

AB INITIO AND DFT CALCULATIONS FOR THE VIBRATIONAL FREQUENCIES AND BARRIER TO PLANARITY OF CYCLOPENTENE AND ITS DEUTERATED ISOTOPOMERS

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Ab initio and DFT calculations have been carried out for the cyclopentene molecule in order to analyze its structure and vibrational frequencies. The structure was calculated with MP2/6-311++G\*\* and MP2/cc-pVTZ basis sets and these predicted puckering angles of 27.1° and 26.1°, respectively, as compared to the experimental far-infrared value of 26°. The barrier to planarity was calculated to be 247 cm<sup>-1</sup>, slightly higher than the 233 cm<sup>-1</sup> far-infrared value. The calculated vibrational frequencies from DFT-B3LYP/cc-pVTZ were compared to the experimental values for the d<sub>0</sub>, d<sub>1</sub>, d<sub>4</sub>, and d<sub>8</sub> isotopomers and several vibrational reassignments were made.