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Vibrational Spectroscopic and Structural Investigations of 2-Amino-6-Methoxy-3-Nitropyridine: a DFT Approach

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Abstract

The conformational analysis of 2-amino-6-methoxy-3-nitropyridine molecule (AMNP) has been carriedout using density functional theory calculations. The vibra-tional spectra of the molecule is simulated theoretically andcompared experimentally, and the vibrational frequencies areassigned on the basis of potential energy distribution calcula-tions. Electronic properties of the molecule derived from thetheoretical ultraviolet–visible spectrum are validated experi-mentally. The higher non-linear optical activity of the mole-cule is indicated in the first-order hyperpolarizability calcula-tions. The natural bond orbital and Mulliken atomic chargedistribution analysis confirm intramolecular charge transfersand intramolecular interactions. The Frontier molecular or-bitals are plotted, and the related molecular properties are cal-culated and discussed. The molecular electrostatic potentialcontour map is simulated. As the presence of intramolecularinteractions and the associated charge transfers between thepyridine ring of AMNP molecule and the lone pair of oxygenis a common molecular feature of a pharmaceutical com-pound, this investigation paves the way for its possible bio-medical applications. Further, the considerably higher non-linear optical (NLO) activity of the molecule identified sug-gests its potential applications in the design of new opticalmaterials.

Keywords

2-Amino-6-methoxy-3-nitropyridine, Vibrational spectral analysis, UV–vis spectral analysis, Density functional theory studies, Natural bond orbitalanalysis, Frontier molecular orbitals analysis.