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Theoretical Studies of Electron-Molecule Collision Processes¹

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Electron collisions with molecules and molecular ions that lead to excitation and dissociation play a key role in a number of environments, since they produce the radicals and molecular fragments that initiate and drive the relevant chemistries. Examples range from the technologically important plasmas used in plasma enhanced chemical vapor deposition, to planetary atmospheres and interstellar clouds, to DNA damage driven by secondary electron cascades produced by radiation. In general, due to the large mass difference between the electron and target, the cross section is dominated by resonant processes, where the electron can temporarily attach to the molecule and change the forces felt between its atoms for a period of time comparable to a vibrational period. This can lead to resonant vibrational excitation and dissociative attachment, for neutral targets, or dissociative recombination in the case of ions. In this talk, I will outline the basic theory that underlies these processes, and our approach to study them. I will illustrate these methods with application to dissociative attachment in ClCN and BrCN, vibrational excitation and dissociative attachment in NO and CF, and dissociative recombination in the HCN⁺ and HNC⁺ systems. This work was supported by DOE-OBES Division of Chemical Sciences and NSF PHY-02-44911.

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