ENERGY THRESHOLDS AND DYNAMICAL REGIMES IN ELECTRON-IMPACT IONIZED MOLECULAR CATIONS

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ABSTRACT

Fragmentation of molecular cations formed by electron-impact ionization is governed primarily by the redistribution of internal energy deposited during the collision event. A detailed understanding of how this energy drives the transition from bound vibrational motion to irreversible bond cleavage is essential for interpreting energy-resolved fragmentation measurements. In this work, we analyze the dependence of dissociation behavior on internal energy using a controlled diatomic benchmark system. Electron-impact ionization is represented through controlled initialization of internal energy on the molecular cation potential energy surface, followed by classical propagation of the nuclear motion. The study focuses on identifying effective dissociation thresholds, characterizing near-threshold dynamical regimes, and examining the scaling of fragmentation times with increasing internal energy. Ensemble simulations are employed to determine dissociation probability as a function of deposited energy and to analyze the redistribution between kinetic and potential energy during bond stretching. The results provide a physically transparent description of energy-driven molecular breakup and offer a reference for interpreting energy-dependent fragmentation phenomena investigated within the ATMOLCOL project.

Keywords: energy redistribution, dissociation threshold, electron-impact ionization, molecular dynamics, fragmentation dynamics.

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