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

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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_6H_6, C_5H_5, CH_4^+, and most recently, the methoxy isotopologues, CH_2DO and CHD_2O. 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.