LASER-INDUCED FLUORESCENCE AND DISPERSED FLUORESCENCE SPECTROSCOPY OF THE TROPYL C_7H_7 RADICAL

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Laser-induced fluorescence (LIF) and dispersed fluorescence (DF) spectra of the cycloheptatrienyl (tropyl) radical (C_7H_7) have been observed under supersonic jet cooling conditions. The DF emission was collected by pumping different vibronic bands of the $\tilde{A}^2E_3'' \leftarrow \tilde{X}^2E_2''$ LIF excitation spectrum. Analysis of the DF spectra yields valuable information about the vibrational levels of the ground $\tilde{X}^2E_2''$ electronic state. In addition to the experimental work, *ab initio* calculations have been performed providing ground and excited state Jahn-Teller parameters; a comprehensive analysis reveals Jahn-Teller activity in 4 e_3' modes for the $\tilde{X}^2E_2''$ state and 3 e_1' modes for the $\tilde{A}^2E_3''$ and provides values for their vibrational frequencies as well as linear Jahn-Teller constants. In addition to the magnitude of the Jahn-Teller distortion, the stabilization energies for both electronic states have been calculated at the CASSCF(7,7) and EOMEA-CCSD levels of theory using different basis sets.