ULTRAVIOLET CAVITY RINGDOWN SPECTRA OF 2-CYCLOHEXEN-1-ONE AND ITS INVERSION POTENTIAL ENERGY FUNCTION

MOHAMED RISHARD, JAAN LAANE, *Department of Chemistry, Texas A&M University, College Station, Texas 877843-3255*; JAEBUM CHOO, *Department of Chemistry, Hanyang University, 425-791 Ansan, Korea*; DANIEL AUTREY, *Department of Natural Sciences, Fayetteville University, Fayetteville, NC 28301*; STEPHEN DRUCKER and EMILY GILES, *Department of Chemistry, University of Wisconsin-Eau Claire, Eau Claire, WI 54702-4004*.

The cavity ringdown spectrum of 2-cyclohexenone vapor has been recorded in the vicinity of the S_0 band, which is at 26 089.1 cm^{-1}. Several very weak low-frequency fundamentals and overtones have been observed. The inversion vibration of the six-membered ring (ν_{39}) occurs at 99.0 cm^{-1}. With the help of far-infrared and Raman spectra, the frequencies for ν_{38} and ν_{37} have also been determined. The barrier to the inversion potential was found to be 1900 ± 300 cm^{-1}, which is very different from previously reported values of 935 and 3379 cm^{-1}. Density functional calculations give a barrier of 2090 cm^{-1} when the B3LYP/6-311+G(d,p) basis set is used. The frequencies calculated by the density functional methods agree very well with the experimental values obtained by liquid and vapor Raman spectra and also with the mid-IR experiments. Investigation of the $T_1(n, \pi*)$ state is currently underway.