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**Spectroscopic Studies and Ab Initio Calculations of 1,3-Benzodioxan in its $S_0$ and $S_1(\pi,\pi^*)$ Electronic States**[1] KATHLEEN MCCANN, JAEBUM CHOO, MARTIN WAGNER, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — Both the ground ($S_0$) and excited [$S_1(\pi,\pi^*)$] states of 1,3-benzodioxan have been studied using molecular spectroscopy and theoretical calculations. Infrared, Raman, ultraviolet absorption, and laser-induced fluorescence (LIF) spectroscopies of the jet-cooled molecules were used to create energy maps for the vibrational and vibronic levels of the molecule, especially for the low-frequency vibrational modes which help to elucidate the conformational energetics of the molecule. The ring-bending, twisting, and flapping motions of the molecule provide the pathways for the conformational changes and were studied in considerable detail. The molecule is twisted with a high barrier to planarity of the equilibrium structure.

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