Abstract Submitted
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Laser Induced Fluorescence and Ultraviolet Absorption Spectra, DFT Calculations, and Structure of 1,3-Benzodioxan[1] KATHLEEN MCCANN, Texas A&M University, College Station, Texas, MARTIN WAGNER, JAEBUM CHOO, JAAN LAANE, Texas A&M University, College Station, Texas — The laser induced fluorescence spectra, both excitation and dispersed, of jet-cooled 1,3-benzodioxan along with ultraviolet absorption spectra of the ambient temperature vapors have been recorded and analyzed. The focus of the study was on the low-frequency out-of-plane vibrational modes which are useful for determining the potential energy surface which governs the molecular structure. In the S_0 electronic ground state these have vibrational frequencies of 107.6 cm^{-1} (ring-bending), 157.3 cm^{-1} (ring-twisting), 275.1 cm^{-1} (ring-flapping), and 350.2 cm^{-1} (ring-twisting at the benzene ring). The corresponding values for the $S_1(\pi,\pi^*)$ excited state are 96.3, 102.2, 194.6, and 255.8 cm^{-1} with the lower values reflecting a less rigid ring structure. DFT calculations predict a twisted structure and a barrier to planarity of 3475 cm^{-1} for the S_0 ground state and this is consistent with the experimental data.

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Jaan Laane
Texas A&M University, College Station, Texas

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