Dissociative Recombination (DR) of H_2O^+

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Abstract

The direct Dissociative Recombination (DR) process of H_2O^+ is studied. DR is a process whereby a low energy electron collides with a molecular ion to form a highly excited neutral state. Since it is an unstable state, it can then dissociate to neutral fragments. Autoionization is also possible while the potential energy surface of the resonant excited state has not crossed the ion ground state surface. However, once the surface have crossed, autoionization is no longer possible, and the molecule continues to dissociate. This is the direct DR mechanism. In the study of the direct DR process, potential energy surfaces and autoionization widths of resonant states are computed using structure and electronic scattering calculations. A quasidibatization is performed by removing electronic states that have a Rydberg configuration. In a 1D model only the breakup of one OH bond is included and the nuclear dynamics is studied quantum mechanically using the Crank-Nicholson method.