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VIBRATIONALLY RESOLVED COLLISIONS OF HYDROGEN IONS AND MOLECULES

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Abstract. Because of its fundamental role in hydrogen plasmas such as those in certain astrophysical (Walker et al, 2018) or fusion reactor environments (Janev at al, 2003), and as a prototype for the study of similar processes in other plasmas, slow collisions (0.1-100 eV) of hydrogen atoms and ions with vibrationally excited hydrogen molecules and molecular ions are studied using fully quantum-mechanical (below 10 eV) and semiclassical (E > 15 eV) approaches, the latter within impact parameter, straight-line approximation. Considered transitions include charge transfer, excitation (Krstić 2002), dissociation (Krstić et al, 2003), three body diatomic association (often referred by the general term three-body recombination) (Krstić et al, 2003), as well as energy and angular spectra of dissociation fragments. Mutual relations of various elastic and inelastic processes, the relevant physical mechanisms governing vibrational dynamics in inelastic channels and comparison of the fully quantal and semi-classical results are also reported. The cross section calculations are performed by solving the Schrödinger equation for the nuclear and electronic motions on the two lowest diabatic electronic surfaces of H_3^+, and by using an expansion of nuclear wave function in a vibrational basis containing all discrete H_2 and H_2^+ states and a large number of pseudo-states from each of the corresponding discretized continua. The rotational dynamics of H_2 and H_2^+ is treated with the infinite order sudden approximation prescription.

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