Molecular structure, Vibrational spectra (FTIR and FT Raman) and Natural bond orbital analysis of 4-Aminomethylpiperidine: DFT study

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Molecular structure, Vibrational spectra (FTIR and FT Raman) and Natural bond orbital analysis of 4-Aminomethylpiperidine: DFT study

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Abstract

The FT-IR and FT-Raman spectra of 4-Aminomethylpiperidine have been recorded using Perkin Elmer Spectrophotometer and Nexus 670 spectrophotometer. The equilibrium geometrical parameters, various bonding features, the vibrational wavenumbers, the infrared intensities and the Raman scattering activities were calculated using Hartree-Fock and density functional method (B3LYP) with 6-311+G(d,p) basis set. Detailed interpretations of the vibrational spectra have been carried out with the aid of the normal coordinate analysis. The spectroscopic and natural bonds orbital (NBO) analysis confirms the occurrence of intra molecular hydrogen bonds, electron delocalization and steric effects. The changes in electron density in the global minimum and in the energy of hyperconjugative interactions of 4-Aminomethylpiperidine (4AMP) were calculated. The theoretical UV-visible spectrum of the compound was computed in the region 200-400 nm by time-dependent TD-DFT approach. The calculated HOMO and LUMO energies show that charge transfer occur within the molecule. The dipole moment (μ) and polarizability (α), anisotropy polarizability (Δα) and hyperpolarizability (β) of the molecule have been reported.

Keywords:

FT-IR
FT-Raman
Intramolecular hydrogen bond
NBO
HOMO-LUMO
4-Aminomethylpiperidine (4AMP)

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