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.