A High-Level Theoretical Study of Hydrogen Abstractions involving the Ethynyl Radical

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The ethynyl radical, C_2H, is one of the most abundant polyatomic radicals in the interstellar medium and plays an important role in fuel-rich hydrocarbon combustion processes. Hydrogen-atom abstraction is among the most prevalent reactions for the ethynyl radical and is often the main reaction pathway. In this study, the $C_2H + HX \rightarrow C_2H_2 + X$, where HX = H_2CO, HNCO, HOCN, HONO, and CH_3OH, reactions have been investigated at a rigorously high level of theory at CCSD(T)-F12a/cc-pVTZ-F12. These molecules were chosen because they can be found in either interstellar or combustion environments. Various additive energy corrections have been included to converge the relative enthalpies of the stationary points to subchemical accuracy ($0.5 \leq$ kcal mol^{-1}). Accuracte kinetics were acquired over a wide range of temperatures (20 - 5000 K), which may be useful for future studies of these reactions.