

화학과 세미나

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Watching Ultrafast Chemistry After Ionization

Ionization initiates chemistry on an electronic timescale, triggering charge redistribution, nuclear motion, bond rearrangement, and fragmentation. Yet a fundamental question remains: what determines which chemical pathway a molecule follows after ionization? We address this question using strong-field ionization, energy- and time-resolved mass spectrometry, femtosecond disruptive probing, and ultrafast X-ray scattering [1–4]. By following many mass-resolved products simultaneously, we determine when competing fragmentation and rearrangement pathways emerge and identify coherent nuclear motion associated with transient structures. Examples include the McLafferty rearrangement [5], retro-Diels-Alder reactions [6], and H_3^+ formation following molecular double ionization, where hydrogen roaming and large-amplitude nuclear motion produce reaction pathways that are difficult to anticipate from equilibrium molecular structure [7–9]. More recent studies of hydrogen-bonded molecular clusters show that the local molecular environment can redirect the chemistry following ionization, favoring proton transfer, molecular reorganization, or covalent bond cleavage. These results point toward a broader principle in which hydrogen-bond topology helps determine the outcome of ionization-induced chemistry. I will also discuss our recent studies of phenyl triflate using disruptive probing [10] and ultrafast X-ray scattering [11], which provide complementary temporal and structural views of fragmentation and reveal the coexistence of rapid nonstatistical bond cleavage with slower statistical dissociation. Together with electronic-structure calculations, molecular dynamics, and quantum wavepacket models, these measurements are moving us from identifying products and reaction times toward molecular movies that reveal how chemistry unfolds from the initial act of ionization through bond breaking, bond formation, and product emergence.

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