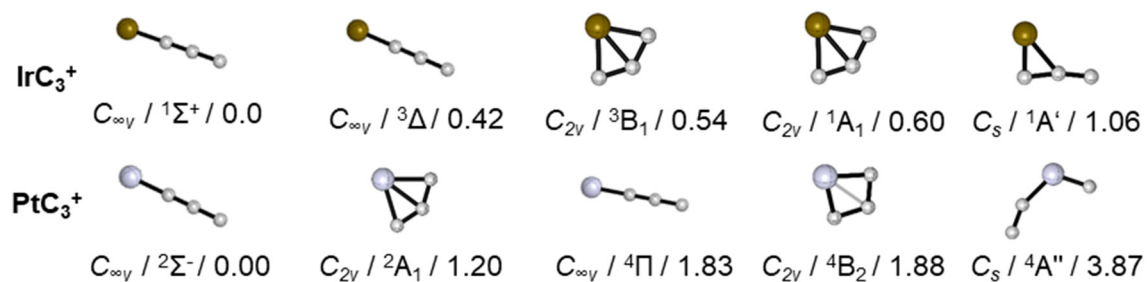


# **The Reactive Sites of Methane Activation: A Comparison of $\text{IrC}_3^+$ with $\text{PtC}_3^+$**

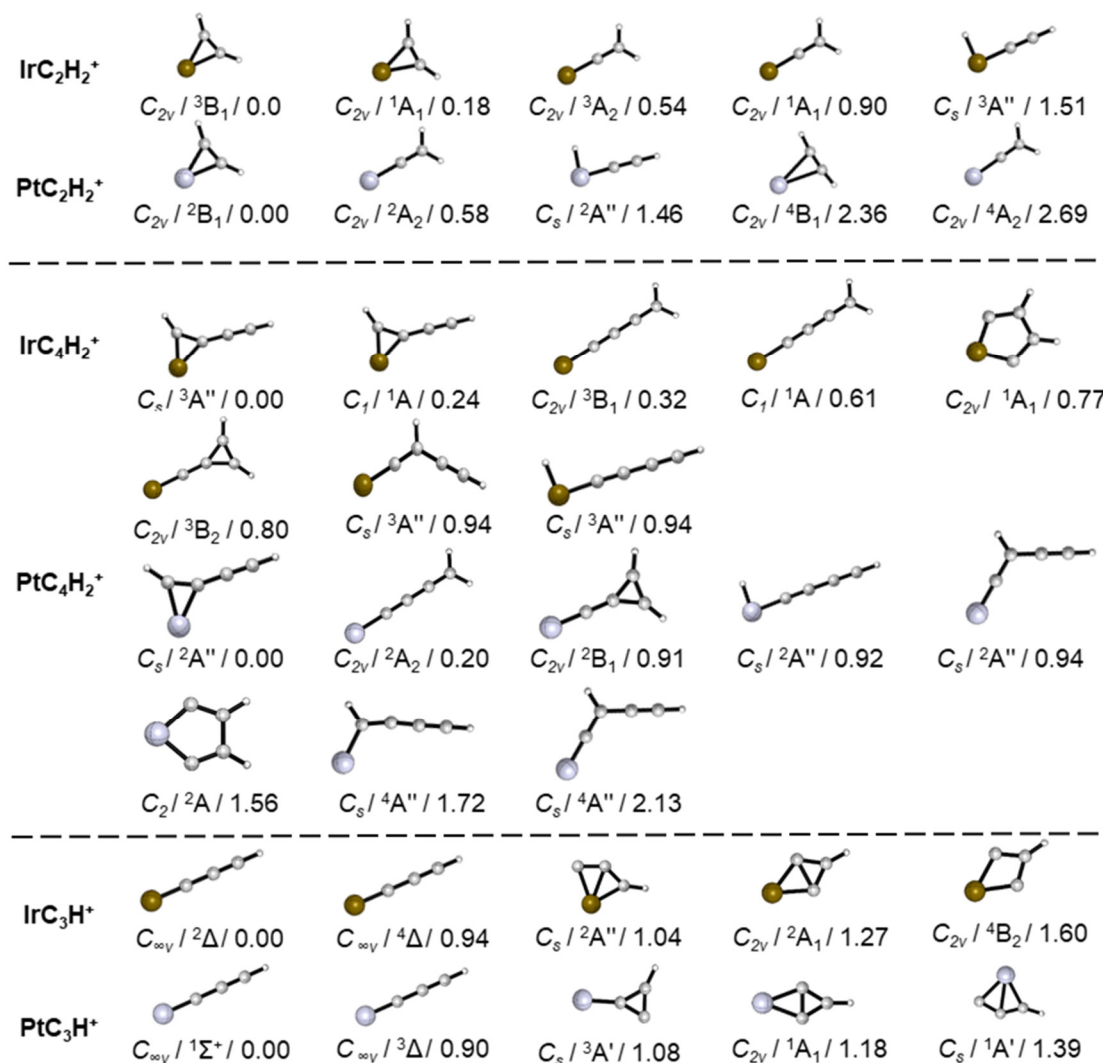
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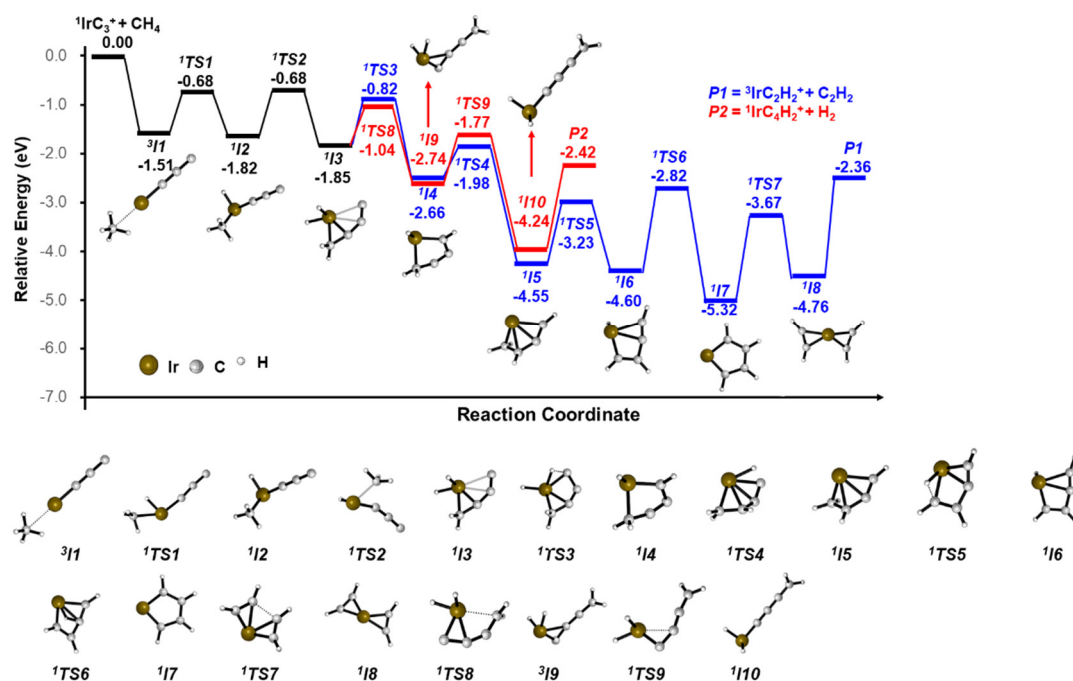
Authors to whom correspondence should be addressed: [wuxiaonan@fudan.edu.cn](mailto:wuxiaonan@fudan.edu.cn)



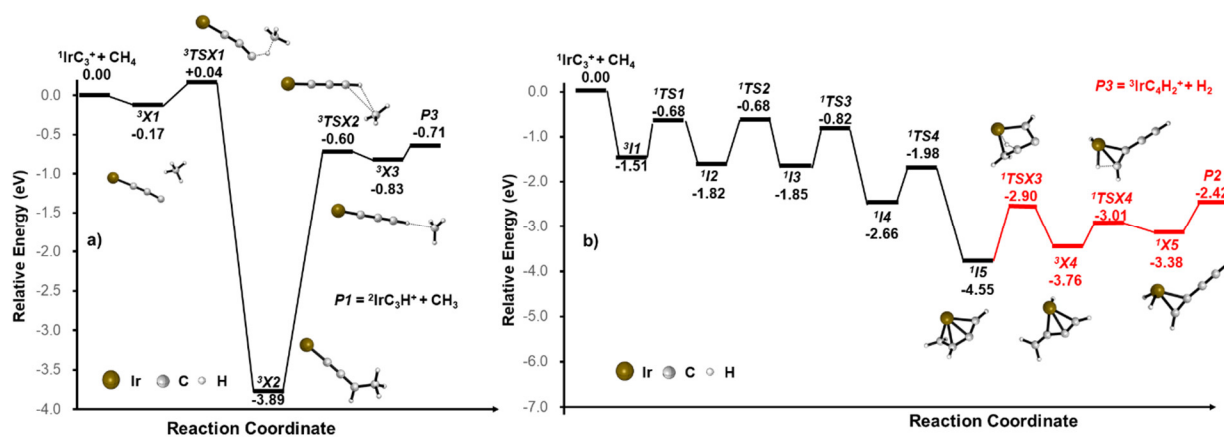
**Figure S1.** The optimized geometries of the [IrC<sub>3</sub>]<sup>+</sup> and [PtC<sub>3</sub>]<sup>+</sup> isomers at the BMK/def2-TZVP level. The relative energies relative to the global minimum structure (in eV), symmetry and electronic states are shown.



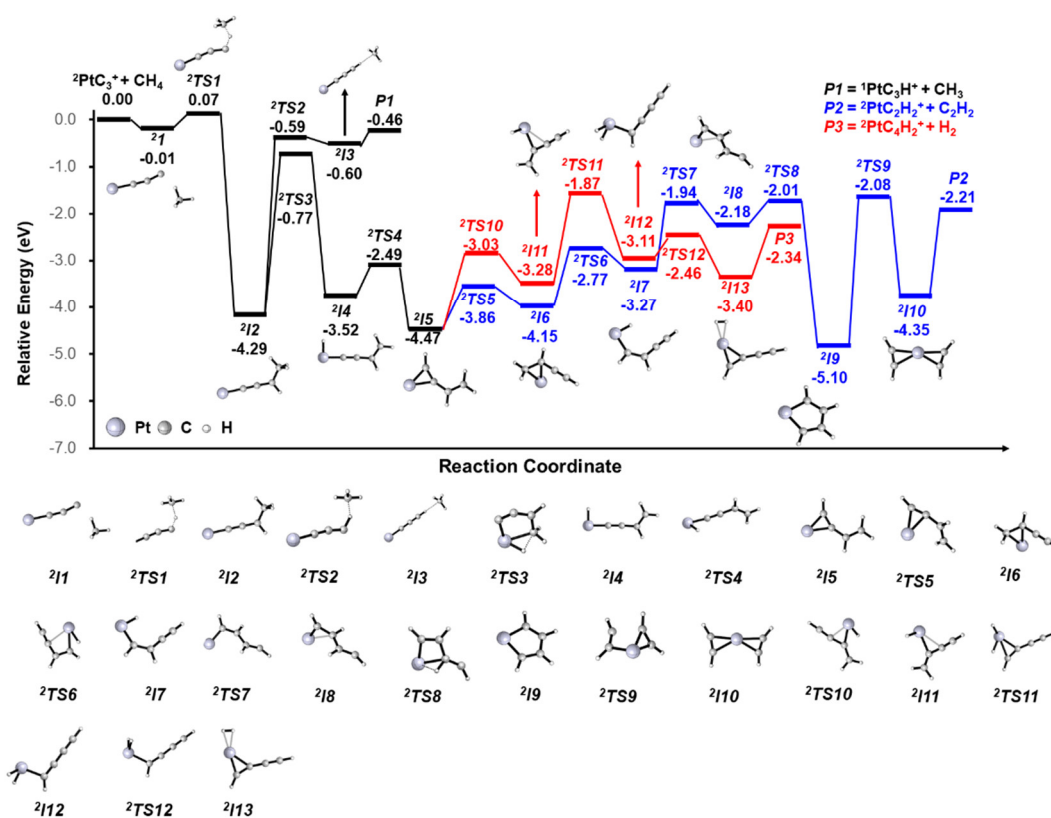
**Figure S2.** The optimized geometries of the [IrC<sub>2</sub>H<sub>2</sub>]<sup>+</sup>/[PtC<sub>2</sub>H<sub>2</sub>]<sup>+</sup> (top), [IrC<sub>4</sub>H<sub>2</sub>]<sup>+</sup>/[PtC<sub>4</sub>H<sub>2</sub>]<sup>+</sup> (middle) and [IrC<sub>3</sub>H]<sup>+</sup>/[PtC<sub>3</sub>H]<sup>+</sup> (bottom) isomers at the BMK/def2-TZVP level. The relative energies relative to the global minimum structure (in eV), symmetry and electronic states are shown.



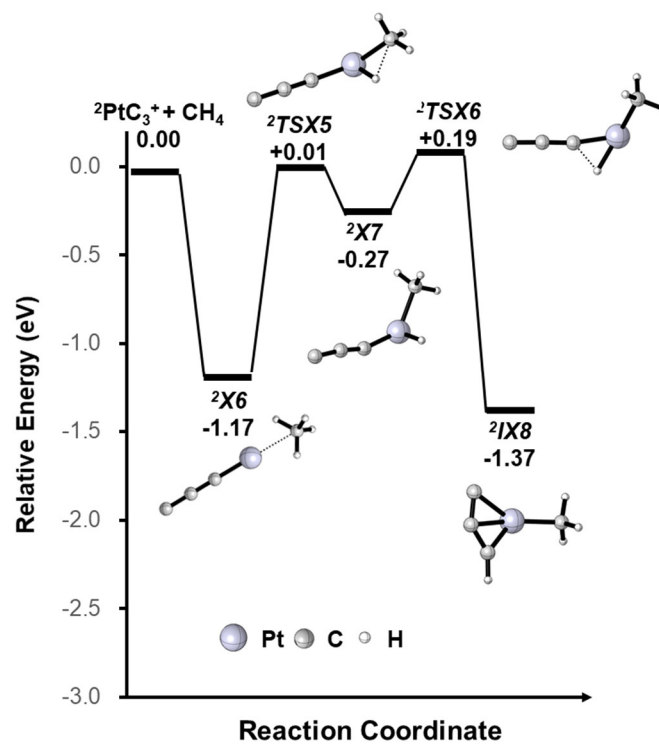
**Figure S3.** The detailed potential energy profiles of the reaction of  $\text{IrC}_3^+$  and  $\text{CH}_4$  in Figure 2. The energies are given in eV.



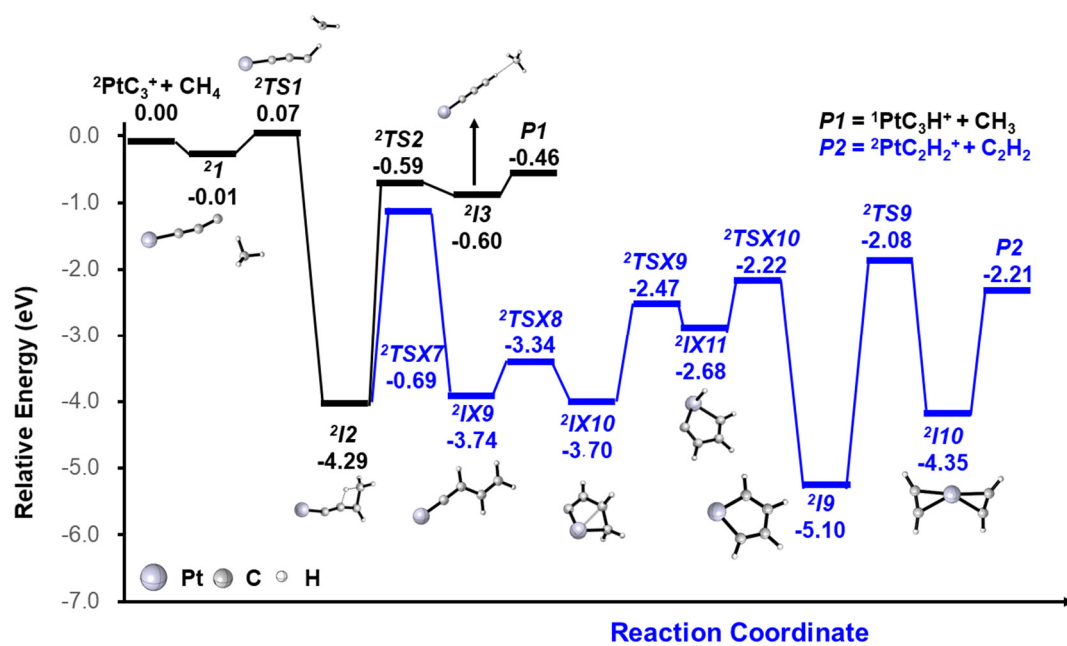
**Figure S4.** The other possible potential energy profiles of the reaction of  $\text{IrC}_3^+$  and  $\text{CH}_4$ . The energies are given in eV.



**Figure S5.** The detailed potential energy profiles of the reaction of  $\text{PtC}_3^+$  and  $\text{CH}_4$  in Figure 3. The energies are given in eV.



**Figure S6.** The other possible potential energy profiles of the reaction of  $\text{PtC}_3^+$  and  $\text{CH}_4$ . The energies are given in eV.



**Figure S7.** The other possible potential energy profiles of the reaction of  $\text{PtC}_3^+$  and  $\text{CH}_4$ . The energies are given in eV.