

THEORETICAL STUDIES OF THE ROLE OF VIBRATIONAL EXCITATION ON THE DYNAMICS OF THE HYDROGEN-TRANSFER REACTION OF  $F(^2P) + HCl \rightarrow FH + Cl(^2P)$

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Hydrogen-transfer reactions are probed through vibrational excitation of the HCl bond in the pre-reactive  $F \cdots HCl$  complex. Such open-shell species provide a challenge for quantum dynamical calculations due to the need to take into account multiple potential energy surfaces to accurately describe the system.

A three-dimensional, fully-coupled potential energy surface has been constructed based on electronic energies calculated at the multireference configuration interaction+Davidson correction (MRCI+Q) level of theory with an aug-cc-pVnZ ( $n = 2, 3, 4$ ) basis.<sup>a</sup> Spin orbit calculations have also been included.<sup>b</sup>

Here we present the results of time-dependent quantum wave packet calculations on the asymmetric hydrogen-transfer reaction of  $F(^2P) + HCl$ . In these calculations, the reaction is initiated by vibrationally exciting the HCl stretching motion in the pre-reactive  $F \cdots HCl$  complex. The wave packet is propagated on the coupled potential energy surfaces. Product state distributions were calculated for reactions initiated in the first three vibrationally excited states of HCl,  $v = 1 - 3$ .

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<sup>a</sup>M. P. Deskevich, M. Y. Hayes, K. Takahashi, R. T. Skodje, and D. J. Nesbitt *J. Chem. Phys.* **124**(22) 224303 (2006)

<sup>b</sup>M. P. Deskevich and D. J. Nesbitt *private communication*(2007)