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Dynamics of the asymmetric D + MuH reaction.

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The dynamics of the asymmetric D + MuH (Mu = Muonium) reaction leading to Mu exchange, DMu + H, and H abstraction, DH + Mu, channels has been investigated using time-independent quantum mechanical (QM) calculations. Quasiclassical trajectory (QCT) calculations were also performed in order to check the reliability of the method for this reaction and to discern genuine quantum effects [1]. Overall, the Mu exchange channel exhibits more structured reaction probabilities and cross sections, with much larger rate coefficients, k(T), than its H abstraction counterpart. Over the 100–1000 K temperature interval considered, the QM k(T) for Mu exchange vary between $5 \times 10^{-15}$ and $2 \times 10^{-11}$ cm$^3$ s$^{-1}$ and those for the generation of DH + Mu between $2 \times 10^{18}$ and $3.5 \times 10^{12}$ cm$^3$ s$^{-1}$. In common with the rest of the isotopologues of the H + H$_2$ system, the height of the respective barriers in the collinear (symmetric stretch) vibrationally adiabatic potential energy curves matches the classical total energy threshold very accurately. The preponderance of the DMu + H channel is determined by its lower and narrower vibrationally adiabatic collinear barrier as compared with that for DH + Mu formation. Comparison of QM and QCT results shows that tunneling accounts for the reactivity at energies below the height of these barriers and that its effect on k(T) becomes appreciable below 300 K. As expected, with growing temperature the contribution of tunneling to the global reactivity decreases markedly, but the rate coefficients are still much higher for the Mu exchange channel due to the effect of MuH rotational excitation that boosts the formation of DMu while diminishing the H abstraction channel that leads to the production DH. The analysis of the thermal cumulative reaction probabilities of the two channels indicates that at the lowest energies/temperatures the reaction into the DH + Mu channel takes place via ‘leakage’ from collisions proceeding along the DMu + H reaction path.