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Infrared, Raman, Ultraviolet Absorption, Fluorescence Excitation and Single Vibronic Level Fluorescence Spectra and Ab Initio Calculations of 1,4-Benzodioxan JUAN YANG, MARTIN WAGNER, DANIEL AUTREY, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — The 1,4-benzodioxan molecule is expected to have a twisted C_2 structure due to the CH_2-CH_2 torsional interaction in the electronic ground state and MP2 calculations confirm that. Mid-infrared (IR) and Raman spectra of this molecule in both liquid and vapor phases were recorded and assigned. Density functional theory (DFT) calculations were carried out to predict the vibrational frequencies. The calculated frequencies, after proper scaling, agreed very well with the experimental values. Ultraviolet (UV) absorption, fluorescence excitation (FES) and single vibronic level fluorescence (SVLF) spectra were also obtained and assigned. From those spectra several energy levels of the ring-bending and ring-twisting vibrations in both the electronic ground and excited states were determined.

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