International Journal of Research in Engineering and Science (IJRES)
ISSN (Online): 2320-9364, ISSN (Print): 2320-9356
www.ijres.org Volume 11 Issue 7 ǁ July 2023 ǁ PP. 419-421

Spectroscopic and electro-optical properties of 4-(5-Pentylpyrimidin-2-yl) benzonitrile molecule: A DFT study

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Abstract
In this article, I have attempted to obtain optimized geometry and calculate the IR and Raman vibration frequencies of ***4-(5-Pentylpyrimidin-2-yl) benzonitrile*** *liquid crystals using the DFT/B3LYP method with the base set 6-311G(d,p). The molecules selected for the present investigation are quite interesting because they show excellent chemical and thermal stability due to the strong and unique physical properties of the C–N bond, which contributes to the performance and photonic applications.*

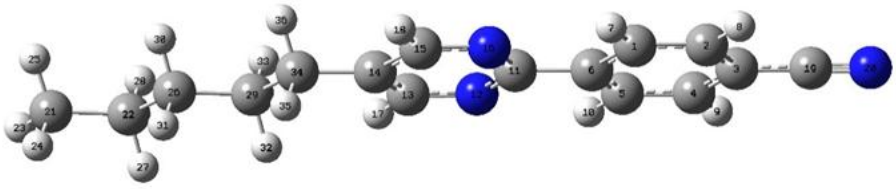

Figure1. Optimized geometry of 4-(5-Pentylpyrimidin-2-yl)benzonitrile molecule.

Keywords: *liquid crystal, IR, Raman, DFT*

I. Introduction

Liquid crystal is an intermediate phase of matter (between isotropic liquid and crystal). These molecules were originally discovered in the chemical and biological systems. For a long time, liquid Crystals (LCs) have been the subject of theoretical and experimental study. By their role in the chemical, biological, and electro-optical systems, they have many industrial applications. Liquid crystals are powerful solvents in holding donor-spacer-acceptor systems as well as in maintaining the fluid and order property over a wide range of temperatures too. Numerous electronic and optical properties of LC vary with the change of substituent. These properties of molecules can be altered by the presence of different substituents. LC molecules have a dipole moment directly perpendicular to the molecular axis [1-5].

The liquid-crystal properties of organic compounds are extremely sensitive to changes in the chemical structure of the molecule. There have been many publications in which changes in the aromatic ring system have been shown not only to lower the lower limit of mesophase survival and to increase thermal stability, and also the criteria governing the type of mesophase established.

In this regard, pyrimidine analogs of the diphenyl and terphenyl systems are of considerable interest [6-8], and have found practical application as components of liquid crystal materials in a variety of electro-optical devices [9-11]. The pyrimidine analogs of the diphenyl and terphenyl systems often extend the operating temperature range, reduce the operating voltage, and enable the material to obtain a lower viscosity-temperature relationship, for devices operating at below 0◌C temperatures [12].

The present report describes the energy, dipole moment, enthalpy, entropy, polarizability, hyperpolarizability, ionization potential, electron affinity, band gap, chemical potential, electronegativity, HOMO-LOMO, IR, and Raman spectra of 4-(5-Pentylpyrimidin-2-yl) benzonitrile molecule.

Computational Methodology

4-(5-Pentylpyrimidin-2-yl)benzonitrile molecules have been optimized with Computational Density Functional Theory (DFT) method using the B3LYP basis set which is a hybrid functional for Gaussian type orbitals (GTOs) and 6-311G basis set using NWChem software package [13-18]. Energy, dipole moment, global reactivity, IR, and Raman are computed using the same theory level.

II. Results and Discussion

A complete vibrational analysis of 4-(5-Pentylpyrimidin-2-yl) benzonitrile molecule liquid crystal molecules has been performed based on DFT/B3LYP/6-311G(d,p) quantum chemical calculations. Optimized structural parameters were used in the calculation of vibrational frequencies to characterize all stationary points as minimums. The IR and Raman spectra of 4-(5-Pentylpyrimidin-2-yl) benzonitrile liquid crystal molecules are shown by figures 2 and 3 respectively. The spectroscopic properties of a molecule like 4-(5-Pentylpyrimidin-2-yl)benzonitrile can provide valuable information about its structure, chemical bonds, and electronic transitions. While I don't have access to a specific database to provide precise values, I can give you an overview of the types of spectroscopic techniques that could be used to study this molecule:

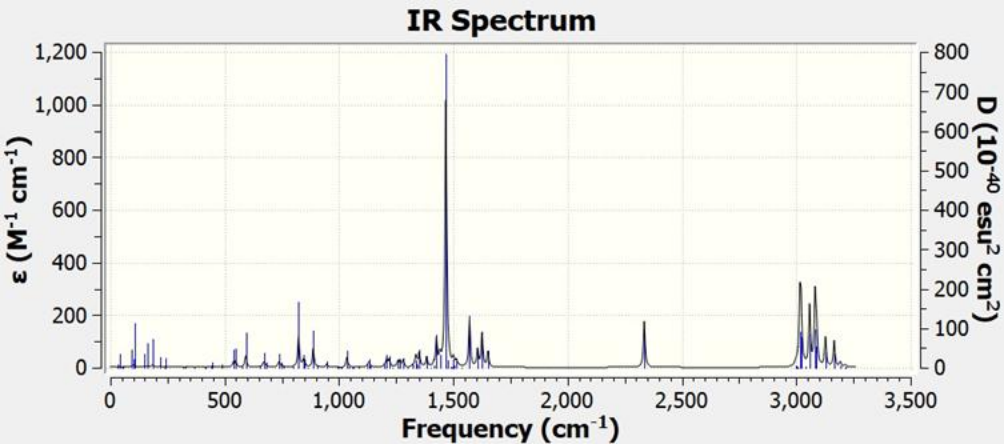

Figure 2: IR spectrum of 4-(5-Pentylpyrimidin-2-yl)benzonitrile molecule.

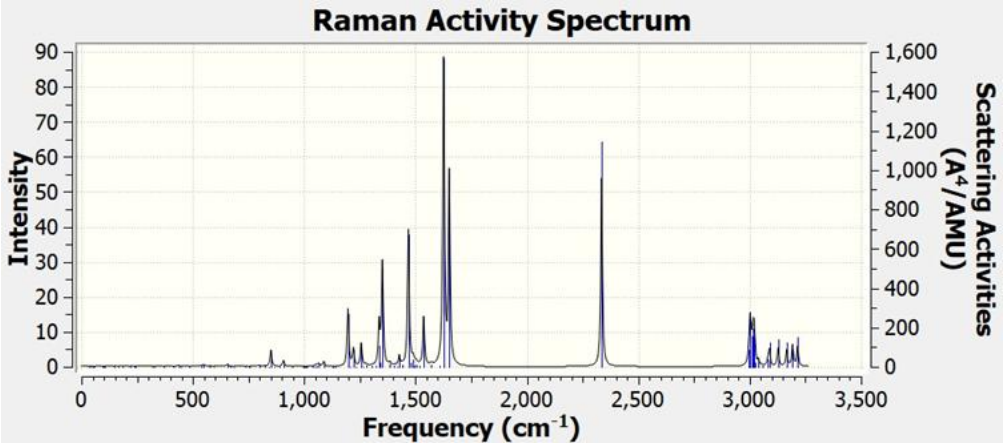

Figure 3: Raman spectrum of 4-(5-Pentylpyrimidin-2-yl)benzonitrile molecule.

Table 1: Global reactivity parameters of 4-(5-Pentylpyrimidin-2-yl)benzonitrile molecule.

Global reactivity parameters (in eV)	
HOMO	-6.90226
LUMO	-2.22099
E_g	4.681264
μ	-4.56163
η	2.340632
S	0.213618

ω	4.445046
ΔN_{max}	1.948887

III. Conclusion

IR spectroscopy can provide information about the functional groups present in the molecule. For example, the nitrile group (-CN) would show characteristic stretching vibrations in the IR spectrum, typically around 2200-2300 cm^{-1}. The presence of functional groups like the nitrile group (-CN) and the aromatic rings (benzene and pyrimidine) suggests potential sites for chemical reactions. For example, the nitrile group can participate in nucleophilic addition reactions, while the aromatic rings can undergo electrophilic aromatic substitution reactions. The IR peaks and Raman activities peaks were explained.

Acknowledgment

The authors are very thankful to Dr. Devendra singh, Dept. of Physics, BBAU, Lucknow for providing computational and scientific discussion.

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