

Study of Molecular Spectroscopy of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine Molecule using Density Functional Theory

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Abstract

The present article deals with IR and Raman spectroscopy of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule. Density functional calculations were carried out at the B3LYP/6-311++G(D,P) level to study the equilibrium geometry and vibrational spectra of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine. The calculated vibrational spectra were analyzed based on the potential energy distribution of each vibrational mode, allowing us to obtain quantitative as well as qualitative interpretations of the IR and Raman spectra.

Keywords: 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine, NLO, IR, Raman, DFT

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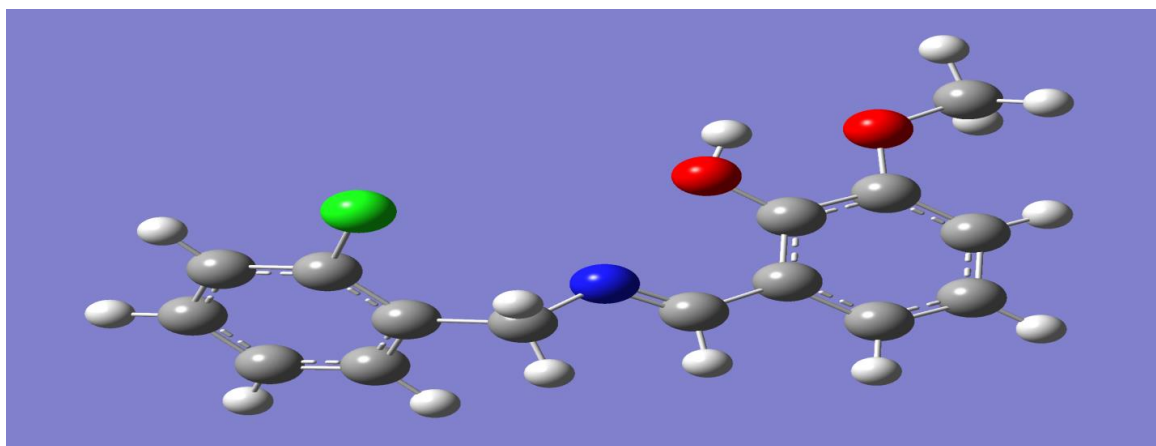


Figure1. Molecular geometry of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule.

I. Introduction

Non-linear optical materials have attracted great interest in recent years because of their future potential applications in the fields of photonics and optoelectronics, such as optical computing, optical data storage, optical switching and dynamic image processing. The superiority of organic NLO materials results from their versatility and the possibility to prepare them for a particular device application [1-3]. Organic NLO materials have higher nonlinear figure-of-merit for frequency conversion, higher laser damage threshold and faster optical response times than inorganic NLO materials. The structure of organic NLO materials is based on a large length-scale extended pi-bond system of the molecule, which can be very easily manipulated by electron donating substituents and electron withdrawing groups around the aromatic moieties, leading to an increased optical non-linearity. Substituted benzyl derivatives with high optical non-linearity are very promising materials for future optoelectronic and nonlinear optical applications. 2-hydroxy-3-Methoxy-N-(2-chloro-benzyl)-benzaldehydeimine is a promising non-linear organic crystal. Vibrational spectroscopy is an advantageous analytical tool to provide information about the structure, composition, structure and intramolecular interactions of complex molecules [3-5]. It can also provide important information on the relationship between molecular architecture and non-linear reactivity/hyperpolarizability [5-7]. IR spectroscopy offers the possibility to measure

different types of inter-atomic bond vibrations at different frequencies, whereas Raman spectroscopy uses inefficient scattering of light to analyze both the vibrational and rotational modes of molecules [7-11]. Thus, vibrational spectroscopy has become an effective tool to elucidate the molecular structure, the nature of chemical bonds, and the intramolecular forces acting between atoms in a molecule. It has been shown that the hyperpolarizability is related to the intensity of the infrared and Raman vibrational modes in these systems. We have calculated, the harmonic vibrational wave number, the absolute Raman scattering activities and the infrared absorption intensity by DFT with the B3LYP functional extended basis set 6-311++G(d,p).

Computational Methodology

The entire calculation was performed on density functional theory using the Gaussian 09 program, applying gradient geometry optimization was performed using Becke's three-parameter hybrid functional, a combination that gives rise to the well-known B3LYP method. The 6-311++ g(d,p) extended basis set was used, augmented by d polarization functions on heavy atoms and p polarization functions on hydrogen atoms, as well as dispersive functions for both hydrogen and heavy atoms. The absolute Raman scattering and infrared absorption intensities were calculated from the derivatives of the polarization and dipole moment associated with each common mode, respectively. Calculations were performed within the harmonic approximation at the same level of theory as that used for optimized geometry.

II. Results and Discussion

In the present work, 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule have been optimized computationally and spectroscopic properties like IR and Raman activity of the molecule are figured out. A complete vibrational analysis of the 93 fundamental vibrational modes of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine has been performed based on its experimental infrared and Raman spectra and DFT/B3LYP/6-311++G(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 spectrum of the 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine shown by figures 2 and 3 respectively. At the frequency of 1720 cm^{-1} , molecule shows the C-N stretching, which is found in IR spectrum of the molecules. The 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule shows asymmetric stretching in the benzene ring in between C-C atom at frequency 1270 cm^{-1} which is found in IR and Raman both spectrum. At frequency 1127 cm^{-1} , molecule shows stretching in between C-O atom which is also found in IR spectrum. The dipole moment and isotropic polarizability of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule are 4.095 debye and 216.11 bohr^3 respectively.

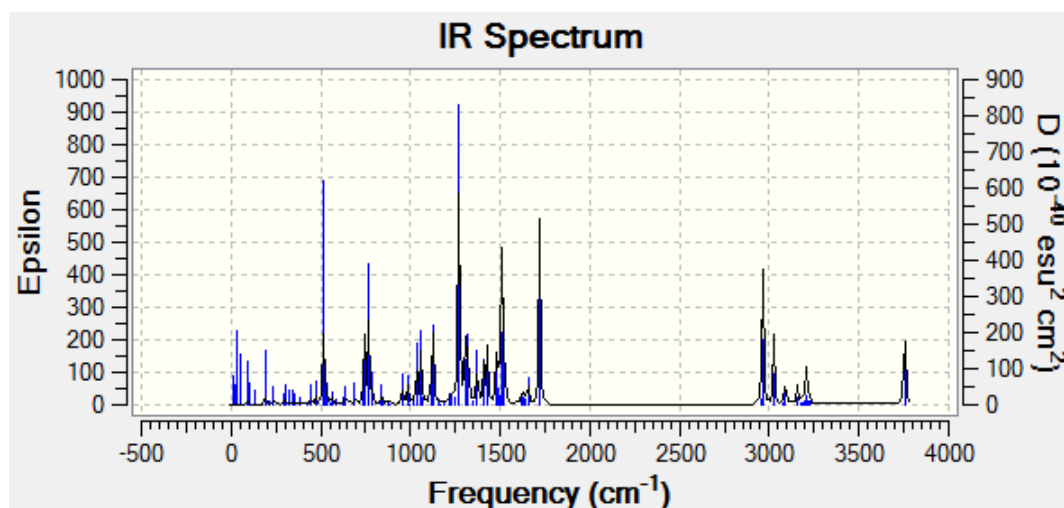


Figure 2: IR activity of the 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule

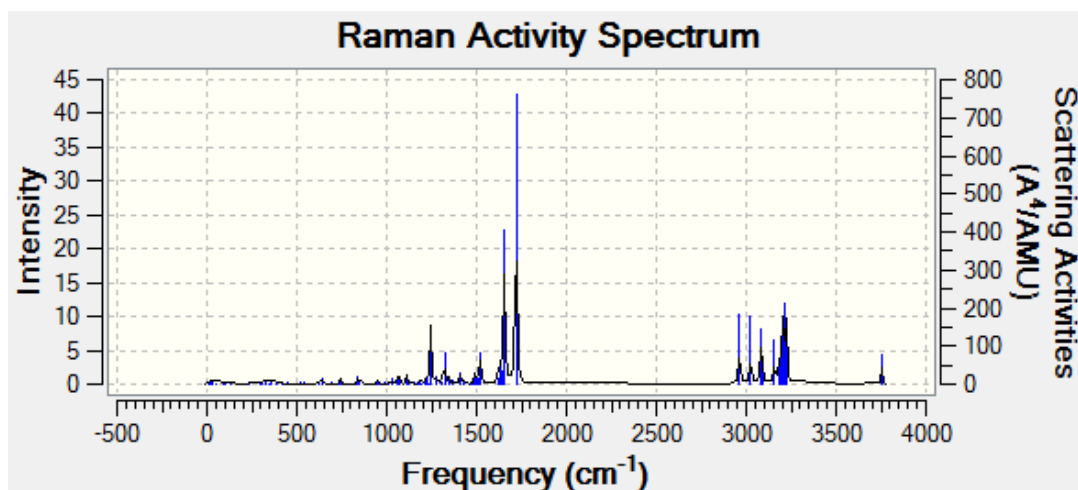


Figure 3: Raman activity of 2-hydroxy-3-methoxy-N-(2-chloro-benzyl)-benzaldehyde-imine molecule

III. Conclusion

The non-linear optical NLO behavior of the investigated molecule was investigated by the determination of the electric dipole moment, polarization and hyperpolarizability. The vibrational modes contributing toward the NLO activity have been identified and analyzed. The rather large hyperpolarizability obtained by theoretical calculations suggests a potential future use of this compound for non-linear optical applications. The IR peaks and Raman activities peaks were explained.

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