DENSITY FUNCTIONAL THEORY STUDIES OF CONFORMATIONAL STABILITIES AND ROTATIONAL BARRIERS OF 2- AND 3-THIOPHENECARBOXALDEHYDES

Y. Umar[1], J. Tijani[2], and S. Abdalla[3]

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The molecular structures, conformational stabilities, and infrared vibrational wavenumbers of 2-thiophenecarboxaldehyde and 3-thiophenecarboxaldehyde are computed using Becke-3–Lee–Yang–Parr (B3LYP) with the 6-311++G** basis set. From the computations, *cis*-2-thiophenecarboxaldehyde is found to be more stable than the transfer conformer with an energy difference of 1.22 kcal/mol, while *trans*-3-thiophenecarboxaldehyde is found to be more stable than the *cis* conformer by 0.89 kcal/mol. The computed dipole moments, structural parameters, relative stabilities of the conformers and infrared vibrational wavenumbers of the two molecules coherently support the experimental data in the literature. The normal vibrational wavenumbers are characterized in terms of the potential energy distribution using the VEDA4 program. The effect of solvents on the conformational stability of the molecules in nine different solvents is investigated using the polarizable continuum model.

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