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Vibrational Spectra, Conformations, and Theoretical Calculations for Cyclohexane, Chlorocyclohexane, Bromocyclohexane and their Isotopomers HYE JIN CHUN, ESTHER OCOLA, JAAN LAANE, Texas AM University, College Station, TX — The infrared and Raman spectra of cyclohexane and its d_{11} and d_{12} isotopomers have been recorded and analyzed. The studies were complemented by *ab initio* (MP2-ccpVTZ) and density functional theory (DFT/B3LYP-ccpVTZ) calculations. The conformational energies of different structures of the molecules were calculated. Vibrational spectra were also recorded for chlorocyclohexane-d_0 and -d_{11} and bromocyclohexane-d_0 and -d_{11}. Theoretical computations were also performed to calculate the spectra and molecular conformational energies of the halocyclohexanes.

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