Experimental (FT-IR, NMR and UV) and theoretical (M06-2X and DFT) investigation, and frequency estimation analyses on (*E*)-3-(4-bromo-5-methylthiophen-2-yl)acrylonitrile

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ABSTRACT

The spectroscopic properties of (*E*)-3-(4-bromo-5-methylthiophen-2-yl)acrylonitrile have been investigated by FT–IR, UV, ^{1}H and ^{13}C NMR techniques. The theoretical vibrational frequencies and optimized geometric parameters (bond lengths and angles) have been calculated using density functional theory (DFT/B3LYP: Becke, 3-parameter, Lee-Yang-Parr) and M06-2X (the highly parametrized, empirical exchange correlation function) quantum chemical methods with 6-311++G(d,p) basis set by Gaussian 09W software, for the first time. The assignments of the vibrational frequencies have been carried out by potential energy distribution (PED) analysis by using VEDA 4 software. The theoretical optimized geometric parameters and vibrational frequencies were in good agreement with the corresponding experimental data, and with the results in the literature. ^{1}H and ^{13}C NMR chemical shifts were calculated by using the gauge-invariant atomic orbital (GIAO) method. The electronic properties, such as excitation energies, oscillator strength wavelengths were performed by B3LYP methods. In addition, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) energies and the other related molecular energy values have been calculated and depicted.

Keywords: FT-IR spectra; Laser-Raman spectra; Vibrational study; Methylthiophene

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