Spin-Vibronic structure of Jahn-Teller active $\tilde{X}\,^2E$ state of CH_3O radical

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Presence of a conical intersection at the three-fold symmetry molecular geometry has lead to significant interest in studying the Methoxy radical. Many studies in the past have analysed both spin-vibronic[1] and high-resolution spectra of the radical[2]. Analysis of the spectra of the $\tilde{X}$ state of CH_3O radical in the CH-stretch region has not been possible in the past because of the computational requirements for the spin-vibronic calculations involved. In addition, analysis of the low-lying levels of the $\tilde{X}\,^2E$ state have clearly indicated the need for potential energy surfaces with upto quartic terms. In this poster, we present our on-going efforts to understand and assign the spin-vibronic levels of $\tilde{X}\,^2E$ state in the 2000 to 3000 cm^{-1} region. The ground state quasi-diabatic PES, with expansions upto and including quartic terms in normal coordinates, has been fitted using machine-learning techniques. Symmetry relationships have been incorporated within the model to significantly reduce the number of fit parameters. Compelling evidence of the improved quality of the new potential is obtained by comparing the predicted rotational parameters for the ground vibrationless level to those experimentally obtained as well as those previously published[3]. Furthermore, improvements to SOCJT3 has enabled us to calculate converged eigenvalues and eigenvectors in 2000-3000 cm^{-1} region, which are used for calculating line-intesities for the spin-vibronic spectra and thereby assist in spectral assignments in the region.

References

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