ELECTRONIC GROUND STATE OF 2-CYCLOHEXEN-1-ONE: STRUCTURE AND INVERSION POTENTIAL ELUCIDATED BY ULTRAVIOLET CAVITY RINGDOWN SPECTROSCOPY AND DFT CALCULATIONS

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The $S_1(n,\pi^*) \leftarrow S_0$ cavity ringdown spectrum of 2-cyclohexen-1-one vapor has been recorded in the vicinity of the origin band, which is at 26,089.1 ± 0.1cm^{-1}. Observation of hot bands in the spectrum has permitted the determination of several low-frequency fundamentals and overtones in the ground electronic state. The lowest two excited quantum states for the inversion vibration, ν_{39}, were found to be at 99.0 and 197.0 cm^{-1}. Together with previously published far-infrared spectra and vapor-phase Raman spectra, the fundamental frequencies for ν_{37} and ν_{38} have also been established. From observed ν_{39} levels, the barrier to inversion was determined experimentally to be 1900 $\pm$300 cm^{-1}, which is very different from values of 935 and 3379 cm^{-1} previously reported from Raman and far-infrared data, respectively. Density functional calculations carried out in the present work give a barrier value of 2090 cm^{-1} when the B3LYP/6-311 + G(d,p) basis set is used.