Quantum and quasiclassical dynamical simulations for the Ar_2H^+ on a new global analytical potential energy surface

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A new analytical potential energy surface (PES) has been constructed for the Ar_2H^+ system from a set of *ab initio* energies computed using the coupled-cluster singles, doubles and perturbative triples (CCSD(T)) method and aug-cc-pVQZ basis set. The long-range interaction is added to the diatomic potentials using a standard long range expansion form to better describe the asymptotic regions. A few low lying vibrational states for the most stable structure which corresponds to a centrosymmetric linear Ar-H-Ar geometry have been calculated for Ar_2H^+ and $^{36}Ar_2H^+$. The states are then assigned to proper quantum numbers. Reactive scattering studies have been performed for the $Ar + Ar'H^+ \rightarrow Ar' + ArH^+$ reaction and for its isotopic variant $^{36}Ar + {}^{36}Ar'H^+ \rightarrow {}^{36}Ar' + {}^{36}ArH^+$ on the newly generated PES. Reaction probability, cross sections, and rate constants are calculated for the Ar + Ar′H+(v = 0, *j* = 0) collisions within 0.001-0.6 eV of relative translational energy using exact quantum dynamical simulations as well as quasiclassical trajectory (QCT) calculations. The effect of vibrational excitation of the reactants is also explored for the reaction. State averaged rate constants are calculated for the proton exchange reaction at different temperatures using the QCT method. The mechanistic aspects for the reaction are understood by analyzing the quasiclassical trajectories.

References:

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