THE H⁺D² REACTION: A COMPARISON BETWEEN THEORY AND EXPERIMENT

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Recent experimental work [1-3] has allowed to investigate the dynamics of the H(n)+D₂→HD+D(n) reaction where H(n) is a hydrogen atom in a highly excited Rydberg state (n~45-50). The strong similitudes presented with the ion-diatom H⁺D₂→HD+D⁺ reaction suggests that the electron of the Rydberg atom behaves as a spectator. Analogously to a previous study on the H⁺H₂(v=0,j=0) process [4], the dynamics of the H⁺D₂(v=0,j=0) reaction on the potential energy surface by Aguado et al. [5] has been theoretically analysed by means of a time-independent exact quantum mechanical (EQM) method [6], a quantum wave packet (QWP) approach [7], a statistical quantum model (SQM) [8] and a quasi-classical trajectory (QCT) method [9]. A detailed comparison with previous experimental data at the E_c = 0.524 eV collision energy has been completed with theoretical predictions at a lower energy, E_c = 0.1 eV, in an attempt to observe possible changes on the reaction mechanism.

References