VIBRATIONAL POTENTIAL ENERGY SURFACES FOR THE RING-PUCKERING AND RING-FLAPPING VIBRATIONS OF 1,3-BENZODIOXOLE IN ITS S_0 AND S_1 (π, π*) ELECTRONIC STATES

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The far-infrared and Raman spectra of 1,3-benzodioxole vapor have been recorded and analyzed to determine the two-dimensional potential energy surfaces for the ring-puckering and ring-flapping vibrations in the S_0 electronic ground state. This molecule is puckered due to anomeric effects which are somewhat suppressed by the presence of the benzene ring. Electronic absorption spectra and laser induced fluorescence spectra of the jet-cooled molecules were recorded to determine the puckering and flapping levels in the $S_1(\pi, \pi^*)$ excited state of this molecule. In the excited state the flapping frequency decreases reflecting the decreased rigidity between the two rings. However, in the $S_1(\pi, \pi^*)$ state the anomeric effect is less suppressed by the benzene ring and the barrier to planarity is increased. *Ab initio* calculations were carried out for both ground and excited states. For the ground state the agreement between observed and predicted barrier heights is excellent.