VIBRATIONAL SPECTRA OF 5-PHENOXY BENZIMIDAZOLE

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ABSTRACT
This work deals with the vibrational spectroscopy of 5-PHENOXY BENZIMIDAZOLE. The mid and far FTIR and FT-Raman spectra were measured in the state. The fundamental vibrational frequencies and intensity of vibrational bands were evaluated using density functional theory (DFT) using standard B3LYP/6-31G methods and basis set combinations. The vibrational spectra were interpreted, with the aid of normal coordinate analysis based on a scaled quantum mechanical force field. The infrared and Raman spectra were also predicted from the calculated intensities. Comparison of simulated spectra with the experimental spectra provides important information about the ability of the computational method to describe the vibrational modes. HOMO and LUMO are types of molecular orbitals. And it is shown that charge transfer takes place within the molecule. The energy difference between the HOMO and LUMO is termed the HOMO–LUMO gap. The detailed study shows that the given compound exhibits the antifungal and antiviral properties.

KEYWORD
Density functional theory, FTIR, FT-Raman, Vibrational spectra, HOMO, LUMO, antifungal, antiviral.

INTRODUCTION
Benzimidazoles have far reaching applications in the field of chemistry and beyond. Benzimidazole and its derivatives are known to possess antibacterial, antifungal, antiviral and antiproliferative properties. They involved in a great variety of biological processes and are used as a procarcinogenic or mutagenic compound. Benzimidazoles have different activities as they can act as bacteriostats or bactericides, anticarcinogens, etc. They are often bioactive. Many anthelmintic drugs (albendazole, mebendazole, triclabendazole etc.) belong to the benzimidazole class of compounds. Benzimidazole fungicides are commercialized. They act by binding to the fungal microtubules and stopping hyphal growth.

Benzimidazole fungicides are a class of fungicides including benomyl, carbendazin (MBC), thiophanate-methyl, thiabendazole and fuberidazole. They can control many ascomycetes and basidionycetes, but not oomycetes. They are applied to cereals, fruits, vegetables and vines, and are also used in post harvest handling of crops. The solubility of Benzimidazole fungicides is low at physiological pH and becomes high at low pH.

Anthelmintics are a group of anti-parasitic drugs that expel parasitic worms (helminths) and other internal parasites from the body by either stunning or killing them and without causing significant damage to the host.
Phenoxy herbicides (or "phenoxies") are a family of chemicals related to the growth hormone indoleacetic acid (IAA). When sprayed on broad-leaf plants they induce rapid, uncontrolled growth ("growing to death"). When sprayed on monocotyledonous (grass) crops such as wheat or corn, they selectively kill broad-leaf weeds, leaving the crops relatively unaffected. The wide variety of phenoxies in use today can be grouped into the phenoxyacetic, phenoxybutyric and phenoxypropionic subtypes, the latter containing the aryloxyphenoxypropionic subtype with the greatest number of commercial variants. Chemically, they are carboxylic acids, typically applied in an ester or salt form.

**METHOD, MATERIAL AND THEORY**

Optimized geometrical structure of 5-PHENOXY BENZIMIDAZOLE using the density functional theory using standard B3LYP/6-31G.

The molecular geometry optimization, energy and Vibrational frequency calculations have been performed for 5-phenoxy bezimidazole using Gauss view 5.0 program packages at the Becke3-Lee-Yang-Parr (B3LYP) level with standard 6-31G basis set. For plots of simulated IR spectra, pure Lorentzian band shapes were used. The Raman activity (Si) calculated by Gaussian program have been suitably adjusted by the scaling procedure with MOLVIB and subsequently converted to relative Raman intensity. DFT calculations allow the prediction and calculation of material behaviour on the basis of quantum mechanical considerations, without requiring higher order parameters such as fundamental material properties.

The optimized structural parameters such as bond lengths, bond angle were determined at B3LYP level theory with 6-31G basis set and are presented in Table given below-

<table>
<thead>
<tr>
<th>ATOMS</th>
<th>BOND LENGTH</th>
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<tbody>
<tr>
<td>C1-C2</td>
<td>1.39516</td>
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<tr>
<td>C1-H7</td>
<td>1.09961</td>
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<tr>
<td>C2-C3</td>
<td>1.39471</td>
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<tr>
<td>C3-C4</td>
<td>1.39543</td>
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<tr>
<td>C3-H8</td>
<td>1.09968</td>
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<tr>
<td>C4-C5</td>
<td>1.39483</td>
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<tr>
<td>C5-C6</td>
<td>1.39514</td>
</tr>
<tr>
<td>C6-H9</td>
<td>1.09960</td>
</tr>
</tbody>
</table>
IR and Raman Frequencies

The vibrational spectral assignments have been carried out with the help of normal coordinate analysis. Non-redundant set of local symmetry coordinates constructed by suitable linear combinations of internal coordinates chosen according to the recommendations of Pulay. The
computed wave numbers are selectively scaled according to the SQM procedure suggested by Rauhut and Pulay, the observed IR and Raman spectra are presented in Figs. 1 and 2 respectively. These calculations were done by using B3LYP/6-31G.

**FIG-1**

**FIG-2**

**Molecular Orbital Energies**

The most important orbitals in a molecule are the frontier molecular orbitals, called highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). These orbitals determine the way the molecule interacts with other species. The frontier orbital gap helps characterize the chemical reactivity and kinetic stability of the molecule. A molecule with a small frontier orbital gap is more polarizable and is generally associated with a high chemical reactivity, low kinetic stability and is also termed as soft molecule.

The HOMO represents the ability to donate an electron, while LUMO as an electron acceptor represents the ability to obtain an electron. The electronic transition absorption corresponds to the transition from ground to the first excited state and is mainly described by one electron excitation from the highest occupied molecular orbital to the lowest unoccupied molecular orbital. Consequently HOMO → LUMO transition implies an energy transfer from the ring. The energy gap between HOMO and LUMO has been used to prove the bioactivity from intramolecular charge transfer. The energy gap measures the kinetic stability of the molecules.
The HOMO and LUMO energy calculated by B3LYP /6-31G method as shown below:

HOMO energy = -0.17286 a.u.
LUMO energy = -0.12154 a.u.

ENERGY GAP (HOMO-LUMO) = -0.05132 a.u.

The HOMO and LUMO energy gap explains the eventual charge transfer interactions taking place within the molecule. The HOMO and LUMO density plots of title compound are shown in Fig. 3 and Fig. 4 respectively.
The IR and Raman Spectra have been recorded and the detailed vibrational assignments are presented for 5-phenoxy benzimidazole. The equilibrium geometries, IR and Raman spectra, HOMO and LUMO analysis of the title compound are determined and analyzed by B3LYP /6-31G level of theory. The lowering of HOMO and LUMO gap clearly explains the charge transfer interactions taking place within the molecule.

CONCLUSION

Thus, the simulation report of 5-phenoxy benzimidazole will be reported soon. The work is still under further research.

REFERENCES

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