



# 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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## 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-(4NP)-AN, C<sub>16</sub>H<sub>12</sub>N<sub>2</sub>O<sub>3</sub>). The spectroscopic properties of the compound were examined by FT-IR, UV–vis and NMR (<sup>1</sup>H and <sup>13</sup>C) techniques. FT-IR spectrum in solid state was observed in the region 4000–400 cm<sup>-1</sup>. The UV–vis absorption spectrum of the compound which dissolved in chloroform was recorded in the range of 200–800 nm. The <sup>1</sup>H and <sup>13</sup>C NMR spectra were recorded in CDCl<sub>3</sub> 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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## 1. Introduction

Organic photochromic compounds having donor and acceptor parts that are conjugated are potential optical materials. Donor–acceptor (D–π–A) dyestuff and colorants represent a vast majority of organic chromogens. Such compounds have found many applications such as in dyeing of fabric, coloring of toners, and in image forming and optical information storage technolo-

gies. Some of these compounds are also used as sources of tunable (dye laser) radiation [1–3].

Theoretical investigations can facilitate the solution to the problems confronted in the experimental techniques, i.e. allowing the determination of molecular properties. The calculations based on DFT have been applied in many areas, and the results also are in great agreement with the experimental ones in calculating spectroscopic properties [4–6]. The calculated harmonic frequencies are usually higher than the corresponding experimental quantities, due to a combination of electron correlation effects and basis set deficiencies. DFT calculations are reported to provide excellent vibrational frequencies of organic compounds if the calculated

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