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Calculations of fast ion collisions with multi-center molecular targets[1]

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The theoretical treatment of ion-molecule collisions is challenging for several reasons: the systems have many degrees of freedom, a rather complex geometry, and the electron dynamics might be nonperturbative and involve electron-electron interaction effects. However, the interest in accurate calculations has been growing recently. An important reason for this development is the relevance of ion-molecule collisions for a number of fields, such as atmospheric science, and the understanding of radiation damage of biological tissue. We have developed a new approach to meet these challenges [1]. It disregards rovibrational motion, but it does address the multi-center geometry of the system and the generally nonperturbative nature of the electron dynamics. The key ingredients are an expansion of the initially populated molecular orbitals in terms of a single-center basis and a spectral representation of the molecular Hamiltonian. This facilitates a separation of molecular geometry and collision dynamics and makes it possible to use well-established ion-atom methods with relatively minor modifications. We have extended our basis generator method to deal with the collision dynamics and report on results for ionization and fragmentation of water molecules by proton and He^+ ion impact over wide ranges of collision energies. For the case of He^+ impact this will include a discussion of effects due to the presence of the projectile electron.

[1] H. J. Lüdde *et al.*, Phys. Rev. A **80**, 060702(R) (2009)

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