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

MAHIR TURSUN, *Department of Physics, Dumlupinar University, Kutahya, 43100, Turkey*; and GURKAN KESAN, *Institute of Physics and Biophysics, Faculty of Science, University of South Bohemia, Branisovsk 31, Cesk Budjovice, 370 05, Czech Republic*; and CEMAL PARLAK, *Department of Physics, Dumlupinar University, Kutahya, 43100, Turkey*; MUSTAFA SENYEL, *Science Faculty, Department of Physics, Anadolu University, Eskisehir, Turkey 26470*.

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.