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Infrared and Raman Spectra, Conformations, and Theoretical Calculations for Isotopomers of Cyclohexane and its Halo Derivatives HYE JIN CHUN, ESTHER J. OCOLA, JAAN LAANE, Department of Chemistry, Texas AM University, College Station, TX 77843-3255, USA — The infrared and Raman spectra of cyclohexane, chlorocyclohexane, bromocyclohexane and their isotopomers have been recorded and analyzed. Theoretical computations have been carried out to calculate the vibrational frequencies and the conformational forms of each molecule using *ab initio* (MP2/cc-pVTZ) and DFT (B3LYP/cc-pVTZ) methods. Cyclohexane can exist in chair or boat conformations and these differ in energy by 32.13 kJ/mol. The chair conformations of chlorocyclohexane and bromocyclohexane both have equatorial and axial forms for the halogen atoms and these differ in energy by 1.06 kJ/mol. The vibrational spectra of cyclohexane-d_{11}, chlorocyclohexane, chlorocyclohexane-d_{11}, bromocyclohexane and bromocyclohexane-d_{11} confirm the presence of the different conformational forms. The observed frequency differences between the different isotopomers are in excellent agreement with the theoretical calculations.

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