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Theoretical studies on dissociative recombination of molecular ions

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In dissociative recombination a molecular ion captures an electron forming a neutral state that dissociates into fragment. Due to the Coulomb attraction between the reactants, the cross section is typically large at low collision energies and the process is important for different types of plasmas. Here, it will be described how the reaction can be studied theoretically. The goal is to compute reaction cross sections and to determine what fragments are formed. The calculations are done in close collaboration with experiments. In the process, the electron may be captured directly into an electronic resonant state that then is dissociated into fragments. An alternative mechanism is driven by an electron capture into a ro-vibrationally excited Rydberg state that then is predissociated. The two mechanisms are competing and should be considered coherently. The study of dissociative recombination requires both the accurate treatment of the electron scattering processes, but must also include an accurate representation of the potential energy curves, both for electronically bound states and the resonant states. In addition, the couplings between these states, both the coupling between the resonant states and the scattering continuum (the autoionization width) and the non-adiabatic coupling between all states are needed to complete describe the cross section including the branching ratios into final states. These are obtained using structure calculations as well as scattering calculations, using the complex Kohn variational method. The electronic states are diabatized before the nuclear dynamics is studied quantum mechanically. The theoretical method will be illustrated with examples on dissociative recombination of small molecular ions such as HF^+, BeH^+, H_2O^+ and N_2H^+.