

VIBRATIONAL SPECTROSCOPIC INVESTIGATION AND CONFORMATIONAL ANALYSIS OF 1-HEPTYLAMINE: A COMPARATIVE DENSITY FUNCTIONAL STUDY

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FT-IR and Raman spectra of 1-heptylamine (1-ha) were experimentally reported in the region of 4000-10 cm⁻¹ and 4000-100 cm⁻¹, respectively. The conformational analysis, optimized geometric parameters, normal mode frequencies and corresponding vibrational assignments of 1-ha (C₇H₁₇N) were theoretically examined by means of Becke-3-Lee-Yang-Parr (B3-LYP) density functional theory (DFT) method together with 6-31++G(d,p) basis set. Furthermore, reliable vibrational assignments were made on the basis of potential energy distribution (PED) calculated and the thermodynamics functions, highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) of 1-ha were predicted. Calculations were carried out with the possible ten conformational isomers (TT, TG, GT, GT1, GG1, GG2, GG3, GG4, GG5, GG6; T and G denote trans and gauge) of 1-ha, both in gas phase and in solution. Solvent effects were investigated using benzene and methanol. All results indicates that B3-LYP method provides satisfactory results for the prediction vibrational wavenumbers, TT isomer is the most stable form of 1-ha and the conformational energy barrier is independent of the solvent whereas the vibrational frequencies and assignments, IR and Raman intensities of 1-ha are solvent dependent.