VIBRATIONAL, ELECTRONIC, AND FLUORESCENCE SPECTRA AND AB INITIO CALCULATIONS OF 1,4-BENZODIOXAN

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The 1,4-benzodioxan molecule has 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, agree 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.