Study of Isomerization of Acetylene after Core Ionization

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ABSTRACT

Recent experiment shows sub -100 fs isomerization of acetylene after carbon K-shell ionization. Past theoretical studies on $HCCH^{2+}$ show a large potential barrier for isomerization to H_2CC^{2+} indicating picosecond isomerization timescale. Here, Energetics of $HCCH^{+}$ and $HCCH^{2+}$ using DIP-STEOM-CCSD have been interpreted to show isomerization occurs from the lower lying states of $HCCH^{2+}$. Two body fragmentation processes have been studied using CCSDT for ground triplet and lowest singlet electronic states of $HCCH^{2+}$ to obtain the potential energy barrier for its isomerization.