Vibration Frequencies, Normal Coordinates and IR Absorption Intensities of 1-; 1,2-Di-; 1,3-Di- and 1,2,3-Trimethylene Cyclobutane

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SCF-MO calculations of the vibration frequencies and IR absorption intensities, applying the MINDO/3-FORCES method, are reported for the four molecules, mono-, di- (1,2- and 1,3-), and 1,2,3-trimethylene cyclobutane. Normal coordinate analysis of all vibration modes is described for each molecule. The obtained results allow interesting correlations between the frequencies of similar modes as calculated for the different methylene cyclobutanes.

Key words: Methylene Cyclobutanes; Vibrations; Normal Coordinates.