Abstract Submitted
for the TSS05 Meeting of
The American Physical Society

Fluorescence and Absorption Spectra and Potential Energy Surfaces of 1,3-Benzodioxole and Coumaran in Their S_0 and $S_1(\pi,\pi^*)$ States
KATSUHIKO OKUYAMA, KEVIN MORRIS, MARTIN WAGNER, JUAN YANG, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — The fluorescence excitation spectra and dispersed fluorescence spectra of jet-cooled molecules along with ultraviolet and far-infrared absorption spectra of the bicyclic molecules 1,3-benzodioxole and coumaran have been recorded. These spectra have allowed us to determine the two-dimensional potential energy surfaces for the ring-puckering and ring-flapping vibrations for the S_0 and $S_1(\pi,\pi^*)$ electronic states. Both molecules are bent with barriers to planarity in both their ground and excited states. The bent structures for coumaran result from $-CH_2$-CH_2- torsional forces while those for 1,3-benzodioxole are caused by the anomeric effect.

Jaan Laane
Department of Chemistry, Texas A&M University, College Station, TX 77843-3255

Date submitted: 04 Feb 2005 Electronic form version 1.4