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Quantum chemical studies and spectroscopic investigations on 22-amino-3-methyl-5-nitropyridine by density functional theory(Article)(Open Access)

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Abstract

Quantum chemical calculations on energy and molecular structure of 2-amino-3-methyl-5-nitropyridine (2A3M5NP) have been attempted by implementing DFT/B3LYP method using 6-311G (d,p), 6-311G++ (d,p) and cc-pVTZ basis sets. The optimized geometry and the vibrational analysis for energetically most stable configuration, are carried out theoretically by using B3LYP/cc-pVTZ basis set. The computed vibrational frequencies were scaled by using scaling factors and compared with the experimental Fourier Transform Infra-Red (FTIR) solid phase spectrum in the region 4000-400 cm^{-1} and FT-Raman spectrum in the region 4000-100 cm^{-1}. The complete vibrational assignments, analysis and correlation of fundamental modes of the compound have been carried out using the potential energy distribution (PED). The intramolecular charge transfer, hyperconjugative interaction of the compound is investigated from natural bonding orbital (NBO) analysis. The UV-Visible spectrum of 2A3M5NP was obtained with ethanol as a solvent. The electronic properties such as HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) energies are determined by B3LYP/cc-pVTZ basis set. The electronic absorption spectrum of the compound was studied from UV-Visible analysis by using time-dependent density functional theory (TD-DFT). The electron density distribution and chemical reactive sites of 2A3M5NP were analyzed from molecular electrostatic potential (MEP) analysis and frontier molecular orbital (FMO) analysis. © 2019

Author keywords

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