Synthesis, investigation of NMR spectra, X-ray crystal structure, vibrational, frontier molecular orbital properties, NLO behaviour and NBO charecteristics of 2-((2-aminopyridine-3-yl) methylene)-N-ethyl hydrazinecarbothioamide using spectroscopic and DFT methods

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ABSTRACT

2-((2-aminopyridine-3-yl) methylene)-N-ethyl hydrazinecarbothioamide was synthesized. It was characterized by, making elemental analysis and recording ^{1}HNMR, ^{13}CNMR, FT-Raman (4000-50 cm^{-1}), FT-IR (4000-400 cm^{-1}), and UV-Vis (200-400 nm) spectra. Crystal and molecular structure of the molecule was determined by means of X-ray diffractometry, which showed that it belongs to triclinic crystal system, with space group P-1, having two molecules per unit cell (z = 2). The dimensions of the unit cell are a = 6.0960(6) Å, b = 7.4119(8)Å, c = 11.9959(13) Å, α = 82.1695(4)°, β = 81.6407(4)°, γ = 88.3283(4)° at 100˚ K. Quantum chemical computations were made using density functional theory (DFT), B3LYP functional and 6-311++G(d,p) basis set in order to determine optimized structure parameters, general valence force field, harmonic vibrational frequencies, potential energy distribution, infrared intensities, NLO properties, frontier molecular orbital parameters, NBO characteristics, and its time-dependent variant (TD-DFT) was used to estimate ^{1}H and ^{13}C NMR chemical shifts employing gauge including atomic orbitals (GIAO) approach in DMSO-d_6 as solvent at room temperature. Similarly, TD-DFT was used to calculate the energy oscillator strength and absorption maxima (λ_{max}) in DMSO-d_6 as solvent, of different electron transitions. There was a good agreement between the theoretical and experimental parameters such as molecular structure parameters, NMR chemical shifts and IR, Raman and

UV-Vis spectra. The rms error between measured and estimated frequencies was 6.9 cm^{-1}. The calculations show that the molecule under investigation was good for NLO applications, which was supported by NBO analysis.

Keywords: Crystal structure; Vibrational spectra; NMR; Raman; Homo-Lumo; UV-Vis spectra; DFT.