

## UNDERSTANDING THE ROTATIONAL AND FINE STRUCTURE OF THE $\tilde{X}^2E$ STATE OF THE METHOXY RADICAL (CH<sub>3</sub>O) IN THE C-H STRETCH REGION

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The preceding talk by Vasilyev et al. focuses on the spin-vibronic structure of the CH-stretch region of the  $\tilde{X}^2E$  ground electronic state of the methoxy radical (CH<sub>3</sub>O). To extract a rotation-free spin-vibronic energy level structure from experimental spectra, one must simulate and fit the rotational and fine structure. The CH-stretch region of the  $\tilde{X}^2E$ -state CH<sub>3</sub>O is a labyrinth of spin-ro-vibronic energy levels. Experimentally, computational, and theoretical techniques have been developed to understand the energy level structure. Experimentally, the fluorescence-depletion infrared (IR) spectroscopy technique was employed to simplify the ro-vibrational spectra. For each vibrational transition within the  $\tilde{X}^2E$  state, only a few transitions were observed, all originating from the same lower rotational level. Theoretically, a spectroscopic model incorporating an effective rotational Hamiltonian was used to account for the spin-orbit interaction coupled with the Jahn-Teller interaction (SOcJT) and simulate the rotational and fine structure. The fit  $B$  rotational constants significantly deviate from that obtained using the undistorted geometry, which may be attributed to strong vibronic interactions. Therefore, the analysis of rotational and fine structures not only provides rotation-free transition frequencies but also illuminates the mechanisms and strengths of spin-vibronic interactions.