SIMULATION OF THE SPIN-VIBRONIC STRUCTURE IN THE GROUND ELECTRONIC STATE AND EMISSION SPECTRA INTENSITIES FOR CH_3O RADICAL.

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Methoxy is a radical ubiquitous in the reactions of combustion and oxidation of hydrocarbon compounds in the atmosphere. Because of its relatively small size and degenerate $\tilde{X}\,^2$E ground electronic state, it presents a benchmark system for theoreticians to study the multimode Jahn-Teller (JT) effect in the presence of spin-orbit interaction. We have coupled an effective Hamiltonian, including Jahn-Teller coupling terms of up to 3^d order, with a powerful computational engine that allows for quick calculations of spin-vibronic eigenstates and, correspondingly, eigenfunctions from which spectrum intensities can be derived. A graphical user interface, coupled with this computational core, helps to visualize the simulated spectra and compare them with the experimental traces. We simulate and discuss the intensities and spin-vibronic level positions, that we have observed in 4 dispersed fluorescence spectra obtained by pumping the $\tilde{A}$ state vibrational levels 3^5, $3^1 4^1$, $3^3 5^1$ and $3^3 6^1$, and complementary data that have been obtained in SEP experiments of Temps and coworkers[c].

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[c]F. Temps, in Molecular Dynamics and Spectroscopy by Stimulated Emission Pumping, edited by Hai-Lung Dai and R. W. Field, World Scientific, NJ, 1995