

JET-COOLED LASER-INDUCED FLUORESCENCE SPECTROSCOPY OF CA-1-PROPOXIDE RADICAL

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Alkaline-earth-metal-containing free radicals, like calcium alkoxides are promising candidates for direct laser cooling with potential applications in precision measurements, cold chemistry, and quantum information science. Our group has studied calcium alkoxide radicals such as CaOCH_3 , CaOC_2H_5 , and $\text{CaOCH}(\text{CH}_3)_2$ using laser-spectroscopic techniques under jet-cooled conditions, revealing their vibronic transition frequencies and relative intensities. The present study focuses on the electronic and vibrational structures of the $\tilde{\text{A}}_2/\tilde{\text{A}}_1-\tilde{\text{X}}$ system of Ca-1-propoxide radicals, particularly examining the effects of gauche (G) and trans (T) conformations on the vibrational branching ratios and the role of C-H stretch modes. In the laser-induced fluorescence (LIF) and dispersed-fluorescence (DF) spectra of Ca-1-propoxide, we identified the $\tilde{\text{A}}_2/\tilde{\text{A}}_1-\tilde{\text{X}}$ origin bands, the spin-orbit (SO) splitting, and distinctive vibrational signatures of the G and T conformers. Vibronic bands of both conformers are assigned based on density functional theory (DFT) and time-dependent (TD-DFT) calculations. Experimentally determined vibronic transitions intensities and the derived Franck-Condon factors reveal the practicality of laser-cooling the Ca-1-propoxide radicals. Notably, transitions to C-H stretch levels, absent in monoalkoxide radicals studied previously, were observed in the LIF and DF spectra of the G conformer C_1 , underlining the critical role of molecular symmetry. Rotationally resolved LIF spectroscopic measurement using narrow-linewidth continuous-wave (CW) ring dye lasers is in process.