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Vibrational Spectra and Structure of Coumaran and Its Ring-Puckering Potential Energy Functions in the S_0 and $S_1(\pi,\pi^*)$ Electronic States[1] JUAN YANG, MARTIN WAGNER, KATSUHIKO OKUYAMA, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — The far-infrared (IR), jet-cooled fluorescence excitation (FES), single vibronic level fluorescence (SVLF), and ultraviolet (UV) absorption spectra of coumaran have been recorded and analyzed. The assignment of those spectra has allowed a detailed energy map of both the S_0 and $S_1(\pi,\pi^*)$ electronic states of the ring-puckering (ν_{45}) vibration to be determined. A one-dimensional potential energy function for the ring-puckering vibration very nicely predicts the experimentally determined energy level spacings for both electronic states. In the S_0 ground state the barrier to planarity is 154 cm^{-1} and the puckering dihedral angle is 25 $^\circ$. In the $S_1(\pi,\pi^*)$ excited state the corresponding values are 34 cm^{-1} and 14 $^\circ$. The decreased barrier in the electronic excited state results from decreased angle strain in the five-membered ring.

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