CONFORMATIONAL, VIBRATIONAL AND ELECTRONIC PROPERTIES OF C5H3XOS (X = H, F, Cl OR Br): HALOGEN AND SOLVENT EFFECTS

MUSTAFA SENYEL, *Department of Physics, Anadolu University, Eskisehir, Turkey*; GUNES ESMA, *Physics, Anadolu University, Eskisehir, TURKEY*; CEMAL PARLAK, *Physics, Dumlupinar University, Kutahya, TURKEY*.

The effects of halogen and solvent on the conformer, vibrational and electronic properties of thiophene-2-carbaldehyde (C5H4OS) and thiophene-2-carbonyl-halogens [C5H3XOS; X = F, Cl or Br] were investigated employing the DFT and TD-DFT methods. The B3LYP functional was used with the 6-31++G(d,p) basis set. Computations were focused on the two conformational isomers of the compounds in the gas phase and both in a non-polar solvent and in a polar solvent. The present work explores the effects of both the halogen and the medium on the conformational preference, geometrical parameter, dipole moment, vibrational spectra, UV spectrum and HOMO-LUMO orbital. The findings of this work can be useful to those systems involving changes in the conformations analogous to the compounds studied.