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Simplified approach to dissociation of polyatomic molecules by electron impact[1]

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Dissociative Recombination (DR) and Dissociative electron attachment (DEA) of molecules are important processes in various plasma environments. Despite several approaches developed for diatomic molecules, the theoretical description of electron-molecule scattering for polyatomic molecules is an extremely complex problem. For both DR and DEA we have used simplified models that highlight the essence of what drives the mechanisms. The DR process can be divided into direct and indirect DR. For indirect DR, which is mostly relevant at energies up to mili electron volts, the simplified approach models the vibrational states using normal modes and the non-adiabatic couplings between them are obtained simply by computing the scattering matrix elements in this vibrational space. Electronic structure calculations, as well as scattering calculations, were carried out entirely from ab initio principles using the MESA program combined with the complex Kohn variational method. At higher energies, up to few electron volts, direct DR becomes more prominent and its treatment starts with carrying out electron scattering calculations as a function of the three internal degrees of freedom to obtain the resonance energy surfaces and autoionizing resonance widths. Then, this data is used as input to form the Hamiltonian relevant to the nuclear dynamics. The multidimensional wave equation is solved using the Multi-Configuration Time-Dependent Hartree (MCTDH) technique. The simplified model has been applied to different systems along the years and the results compare surprisingly well with available experimental data. In this talk I will focus on the DR results obtained for H_2O^+, N_2H^+ and HCl^+. The DEA approach follows the treatment proposed by Bardsley (1968) developed for diatomic molecules. The formalism of resonant scattering has been adapted to polyatomic molecules and applied to the H_2CN molecule, which has six normal modes and is believed to be responsible for the formation of the CN^- and H^- ions and the HCN molecule in the interstellar space. The relevant electronic states are calculated from ab initio principles by combining electron scattering calculations to obtain resonance positions and autoionization widths with multi-reference configuration interaction calculations of the Rydberg states and the ion.

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