Vibrational spectra of 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole: anti viral & anti fungal

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ABSTRACT

5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole is a chemical compound of anti viral and anti fungal drug. Antifungal drugs work by exploiting differences between mammalian and fungal cells to kill the fungal organism with fewer adverse effects to the host and antiviral drugs is used specifically for treating viral infections.

The molecular geometry , molecular structure and vibrational spectra of 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole from X-ray determination of the compound in the ground state has been compared using the *Ab initio* Hartree−Fock and density functional theory (DFT) calculations using the 6-31G basis set. Vibrational spectra reveals that the B3LYP (Becke 3-Lee−Yang−Parr) calculations are quite accurate in predicting the vibrational frequencies, modes and also calculate raman, IR, & normal mod analysis. The calculated highest occupied molecular orbital and lowest unoccupied molecular orbital energies show that charge transfer occurs within the molecule. The lowering of highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap appears to be the cause of its enhanced charge transfer interaction.

KEYWORDS

DFT, HOMO, LUMO, Raman, IR, Vibrational spectra.

INTRODUCTION

Benzimidazole and its derivatives are known to possess antifungal and antiviral properties. They involved in a great variety of biological processes and are used as a procarcinogenic or mutagenic compound. They contain both the imidazole ring and a larger conjugated π system, capable of acting as hydrogen-bond donors and for π–π stacking interaction. Benzimidazoles have different activities. Almost all antifungal agents currently in use in human mycoses target the ergosterol biosynthetic pathway, an important component of fungal membranes. Many antiviral drugs are Purine or Pyrimidine analogs. Many antiviral drugs are Prodrugs. They must be phosphorylated by viral or cellular enzymes in order to become active. Anti-viral agents inhibits active replication so the viral growth resumes after drug removal.

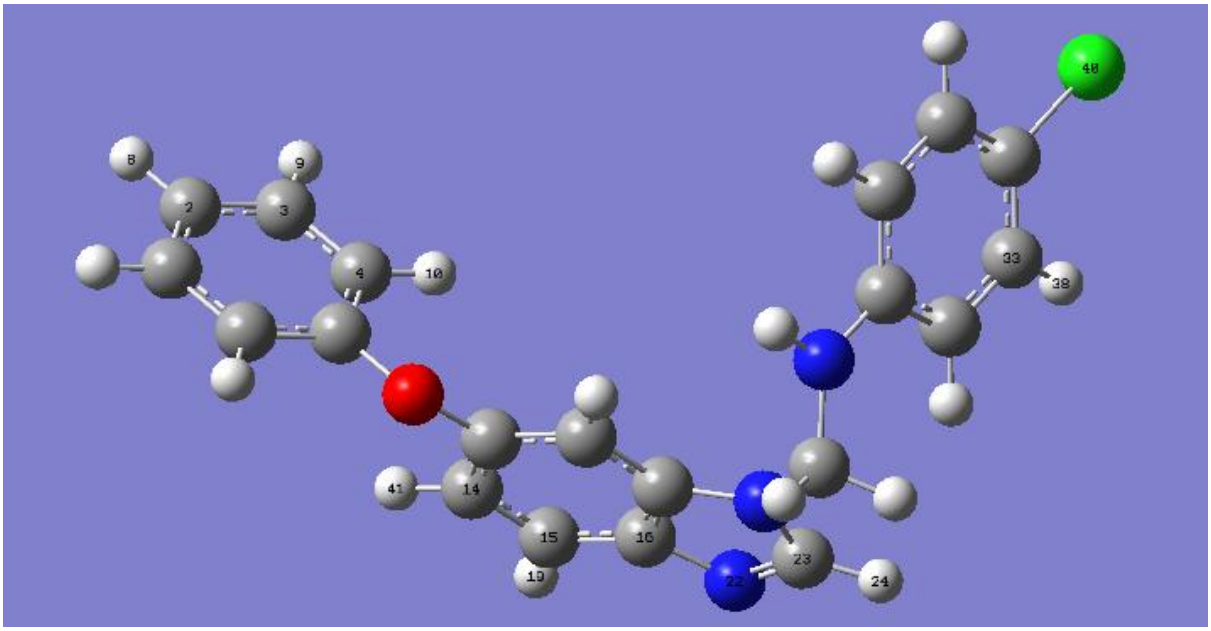
Vibrational spectroscopy is used extensively in organic chemistry for the identification of functional groups of organic compounds, for studies on molecular confirmation, the results based on quantum chemical calculations, HOMO-LUMO analysis on 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole have no reports. In the present work, we have attempted to study vibrational spectra and bonding nature of 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole by using B3LYP level of theory with the 6-31G basis set. The optimized geometry obtained from DFT calculation. DFT calculations are known to provide excellent vibrational wave numbers of organic

compound. In this work by using B3LYP methods we calculate the vibrational wave numbers of the title compound in the ground state to distinguish the fundamentals from many vibrational assignments and geometrical parameter. Quantum chemical calculations were used to carry out the optimized geometry and vibrational wave numbers.

The optimized structural parameters are used in the vibrational frequency calculations at DFT level. At the optimized geometry of the compound no imaginary frequency modes are obtained, so there is a true minimum potential energy surface is found. The assignments of the normal modes of vibration for the compound have been made by visual inspection of the individual mode using the Gauss. Finally the calculated normal mode vibrational frequencies provide atomic charges through the principle of statistical mechanics. A detailed description of vibrational modes can be given by means of normal coordinate analysis. Natural Bond Orbital analysis was also performed by the Gaussian 09 program. This transforms the canonical delocalized molecular orbital's into localized molecular orbital's that are closely tied to chemical bonding concepts. Harmonic vibrational wave numbers we are calculated using analytic second derivatives to confirm the convergence to minima on the potential surface. Then frequency calculations were employed to confirm the structure as minimum points in the energy. At the optimized structure of the examined species, no imaginary wave number modes were obtained, providing that a true minimum on the potential surface was found.

METHOD, MATERIAL & THEORY

Density functional theory (DFT) is a computational quantum mechanical modeling method used in physics, chemistry and material sciences. In the present contribution, the properties that can be calculated with DFT, such as geometries, energies, spectroscopic properties. Using this theory, the properties of a many-electron system can be determined by using functional, i.e. functions of another function, which in this case is the spatially dependent electron density. Hence the name density functional theory comes from the use of functional of the electron density.



Density functional theory (DFT) calculations have been performed to predict the IR and Raman spectra for the molecule. Fourier transform infrared (FTIR) and Raman spectra of the compound have been obtained experimentally. All FTIR and Raman bands of the compound obtained experimentally were assigned based on the modeling results obtained at the B3LYP/6-31G level. Normal coordinate analysis is the mathematical procedure that gives the normal coordinates, their frequencies and force

constant. The detailed description of vibrational mode can be given by mean of normal coordinate analysis. The internal coordinate describe the position of the atoms in terms of distance, angles and dihedral angles with respect to an origin atom.

Obtain the vibrational spectra and bonding nature of 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole by using B3LYP level of theory with the 6-31G basis set from the Density function theory method. Optimized geometric structure of 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole is given above-

BOND LENGTH AND BOND ANGLE-

The distance between the centers of two nuclei of atoms connected by a chemical bond is known as 'bond length'. The angle between the directions of two bonds in a molecule is called the 'bond angle'. Bond angle depend upon factors, charge distribution, geometry of the molecules, symmetry, etc. These optimized structural parameters were determined at B3LYP level theory with 6-31G basis set and are presented as-

BOND LENGTH	**DFT**	**BOND ANGLE**	**DFT**
C2-H8	1.084821	C3-H9-C2	34.133
C5-O12	1.40776	C5-C4-O12	28.635
C14-C15	1.39276	O12-C13-C5	29.180
C16-N22	1.40648	C17-N21-C18	23.739
C17-N21	1.39576	C25-H26-N21	41.732
N28-H29	1.00752	C32-C31-N28	122.476
Cl40-C34	1.82921	C30-C35-C34	119.201
O12-C13	1.40828	N22-C23-H24	125.163
N21-H26	2.09539	C16-N22-C23	104.993
N28-C31	1.39757	H38-C33-C32	120.043
N22-C23	1.31945	C18-C13-C14	122.567
C15-C16	1.39977	N28-C31-H29	25.831
C25-N28	1.43891	H26-N21-C23	135.330
C3-H9	1.08540	C6-C5-O12	115.925
		N21-C23-N22	113.405
		Cl40-C34-C35	119.340
		C33-C34-CL40	119.486

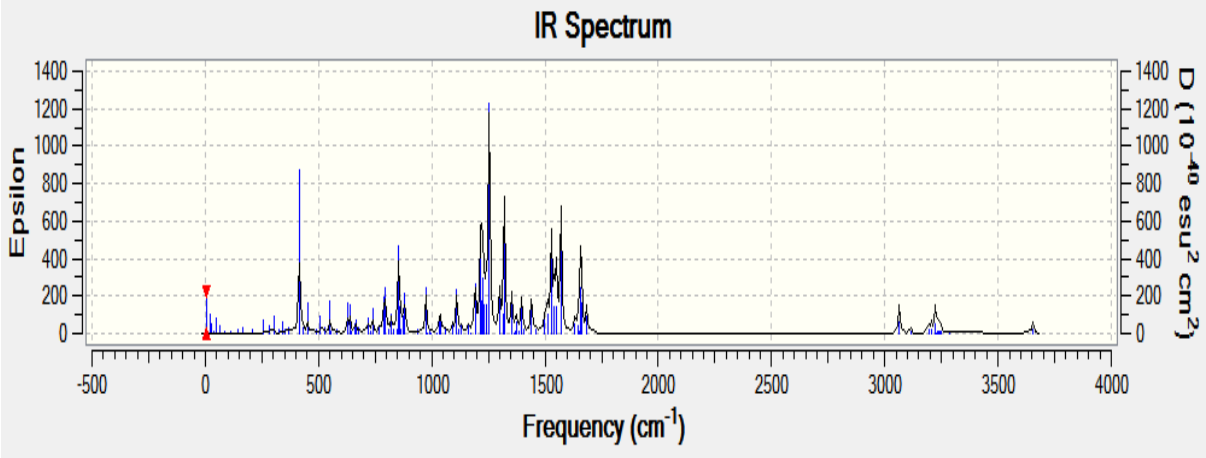
DIPOLE MOMENT-

When atoms in a molecule share electrons unequally, they create what is called a dipole moment. Dipole moment of the compound 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole is 3.8471debye.

(1 Debye equals 3.34×10−30Cm)

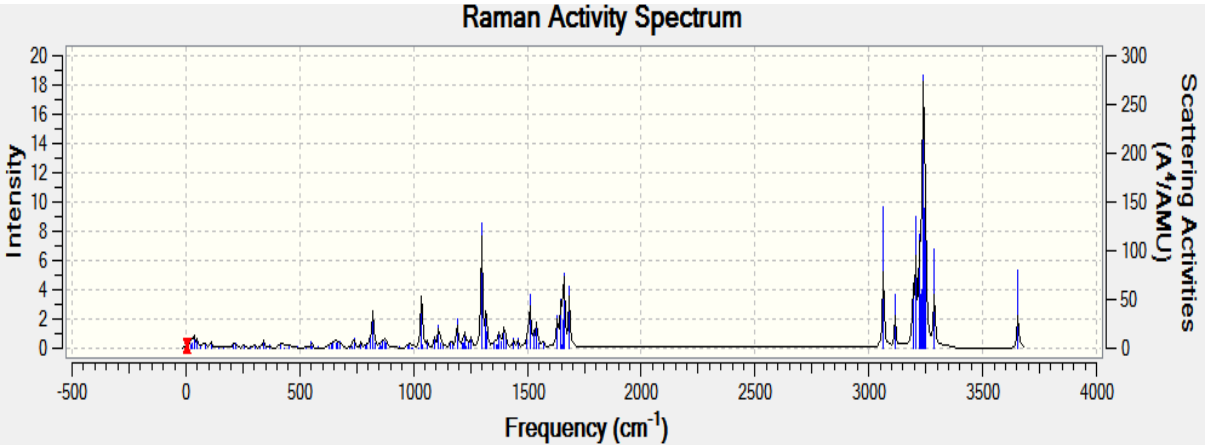
IR SPECTRA-

IR spectroscopy exploits the fact that molecules absorb frequencies that are characteristic of their structure. These absorptions occur at resonant frequencies I.e. the frequency of the absorbed radiation matches the vibration frequency.



RAMAN SPECTRA-

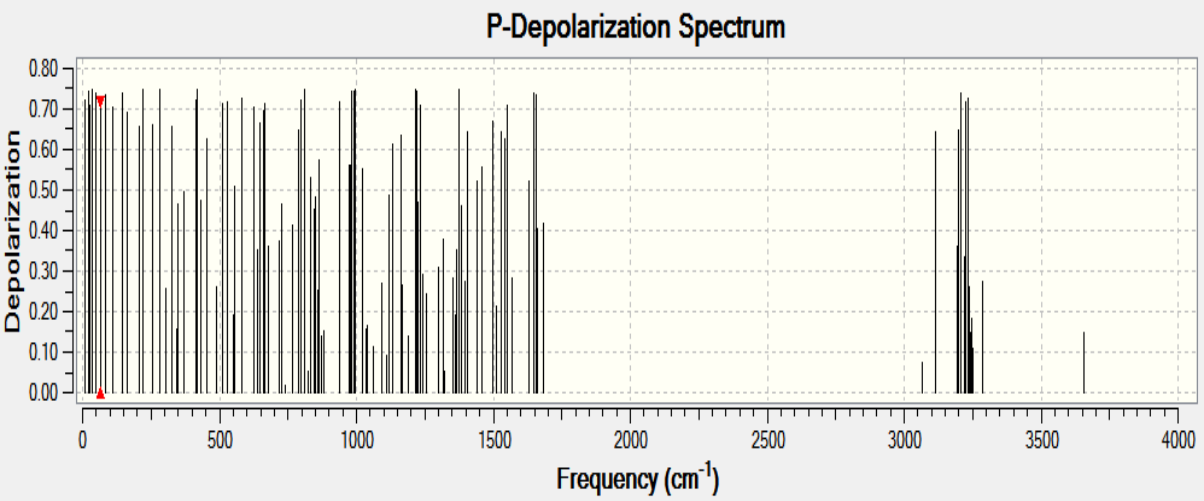
Raman spectroscopy used to observe vibrational and low frequency modes. The raman spectra is expressed in a form of intensity of a scattering light and wave number or frequency.

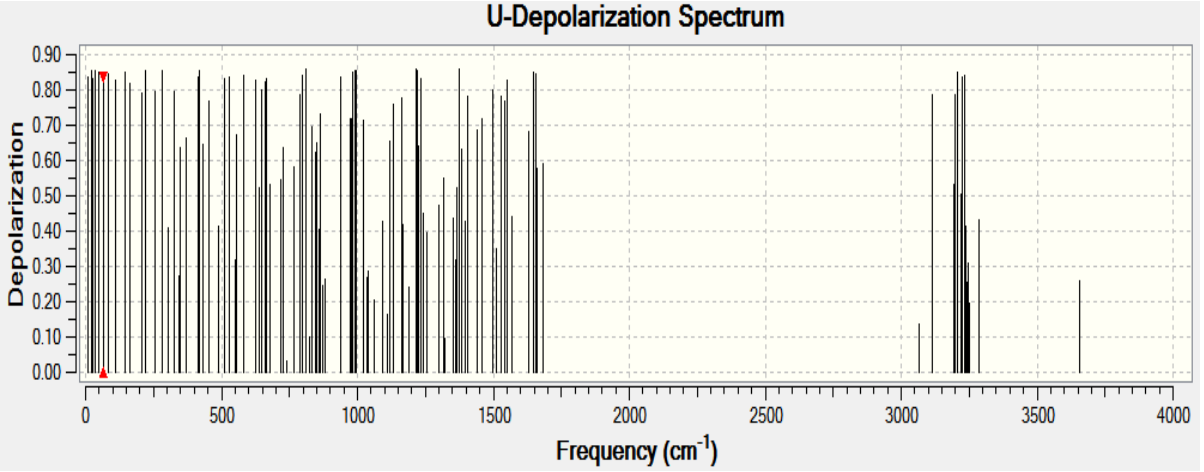


DEPOLARIZATION SPECTRA-

The depolarization ratio is the intensity ratio between the perpendicular component and the parallel component of the raman scattered light. Two type of polarization occur i.e. p- polarization and u-polarization.

The optimised spectra of p-depolarization and u-depolarization is shown in the figure-





MOLECULAR ORBITAL ENERGIES-

HOMO and LUMO are type of molecular orbital. HOMO stand for highest occupied molecular orbital and LUMO stand for lowest unoccupied molecular orbital. The energy difference between the HOMO and LUMO is known as HOMO-LUMO Gap.

HOMO is most available for bonding and most weak held electrons. The electrons of the HOMO are donated and characteristic for nucleophilic component.LUMO receives electrons and lowest energy orbital available. And also characteristic for electrophilic component.

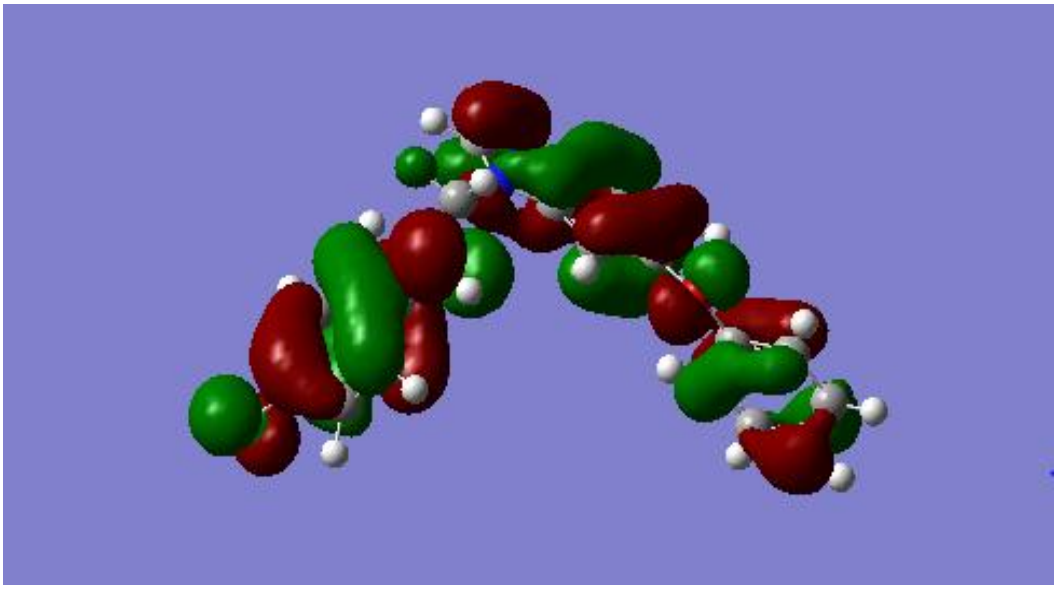
The HOMO of π nature, are well localized within the ring. By contrast, LUMO of π* nature is delocalized over the entire part of the molecule. Consequently HOMO → LUMO transition implies an energy transfer from the aromatic heterocyclic ring. The energy gap between HOMO and LUMO has been used to prove the bioactivity from intramolecular charge transfer [45]. The energy gap measures the kinetic stability of the molecules. A molecule with a small frontier orbital gap is more polarizable and it implies high chemical reactivity and low kinetic stability.

The HOMO and LUMO energy calculated by B3LYP /6-31G method -

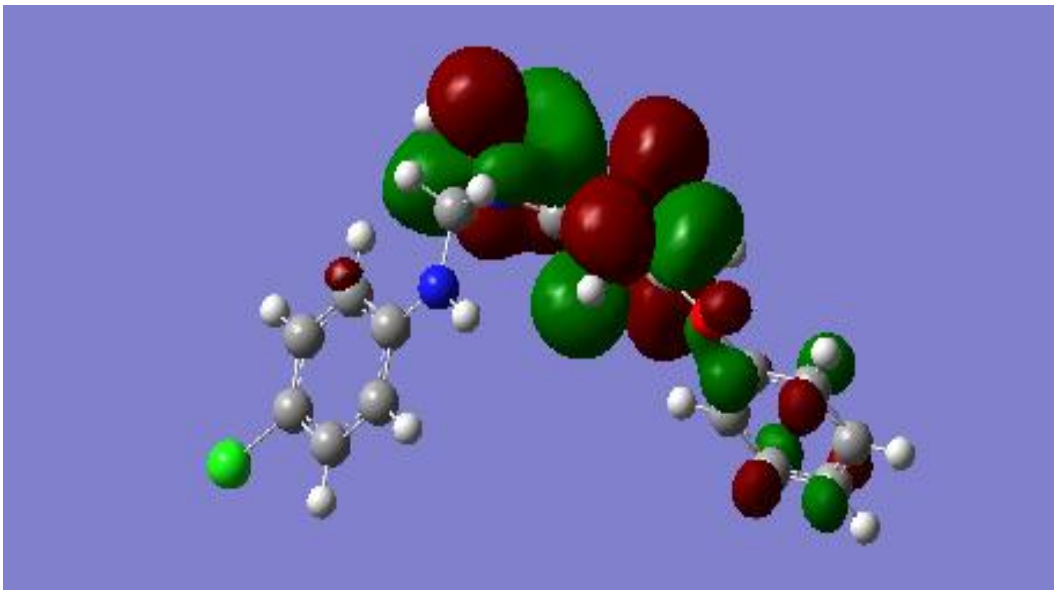
HOMO energy = -0.21563 a u.

LUMO energy = -0.02607 a.u.

HOMO – LUMO energy gap=-0.18956 a.u.



HOMO



LUMO

CONCLUSION

The simulation report of 5(6) phenoxy-1-aryl aminomethyl-1-chlorobenzimidazole , we will reported very soon.

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