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FT-IR, UV/Vis and Fluorescence spectra studies and Quantum Chemical Calculations on 3-Amino-5-(4-fluorophenyl)isoxazole

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Abstract

*In this investigation, the molecular structural properties of 3-Amino-5-(4-fluorophenyl) isoxazole (3AFPI) have been verified experimentally by using FT-IR (400-4000 cm^{-1}), UV-Visible (300-1100 nm) and Fluorescence spectroscopies. Furthermore, the experimentally obtained values were compared with theoretically calculated values of 3AFPI by using DFT/B3LYP/6-311++G** method. Thereafter, the least energy and more stable conformation of the investigated molecule were calculated by using potential energy surface (PES) scan method. Stabilization energy of the molecule, charge transfer within the molecule and hyperconjugative structure of the molecule was calculated by using natural bonding orbital (NBO) analysis. The non-linear optical (NLO) performance of the molecule was examined by calculating the polarizability (α), hyperpolarizability (β), and dipole moment (D) values of the titled molecule and results were compared with standard compound Urea. According to Koopman's theorem, Ionization potential and Electron affinity of the molecule was calculated by using frontier molecular orbital analysis. Molecular electrostatic potential (MEP) map analysis of the tiled compound have been calculated and analysed. All theoretical values were compared with experimental results by which a good agreement was obtained.*

Keywords: 3-Amino-5-(4-fluorophenyl) isoxazole, NBO, NLO, MEP, IP, EA.

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