Molecular Spectroscopy of 4 Nitroso Benzonitrile Liquid Crystal Molecule Studied by DFT Methodology

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Abstract

In the present work, the spectroscopic properties of 4-nitroso benzonitrile are studied. The different modes of vibration in this molecule are studied from the IR spectrum. Here, due to the C-N group, the molecule shows different types of vibration at different frequencies. In the IR spectra of the molecule, the frequencies are found at 2338 cm^{-1} (stretching in C-N atom), 1630 cm^{-1} (scissoring in C-H atom), 1536 cm^{-1} (rocking in C-H atom), 3241 cm^{-1} (stretching in C-H atom) associated with different type of vibration of the molecule. The dipole moment of 4-nitroso benzonitrile is found to be 0.6197 debye and HOMO-LUMO gap is 0.11049. This molecule is useful in biological and medicinal purposes.

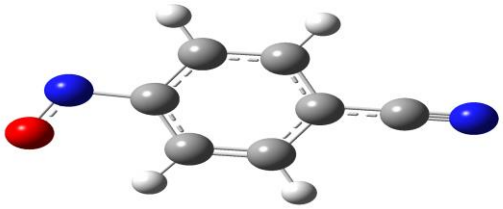

Fig 1. Molecular structure of 4-nitroso benzonitrile

Introduction

4- nitroso benzonitrile is useful in liquid crystal display devices as it contains substituent in ortho and para positions of the benzene ring. The organic molecules have lower value of refractive indices as compared to inorganic molecules. The presence of weak bonds in 4 nitroso benzonitrile makes it more reliable for telecommunication purposes. The extent of charge delocalization helps in getting high value of conversion efficiency [1]. In organic synthesis, nitroso compounds act as synthetic building blocks and are capable in the formation of natural product like molecules. The N-O group in 4 nitroso benzonitrile act as a directing group. A selective C-N cleavage reaction helps in the formation of nitroso compounds [2]. The aromatic nitriles are polar in nature and hence they act as polar narcotics. Due to the inductive effect of the substituent at the ortho position, these nitriles show narcotic behavior. Also, the halogenated derivatives show toxicity up to some extent due to the steric hinderance and polarity of nitrile group [3]. In many biological and medicinal applications, the nitroso compounds are widely preferred. The nitroso compounds are classified in different groups like C-nitroso, O- nitroso and this classification is dependent on the type of atom attached to N-O group [4]. Another method of formation of benzonitrile is from the pyrolysis of different nitrosobenzene at a temperature above 700^0C. The major part of a benzonitrile consists of nitrogen and for greater benzonitrile conversions the thermolysis of methyl aniline is utilized [5]. In liquid crystal display devices, lamellar smectic A phase are extensively used over the nematic phase. This leads to lower value of power consumption as there is no need of backlight as in case of nematics. Under the application of fields, the material showing superior behavior is highly required [6]. The charge transfer abilities of aromatic nitrile are weak and the stretching vibration of N-O bond occurs at higher frequency. The benzonitrile at high intensity exhibit absorption band [7]. A technique known as solvent crystallization is used to separate benzonitrile from crude organic compounds. It is due to the reason that solubility is the most basic thermodynamic property [8].

Computational methodology

4 nitroso benzonitrile liquid crystal molecule have been optimized with Computational Density-Functional -Theory (DFT) method using B3LYP basis set which is a hybrid functional for Gaussian type orbitals (GTOs) and 3-21g basis set using NWChem software package [9-16].

Results and discussion

In the present work, 4-nitroso benzonitrile liquid crystal molecule have been optimized computationally and the spectroscopic properties like IR and Raman spectra of the molecule are figured out. The IR and Raman spectra of the molecule are shown in Fig. 2 and 3 respectively. At the frequency 2338 cm^{-1}, this molecule shows C-N stretching which is found in IR spectra of the molecule. The 4-nitroso benzonitrile shows symmetric stretching in benzene at 822 cm^{-1}. This peak appears in IR spectra of the molecule. At the frequency 1096 cm^{-1}, molecule shows asymmetric stretching in benzene ring in between C-C atom which is also found in IR spectrum of the

molecule. The molecule shows rocking in the C-H bond at the frequency 1536 cm^{-1} and at the frequency 1630 cm^{-1}, the molecule shows the scissoring in C-H bond. At maximum frequency 3241 cm^{-1}, the molecule shows stretching in C-H atom.

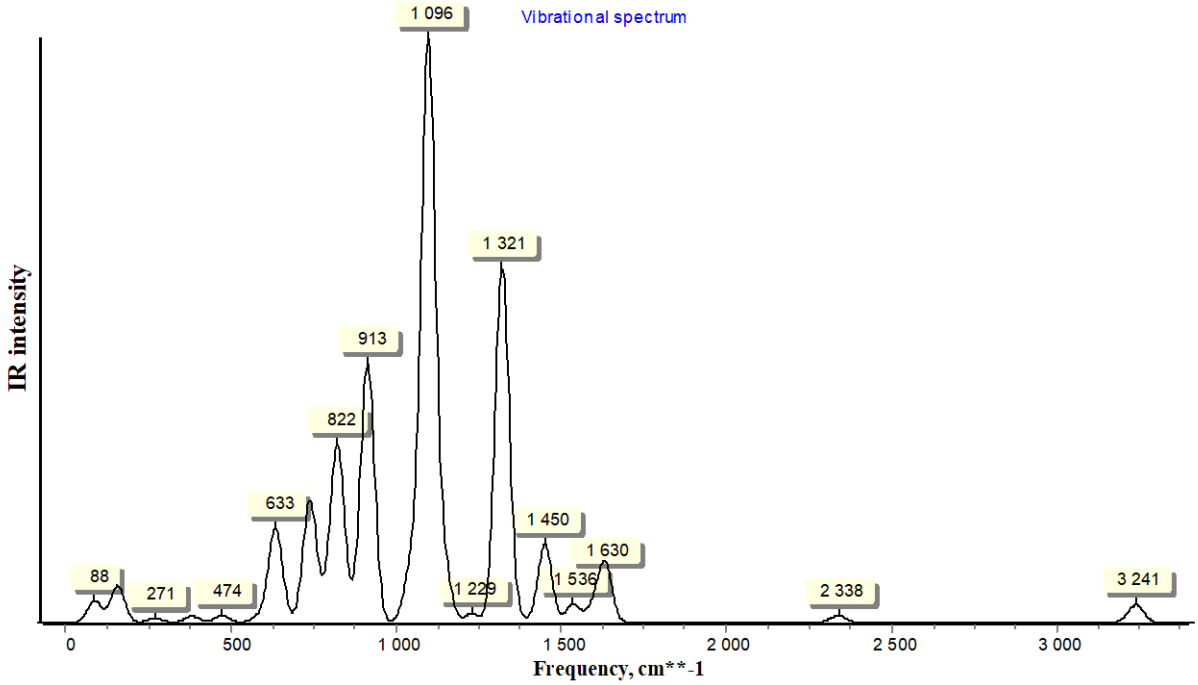

Fig. 2 IR activity of 4-nitroso benzonitrile molecule

Table 1. Molecular stretching of 4-nitroso benzonitrile liquid crystal

S.No.	Frequency(cm^{-1})	Modes of Vibration
1.	88	C-H atom wagging in benzene ring
2.	271	Scissoring in N-O bond attached to the benzene ring
3.	474	Twisting in C-H bond of benzene ring
4.	633	Twisting in C-H bond of benzene ring
5.	822	C-C atom stretching in benzene ring
6.	913	C-H atom wagging in benzene ring
7.	1096	C-C atom asymmetric stretching in the benzene ring
8.	1229	C-H atom scissoring in benzene ring
9.	1321	Stretching in N-O atom
10.	1450	C-H atom scissoring in benzene ring
11.	1536	Rocking in C-H bond
12.	1630	C-H atom scissoring in benzene ring
13.	2338	Stretching in C-N atom
14.	3241	Stretching in C-H atom

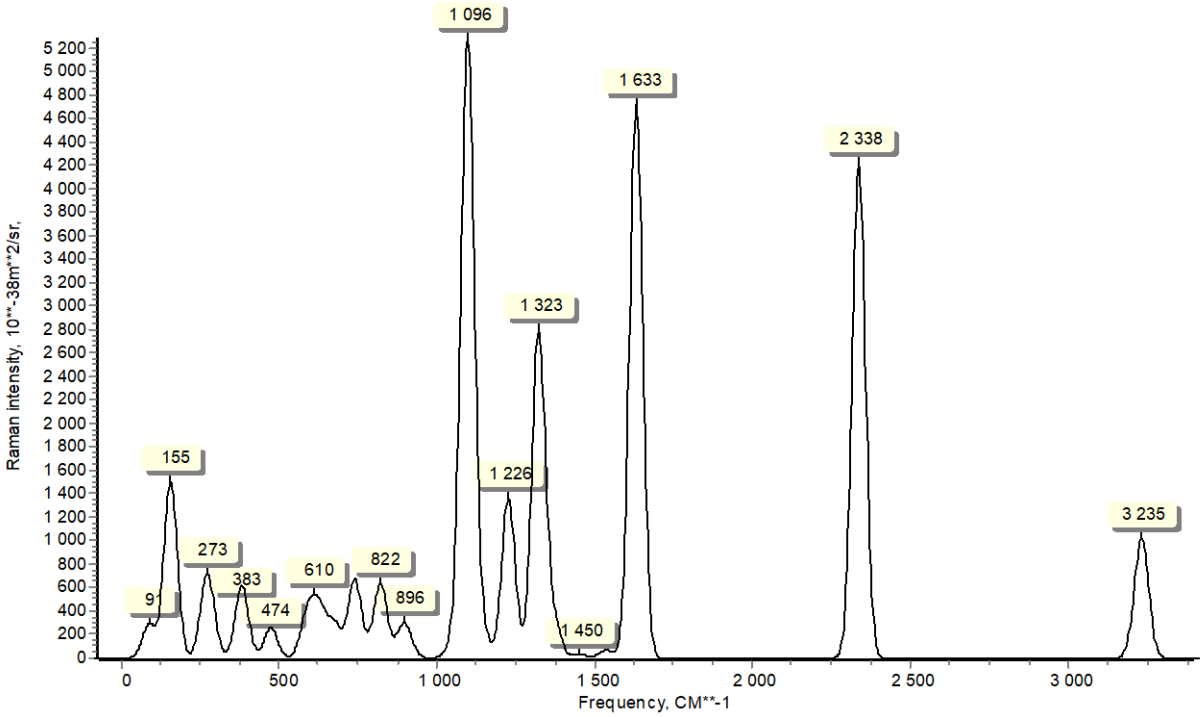

Fig. 3 Raman activity of 4-nitroso benzonitrile molecule

Conclusion

The stretching in C-N atom at the frequency of 2338 cm^{-1} makes 4-nitroso benzonitrile liquid crystal molecule potent enough be used in biological and medicinal purposes. This frequency is found in both the spectrum.

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