The FTIR Study of the UV Irradiation of Amorphous and Crystalline Acetyl Chloride

Brad Rowland and Wayne Hess, *Battelle Pacific Northwest Laboratories, PO Box 999, Richland, WA. 99352, Mail Stop K2-14.*

The UV irradiation of amorphous and crystalline acetyl chloride samples at 10K produces dimer complexes of ketene and HCl molecules. We use infrared spectroscopy to study the vibrational spectra of the ketene-HCl complexes formed by the elimination of HCl within the 3 um thick acetyl chloride film. Ab-Initio calculations are used to facilitate the interpretation of the infrared spectra and to obtain optimized geometries for the complexes. The formation of ketene-HCl complexes is reversible at temperatures that exceed 50K. Rate information and an activation energy are obtained for the reverse reaction of the most abundant ketene-HCl conformation.