COUPLING OF LARGE AMPLITUDE INVERSION WITH OTHER STATES

JOHN PEARSON, SHANSHAN YU, Jet Propulsion Laboratory, California Institute of Technology, Pasadena, CA, USA.

The coupling of a large amplitude motion with a small amplitude vibration remains one of the least well characterized problems in molecular physics. Molecular inversion poses a few unique and not intuitively obvious challenges to the large amplitude motion problem. In spite of several decades of theoretical work numerous challenges in calculation of transition frequencies and more importantly intensities persist. The most challenging aspect of this problem is that the inversion coordinate is a unique function of the overall vibrational state including both the large and small amplitude modes. As a result, the r-axis system and the meaning of the K-quantum number in the rotational basis set are unique to each vibrational state of large or small amplitude motion. This unfortunate reality has profound consequences to calculation of intensities and the coupling of nearly degenerate vibrational states. The case of NH3 inversion and inversion through a plane of symmetry in alcohols will be examined to find a general path forward.