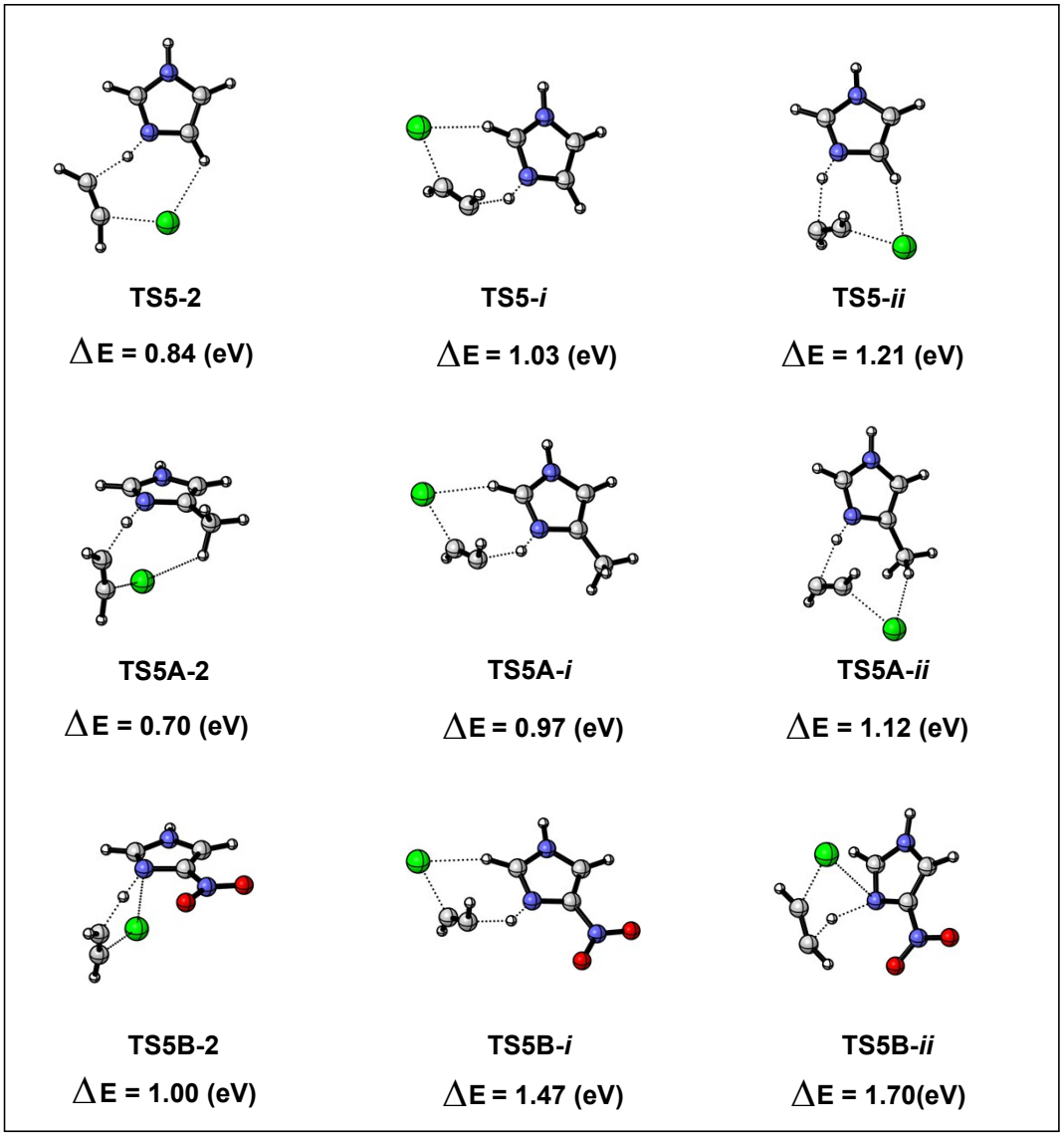

Fig. S3 Optimized geometries of another possible transition states.

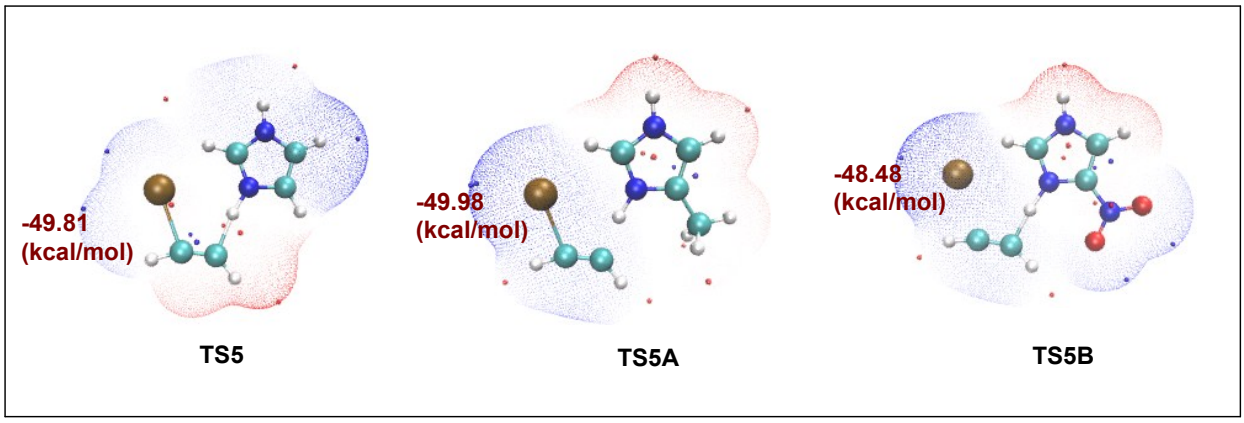

Fig. S4 ESP-mapped molecular vdW surface of **TS5**, **TS5A** and **TS5B**.

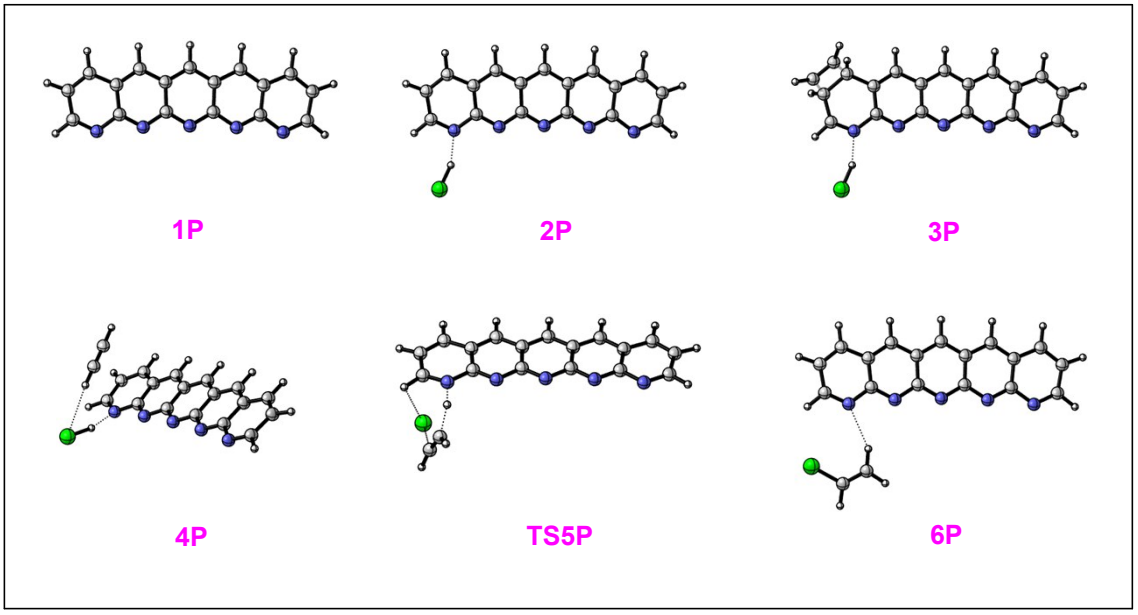

Fig. S5 Optimized geometries of intermediates and transition states for acetylene hydrochlorination with **1P**.

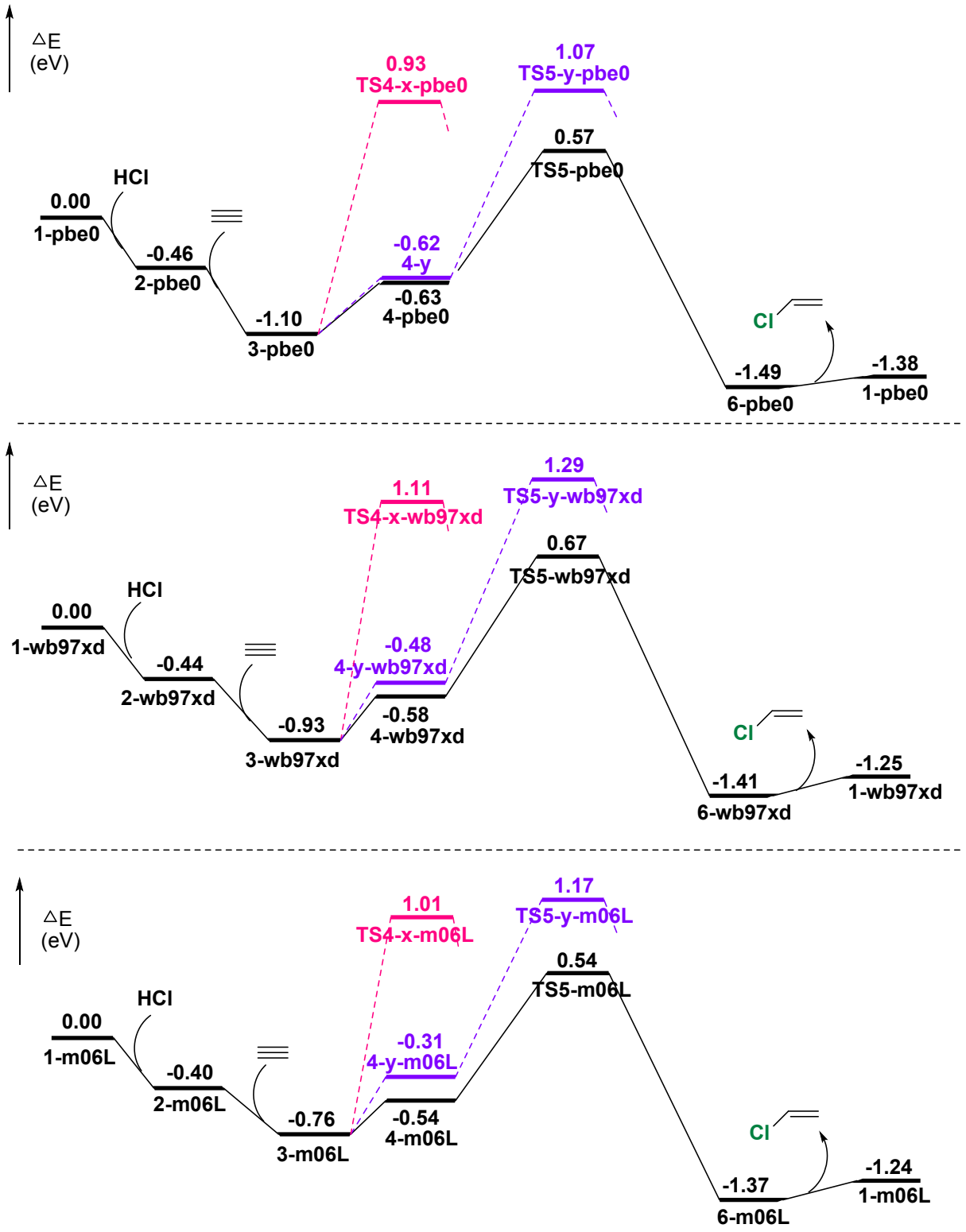

Fig. S6 Energy profiles of different DFT results for the acetylene hydrochlorination between C_2H_2 and HCl with catalyst **1**. Values are given in eV.

To investigate whether this discrepancy is due to the employed functional, we recalculated the energy profile using the PBE0, ωB97XD and M06-L methods by performing single-point calculations on the PBE0, ωB97XD and M06-L optimized geometries, respectively. The computation results indicate that when different functional are taken into consideration, the fluctuation tendency of energy in this pathway is almost the same among these functionals. We can draw the conclusion that the M06-2X functional could provide great accuracy in energetic information for this work and the use of other functionals will not affect the over conclusions.