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Surprising reaction dynamics of radical cations following electron ionization

Thursday 7 September 2023 14:30 (40 minutes)

Femtosecond time-resolved measurements have provided the timescales of bond breaking and bond forming processes for a wide range of chemical reactions. Some chemical reactions such as those that involve a collision with an atom or an electron, however, are very difficult to study by time resolved methods. This talk will focus on the reaction dynamics of radical cations far from equilibrium following electron scattering, a situation that occurs in electron-ionization mass spectrometry. These types of measurements are important because they can help refine methods for predicting molecular fragmentation patterns, which are essential for molecular identification. Lack of experimental dynamic information has prevented scientists from determining how fast the energy distributes and how it affects bond breaking and bond forming processes. Therefore, currently predicting the fragmentation pattern of a given molecule remains a challenge. We have developed a method for tracking multiple fragmentation pathways simultaneously following strong-field ionization. This talk will include examples of unexpected pathways that include roaming moieties, concerted dynamics, and intramolecular rearrangements, many occurring prior to intramolecular energy redistribution.

References:

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