



Contents lists available at ScienceDirect

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy

journal homepage: www.elsevier.com/locate/saa

Synthesis, molecular conformation, vibrational and electronic transition, isometric chemical shift, polarizability and hyperpolarizability analysis of 3-(4-Methoxy-phenyl)-2-(4-nitro-phenyl)-acrylonitrile: A combined experimental and theoretical analysis

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ARTICLE INFO

Article history:

Received 16 March 2011

Received in revised form 18 July 2011

Accepted 21 July 2011

Keywords:

FT-IR

UV–vis

¹³C and ¹H NMR

NLO

DFT

ABSTRACT

This work presents the synthesis and characterization of a novel compound, 3-(4-Methoxy-phenyl)-2-(4-nitro-phenyl)-acrylonitrile (abbreviated as 3-(4MP)-2-(4-NP)-AN, C₁₆H₁₂N₂O₃). The spectroscopic properties of the compound were examined by FT-IR, UV–vis and NMR (¹H and ¹³C) techniques. FT-IR spectrum in solid state was observed in the region 4000–400 cm⁻¹. The UV–vis absorption spectrum of the compound which dissolved in chloroform was recorded in the range of 200–800 nm. The ¹H and ¹³C NMR spectra were recorded in CDCl₃ solution. To determine lowest-energy molecular conformation of the title molecule, the selected torsion angle is varied every 10° and molecular energy profile is calculated from 0° to 360°. The structural and spectroscopic data of the molecule in the ground state were calculated using density functional theory (DFT) employing B3LYP/6-31G(d,p) basis set. The dipole moment, linear polarizability and first hyperpolarizability values were also computed using the same basis set. A study on the electronic properties, such as HOMO and LUMO energies, were performed by time-dependent DFT (TD-DFT) approach. The HOMO and LUMO analysis were used to elucidate information regarding charge transfer within the molecule. The vibrational wavenumbers were calculated and scaled values were compared with experimental FT-IR spectrum. The complete assignments were performed on the basis of the experimental results and total energy distribution (TED) of the vibrational modes, calculated with scaled quantum mechanics (SQM) method. Isotropic chemical shifts were calculated using the gauge-invariant atomic orbital (GIAO) method. Comparison of the calculated frequencies, NMR chemical shifts, absorption wavelengths with the experimental values revealed that DFT and TD-DFT method produce good results. The linear polarizabilities and first hyperpolarizabilities of the studied molecule indicate that the title compound can be used as a good nonlinear optical material. The thermodynamic properties of the studied compound at different temperatures were calculated, revealing the correlations between standard heat capacity, standard entropy, standard enthalpy changes and temperatures.

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