Distinct influence of vibration on the two channels of the D+MuH(ν=1) reaction

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Muonic chemistry has provided most useful information, not always free from controversy, for the investigation of tunneling, zero point energy effects, and vibrational adiabaticity in reaction dynamics [1, 2]. Recently, the possibility of inducing a fundamental change in the nature of chemical bonding (vibrational bonding) upon muonic substitution [3] has been also stressed.

The present study extends a previous work by the authors on the dynamics of the asymmetric D+MuH (ν=0) isotopic variant [4] of H+H₂. Quantum mechanical calculations of integral (ICS) and differential reaction cross sections (DCS), as well as cumulative reaction probabilities (CRPs) and rate constants k(T) have been performed for the two channels of the D+MuH(ν=1) reaction leading respectively to DMu and DH. Vibrational excitation is found to be globally more efficient than translational energy for promoting the reaction. This is particularly so for the DMu channel whose reactivity increases rapidly, showing a sharp resonance peak, as soon as the MuH (ν=1) channel is energetically open. No peak was observed in the ICS for ν=0. In comparison with the DH channel, the DMu exit path has a more “quantal” nature, with marked structures in its ICS and DCS. The dynamical implications of these results are analyzed in terms of the vibrationally adiabatic potentials.

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