

Abstract Submitted
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Ultraviolet Cavity Ringdown Spectra of 2-Cyclohexen-1-one MOHAMED RISHARD, JAEBUM CHOO, DANIEL AUTREY, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255, STEPHEN DRUCKER, 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 $26\,089.1\text{ cm}^{-1}$. Several low-frequency fundamentals and overtones have been observed using this very sensitive technique which also allows even weak bands to be detected. The inversion 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 $1900\pm 300\text{ cm}^{-1}$, 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 $T_1(n,\pi^*)$ is currently underway.

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