Title:	HeH+ Collisions with H2: Rotationally Inelastic Cross Sections and Rate Coefficients from Quantum Dynamics at Interstellar Temperatures
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Abstract:	We report for the first time an accurate ab initio potential energy surface for the HeH+–H2 system in four dimensions (4D) treating both diatomic species as rigid rotors. The computed ab initio potential energy point values are fitted using an artificial neural network method and used in quantum close coupling calculations for different initial states of both rotors, in their ground electronic states, over a range of collision energies. The state-to-state cross section results are used to compute the rate coefficients over a range of temperatures relevant to interstellar conditions. By comparing the four dimensional quantum results with those obtained by a reduced-dimensions approach that treats the H2 molecule as an averaged, nonrotating target, it is shown that the reduced dimensionality results are in good accord with the four dimensional results as long as the HeH+ molecule is not initially rotationally excited. By further comparing the present rate coefficients with those for HeH+–H and for HeH+–He, we demonstrate that H2 molecules are the most effective collision partners in inducing rotational excitation in HeH+ cation at interstellar temperatures. The rotationally inelastic rates involving o-H2 and p-H2 excitations are also obtained and they turn out to be, as in previous systems, orders of magnitude smaller than those involving the cation. The results for the H2 molecular partner clearly indicate its large energy-transfer efficiency to the HeH+ system, thereby confirming its expected importance within the kinetics networks involving HeH+ in interstellar environments.
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