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

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Open-shell species provide a new challenge when it comes to quantum mechanical calculations due to the need to take into account multiple potential energy surfaces to accurately describe the system. An example of such a system is $Cl(^2P)$ + HCl. Previous studies on the hydrogen-transfer reaction of this system investigated whether vibrational excitation would promote the reaction and if so, how the reaction dynamics were affected by the potentials and the coupling between them.[a] In these studies, we found that exciting the HCl to its first overtone did indeed lead to reaction. The reaction mechanism involved coherent oscillations of the wave packet between the reactant and product channels. Interestingly, if we removed the coupling between the three diabatic potential surfaces, the reactivity decreased substantially.

Here, we present results of a similar nature when looking at the asymmetric hydrogen-transfer reaction of $F(^2P)$ + HCl. A primary point of interest in this system compared to $Cl(^2P)$ + HCl is to see what happens when we break the symmetry since this means we can no longer see coherent oscillations. Due to it's simplicity, full-scale *ab initio* calculations have been executed in order to construct the potential energy surfaces.[b] We performed time-dependent quantum propagations involving all three potential surfaces, initiating the reaction with HCl in each of its three lowest vibrationally excited states. A primary point of interest in this system compared to $Cl(^2P)$ + HCl is to see what happens when we break the symmetry.

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

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