BREAKING THE SYMMETRY IN JAHN-TELLER ACTIVE MOLECULES BY ASYMMETRIC ISOTOPIC SUBSTITUTION: SPLITTING THE ZERO-POINT VIBRONIC LEVEL.

DMITRY G. MELNIK, JINJUN LIU, TERRY A. MILLER, Laser Spectroscopy Facility, Department of Chemistry, The Ohio State University, 120 W. 18th Avenue, Columbus, Ohio 43210; ROBERT F. CURL, Department of Chemistry and Rice Quantum Institute, Rice University, Houston, Texas 77005.

Analysis and understanding of the vibronic spectra of Jahn-Teller active molecules have been challenging tasks due to the complex interaction patterns between vibronic levels even if the density of vibronic states is not too high. An example of a spectral feature that draws attention is the splitting of the ground vibronic level, as reported for degenerate electronic states of asymmetrically deuterated C$_6$H$_6$, C$_5$H$_5$, CH$_4^+$, and most recently, the methoxy isotopologues, CH$_3$DO and CHD$_2$O. Understanding such splittings plays a crucial role for the analysis of the vibronic spectra of these species. We have developed a simplified model emulating vibronic interactions involving a single doubly-degenerate vibrational mode and one totally symmetric mode in a degenerate electronic state. The extension of this model to more complex, realistic cases and comparison with experiment and quantum chemical calculations will also be presented.