VIBRATIONAL OVERTONE SPECTROSCOPY OF CYCLOHEPTATRIENE.NEW METHOD FOR SPECTRAL ASSIGNMENTS IN THE OVERTONE SPECTROSCOPY

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The spectrum of the first through fifth vibrational overtone absorptions of cycloheptatriene is reported. The spectrum for the first and second overtones was recorded using a liquid sample while the third, fourth and fifth overtones were recorded for gaseous samples. A Direct Correlation (DC) method is developed using the correlation between ab initio CH bond lengths and the local mode transition energy to predict the experimental spectra for the third, fourth and fifth overtones. These predictions were used to assign the absorption peaks for the boat conformer of cycloheptatriene in the gaseous spectrum. Progressions belonging to the olefinic and methylenic CH bond stretches are identified for both the gaseous and liquid data. The description of the DC method and interpretation of the cycloheptatriene spectrum will be presented.