CYCLOHEXANE VIBRATIONS: HIGH RESOLUTION SPECTRA AND ANHARMONIC LOCAL MODE CALCULATIONS

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High resolution infrared absorption spectra of cyclohexane (C_6H_{12}) have been recorded from 1100 to 4000 cm^{-1} at room temperature and 241 K. Cyclohexane is an oblate symmetric top with D_{3d} symmetry. A rotational analysis was obtained for the ν_{27} (e_u) and ν_{14} (a_{2u}) CH_2 scissor modes at 1452.9 cm^{-1} and 1456.4 cm^{-1}, respectively. Several combination modes were also assigned and rotationally analyzed. The C-H stretching modes are perturbed by overtone and combination modes of the CH_2 scissor vibrations, and an anharmonic local mode calculation was needed to interpret the spectra. The 4 main strong allowed C-H stretching modes appear as two e_u a_{2u} pairs near at 2862 cm^{-1} and 2933 cm^{-1}. The Fermi-resonance local mode model coupling terms give physical insight into the effects that organize the cyclohexane vibrational energy levels. The unstrained cyclohexane molecule is a useful paradigm for six-membered rings in larger chemical and biological systems.