Vibrational Spectra, *Ab Initio* Calculations, and Ring-Puckering Potential Energy Function for γ-Crotonolactone

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ABSTRACT

The infrared and Raman spectra of liquid and vapor γ-crotonolactone have been collected. Both the experimental data and *ab initio* calculations show that the molecule is rigidly planar in its electronic ground state. This conclusion agrees with the previously reported microwave studies and is attributed to the conjugation between the C=C and C=O double bonds of the ring. The ring-puckering potential energy function was generated from *ab initio* calculations and was confirmed by the vapor-phase Raman spectra to be nearly harmonic. DFT calculations predict a harmonic ring-puckering frequency of 203 cm^{-1} as compared to the observed vapor-phase Raman value of 208 cm^{-1}. The DFT calculations were also used to compute the infrared and Raman spectra of γ-crotonolactone, and these agree very well with the experimental spectra.

Keywords: γ-crotonolactone, *ab initio* calculations, vibrational spectra, ring-puckering potential energy function.