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

ABDULAZIZ AL-SAADI and 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° and 26.1°, respectively, as compared to the experimental far-infrared value of 26°. 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.