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Title:	Importance of Coriolis Coupling in Isotopic Branching in (He, HD ⁺) Collisions
Authors:	Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Chemical reactions Mathematical methods Quantum mechanics Chemical calculations
Issue Date:	2009
Publisher:	ACS Publications
Citation:	J. Phys. Chem. A 2009, 113(34), p. 9568–9574.
Abstract:	A three-dimensional time-dependent quantum mechanical wave packet approach is used to calculate the reaction probability (PR) and integral reaction cross section values for both channels of the reaction $\text{He} + \text{HD}^+(\nu = 1; j = 0) \rightarrow \text{HeH}(\text{D})^+ + \text{D}(\text{H})$ over a range of translational energy (Etrans) on the McLaughlin–Thompson–Joseph–Sathyamurthy potential energy surface including the Coriolis coupling (CC) term in the Hamiltonian. The reaction probability plots as a function of translational energy for different J values exhibit several oscillations, which are characteristic of the system. The σ_R values obtained by including CC and not including it are nearly the same over the range of Etrans investigated for the HeD ⁺ channel. For the HeH ⁺ channel, on the other hand, σ_R values obtained from CC calculations are significantly smaller than those obtained from coupled state calculations. These results are compared with the available experimental results. The computed branching ratios ($\Gamma\sigma = \sigma_R(\text{HeH}^+)/\sigma_R(\text{HeD}^+)$) are also compared with the available experimental results.
URI:	https://pubs.acs.org/doi/full/10.1021/jp9049523 (https://pubs.acs.org/doi/full/10.1021/jp9049523) http://hdl.handle.net/123456789/3691 (http://hdl.handle.net/123456789/3691)
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