EIGENSTATE RESOLVED INFRARED SPECTROSCOPY OF 1,1,1-d_3-ETHANE IN THE REGION AROUND 5900 CM^{-1}

J. W. DOLCE, A. CALLEGARI, H. K. SRIVASTAVA, K. K. LEHMANN, and G. SCOLES, *Princeton University, Department of Chemistry, Princeton, NJ, 08544.*

This talk will describe results which are part of a series of experiments studying intramolecular vibrational energy redistribution (IVR) in medium size molecules containing a methyl group. Last year we reported on methylsilane[a], while this year we will discuss the results for 1,1,1-d_3-ethane also obtained using optothermal detection, cavity enhanced, molecular beam laser spectroscopy. A 9 cm^{-1} wide section in the 5900 cm^{-1} C-H stretch overtone region was observed. All molecules we have studied with an axial methyl group have a strong parallel band in this region with band orgins within a few cm^{-1} of each other. We believe the best zero order assignment for these bands is as the first overtone of the assymetric methyl CH stretch. For the CH_3CD_3 band, Lawrence-Knight deconvolution of the rotationally assigned transitions reveals that the coupling strengths of this state to the nearly isoenergetic background of vibrational states range from 1×10^{-3} to 25×10^{-3} cm^{-1}. The observed coupling strengths do not show a systematic dependence from the rotational quantum number for the low J,K values that we have observed in our beam experiment, and therefore appear to be dominated by anharmonic forces. These results will be discussed in light of those previously obtained for methylsilane and other similar molecules.

[a]Talk RK11, 1995.