Title:	Importance of coriolis coupling in isotopic branching in (He, HD+) collisions
Authors:	Tiwari, Ashwani Kumar (/jspui/browse?type=author&value=Tiwari%2C+Ashwani+Kumar) Kolakkandy, Sujitha (/jspui/browse?type=author&value=Kolakkandy%2C+Sujitha) Sathyamurthy, N. (/jspui/browse?type=author&value=Sathyamurthy%2C+N.)
Keywords:	Branching ratio Coriolis coupling Coupled state J value Quantum mechanical
Issue Date:	2009
Publisher:	American Chemical Society.
Citation:	Journal of Physical Chemistry A, 113 (34), pp. 9568-9574.
Abstract:	A three-dimensional time-dependent quantum mechanical wave packet approach is used to calculate the reaction probability (P R) and integral reaction cross section values for both channels of the reaction He + HD +(v = 1;j = 0) -- HeH (D) + + D (H) over a range of translational energy (E trans) on the McLaughlin-ThompsonJoseph- 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 E trans 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 (T = σ R(HeH +) / σ R(HeD +)) are also compared with the available experimental results.
URI:	http://www.ncbi.nlm.nih.gov/pubmed/19642652 (http://www.ncbi.nlm.nih.gov/pubmed/19642652) http://pubs.acs.org/doi/abs/10.1021/jp9049523 (http://pubs.acs.org/doi/abs/10.1021/jp9049523)
Appears in Collections:	Research Articles (/jspui/handle/123456789/9)

Files in This Item:

File	Description	Size	Format	
Need to add pdf.odt (/jspui/bitstream/123456789/95/3/Need%20to%20add%20pdf.odt)		8.63 kB	OpenDocument Text	View/Open (/jspui/bitstream/1234567

Show full item record (/jspui/handle/123456789/95?mode=full) (/jspui/handle/123456789/95/statistics)