

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Modeling the transient vibrational dynamics of photofragments**

STEVE YOUNG, SARA MASON, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania, HAI-LUNG DAI, Department of Chemistry, University of Pennsylvania, ANDREW RAPPE, The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania — Knowledge of radical spectroscopy and the structure of radicals is important in many scientific areas, such as atmospheric systems, combustion reactions, biological processes, and more. Because many radicals are transient, unstable, and generally produced in small quantities, they are often difficult to characterize spectroscopically. In this talk, we will present our synthesis of theoretical and experimental data to understand the behavior of radical photofragments. The first part of the talk outlines our approach to understanding vibrationally hot but electronically cold radical dynamics, with direct molecular dynamics and performing electronic structure calculations using DFT within the GAMESS package. We will then summarize our recent development and application of time-resolved FTIR emission spectroscopy for the study of photofragments. Finally, we will present a joint theoretical and experimental investigation of the dynamics of the vinyl radical, including characterization of the complex interaction of rotation, alpha-proton motion, and anharmonic effects, and discuss their influence on the IR spectrum.

Steve Young

The Makineni Theoretical Laboratories, Department of Chemistry, University of Pennsylvania

Date submitted: 03 Dec 2006

Electronic form version 1.4