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Ab Initio Calculations for the Structure, Vibrational Frequencies, and Barrier to Planarity of Cyclopentene ABDULAZIZ AL-SAADI, JAAN LAANE, Department of Chemistry, Texas A&M University, College Station, TX 77843-3255 — 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 $^\circ$ and 26.1 $^\circ$, respectively, as compared to the experimental far-infrared value of 26 $^\circ$. The barrier to planarity was calculated to be 247 cm^{-1}, slightly higher than the 233 cm^{-1} far-infrared value. The calculated vibrational frequencies from DFT-B3LYP/cc-pVTZ were compared to the experimental values for the $d_{0,}d_1$, d_4, and d_8 isotopomers and several vibrational reassignments were made.

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