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

SARA E. RAY, GÉ W. M. VISSERS and ANNE B. McCOY, *Department of Chemistry, The Ohio State University, Columbus, OH 43210*.

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.[a] Spin orbit calculations have also been included.[b]

Here we present the results of time-dependent quantum wave packet calculations on the asymmetric hydrogen-transfer reaction of F(^{2}P) + 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, $v = 1 - 3$.

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

[b] M. P. Deskevich and D. J. Nesbitt *private communication*(2007)