*Ab Initio* and DFT Calculations for the Structure and Vibrational Spectra of Cyclopentene and its Isotopomers

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Abstract

*Ab initio* calculations using the MP2/cc-pVTZ basis set do an excellent job of predicting the inversion barrier (247 vs. 232 cm\(^{-1}\)) and dihedral angle (26°) of cyclopentene. DFT calculations also do an excellent job of predicting the vibrational frequencies of the \(d_0\), \(d_1\), \(d_4\), and \(d_8\) isotopomers. They have also allowed the reassignments of several of the vibrational frequencies.