

VIBRATIONAL DYNAMICS AROUND THE CONICAL INTERSECTION RESULTING FROM THE $\tilde{A} \rightarrow \tilde{X}$ LASER INDUCED FLUORESCENCE OF THE METHOXY (CH_3O) RADICAL

JAYASHREE NAGESH and EDWIN L. SIBERT III, *Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin-Madison, WI 53706.*

The results of a theoretical calculation of the spectra associated with the laser induced fluorescence $\tilde{A}^2A_1 \rightarrow \tilde{X}^2E$ of both the methoxy molecule and CH_2DO are presented and discussed. The form of the vibronic dipole moment is determined by symmetry and the corresponding dipole expansion coefficients are calculated using *ab initio* methods. The calculated spectra include states up to 3000 cm^{-1} above the zero point energy. We describe how the various features of the spectrum are related to coordinate dependent terms in the dipole expansion as well as the spin-orbit couplings, Jahn-Teller couplings, and vibrational anharmonicities.