SPIN-VIBRONIC CALCULATIONS FOR JAHN-TELLER ACTIVE MOLECULES IN QUASI-DIABATIC BASIS WITH SOCJT3

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Jahn-Teller active molecules demonstrate significant vibronic and spin-orbit couplings which has always posed a computational challenge in quantum chemistry. The presence of a conical intersection in the adiabatic potential energy surfaces makes getting a reliable quantum chemistry calculation of these terms challenging due to breakdown of Born-Oppenheimer (BO) approximation. Calculating experimentally observable parameters for rotationally resolved spectra of such molecules involves three basic steps, a) generating a potential energy surface in quasi-diabatic basis, b) transformation of the potential energy surface from Cartesian to cylindrical coordinates c) diagonalizing the spin-vibronic Hamiltonian. One of the major obstacles in these calculations is solving the eigenvalue problem in quasi-diabatic basis due to the size of matrices that need to be diagonalized. In this talk we talk about pushing the boundaries for such calculations with our program package (SOCJT3). We have implemented new algorithms that diagonalize huge matrices and include coupling terms up to quartic order. This is further utilized to calculate experimentally observable rotational parameters. The primary objective of our work is to generate a simulation to understand and characterize the previously unanalyzed rotationally resolved spectra of open-shell radicals.