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

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Recently, open-shell systems have gained interest in experimental and theoretical science. What proves interesting about these open-shell systems is that the potential energy surfaces often contain a van der Waals well in the reactant or product channel that allows researchers to probe the pre-reactive species. 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 of the pre-reactive $F\cdots HCl$ complex in the van der Waals well. The wave packet is propagated on a three-dimensional, fully coupled potential energy surface that has been constructed based on electronic energies calculated at the multi-reference configuration interation+Davidson correction (MRCI+Q) level of theory with an aug-cc-pVnZ (n=2,3,4) basis.[a] Product state distributions were calculated for reactions initiated in the first three vibrationally excited states of HCl, v=1, 2, and 3. Specifically, we analyzed the final electronic, vibrational, and rotational distributions.

Previous studies on the hydrogen-transfer reaction of the $Cl(^2P)$ + HCl system focused on whether vibrational excitation of the HCl stretch would promote the reaction and if so, how the reaction dynamics reflect the coupling among the diabatic potential surfaces that describe this system.[b] We also compare our $F(^2P)$ + HCl results to those of this related system.

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

[b] G. W. M. Vissers and A. B. McCoy *J. Phys Chem. A* **110** 5978 (2006)