DFT STUDY OF SOLVENT EFFECTS ON CONFORMATIONAL EQUILIBRIA AND VIBRATIONAL SPECTRA OF 4-(1-PYRROLIDINYL)PIPERAZINE

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The optimized structural parameters (bond lengths, bond and dihedral angles), conformational equilibria and normal mode frequencies and corresponding vibrational assignments of 4-(1-Pyrrolidinyl)piperazine (4-pypp) have been examined by means of B3LYP hybrid density functional theory (DFT) method with 6-31++G(d,p) basis set. Furthermore, reliable vibrational assignments have 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 4-pypp ($C_8H_{17}N_3$) have been predicted. Calculations are employed for different conformations of 4-pypp both in gas phase and in solution. Solvent effects are investigated using chloroform and dimethylsulfoxide. Results from the theoretical values are showed that the structural parameters, mole fractions of stable conformers, vibrational frequencies, IR intensities and Raman activities of 4-pypp are solvent dependent.

Keywords: 4-(1-Pyrrolidinyl)piperazine, vibrational spectra, solvent effect, DFT.