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Normal Coordinate Analysis, Molecular Structure, Vibrational, Electronic Spectra, and NMR Investigation of 4-Amino-3-Phenyl-1H-1,2,4-Triazole-5(4H)-Thione by Ab Initio HF and DFT Method

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Abstract : In the present work, the characterization of 4-Amino-3-phenyl-1H-1,2,4-triazole-5(4H)-thione (APTT) molecule was carried out by quantum chemical method and vibrational spectral techniques. The FT-IR (4000–400 cm_1) and FT-Raman (4000–100 cm_1) spectra of APTT were recorded in solid phase. The UV–Vis absorption spectrum of the APTT was recorded in the range of 200–400 nm. The molecular geometry, harmonic vibrational frequencies and bonding features of APTT in the ground state have been calculated by HF and DFT methods using 6-311++G(d,p) basis set. The complete vibrational frequency assignments were made by normal coordinate analysis (NCA) following the scaled quantum mechanical force field methodology (SQMF). The molecular stability and bond strength were investigated by applying the natural bond orbital analysis (NBO) and natural localized molecular orbital (NLMO) analysis. The electronic properties, such as excitation energies, absorption wavelength, HOMO and LUMO energies were performed by time depended DFT (TD-DFT) approach. The 1H and 13C nuclear magnetic resonance chemical shift of the molecule were calculated using the gauge-including atomic orbital (GIAO) method and compared with experimental results. Finally, the calculation results were analyzed to simulate infrared, FT-Raman and UV spectra of the title compound which shows better agreement with observed spectra.

Keywords : 4-amino-3-phenyl-1H-1,2,4-triazole-5(4H)-thione, vibrational assignments, normal coordinate analysis, quantum mechanical calculations
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