Theoretical study of the D− + H2 → H− + HD reaction at low energies

CHI HONG YUEN, University of Central Florida, MEHDI AYOUZ, LGPM, CentraleSupelec, Universit Paris-Saclay, VIATCHESLAV KOKOOULINE, University of Central Florida — The rearrangement reaction D− + H2 → H− + HD has been studied in a recent experimental work at low temperatures (10, 19, and 23K) [1]. An upper limit of about 10−18 cm3/s for the rate coefficient is obtained. A fully-quantum reactive scattering calculation of the rate coefficient is performed using the hyperspherical coordinates and the potential energy surface in Ref. [2]. Eigenchannel R-matrix approach with modified slow variable discretization [3] is used to represent continuum wave functions of the system to obtain the scattering matrix describing the scattering from the initial rovibrational channel of the H2+D− into possible channels of H− + HD. At low collision energies between H2 in the ground state and D−, only three rotational channels of HD(v, j) + H− are open for the reaction with v = 0 and j = 0, 1, 2. Formulas for the cross section and rate coefficient for reactive scattering in hyperspherical coordinates are derived. Preliminary results for the rate coefficient of the D− + H2 → H− + HD reaction is obtained. [1]Endres et al, in press, PRA (2017) [2] Ayouz et al, JCP 132, 19 (2010) [3] Yuen and Kokoouline, EPJD, 71, 19 (2017)

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Chi Hong Yuen
University of Central Florida

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