DFT, FT-RAMAN AND FT-IR INVESTIGATIONS OF 1-CYCLOPENTYLPIPERAZINE

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FT-IR and FT-Raman spectra of 1-cyclopentylpiperazine (1cppp) have been experimentally reported in the region of 4000-50 cm^{-1}. The optimized geometric parameters (bond lengths, bond and dihedral angles), conformational analysis, normal mode frequencies and corresponding vibrational assignments of 1cppp ($C_9H_{18}N_2$) are theoretically examined by means of B3LYP hybrid density functional theory (DFT) method together with $6-31++$G(d,p) basis set. Furthermore, reliable vibrational assignments have been made on the basis of potential energy distribution (PED) and the thermodynamics functions, highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) of 1cppp have been predicted. Calculations are employed for four different conformations of 1cppp both in gas phase and in solution. Solvent effects are investigated using chloroform and dimethylsulfoxide. All results indicates that B3LYP method is able to provide satisfactory results for predicting vibrational frequencies and the structural parameters, mole fractions of stable conformers, vibrational frequencies and assignments, IR and Raman intensities of 1cppp are solvent dependent.

Keywords: 1-cyclopentylpiperazine; Vibrational spectra; Solvent effect; PED; DFT; B3LYP