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# DFT Studies on Molecular Structure, Thermodynamics Parameters, HOMO-LUMO and Spectral Analysis of Pharmaceuticals Compound Quinoline (Benzo[b]Pyridine)

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## Abstract

Advances in computational chemistry have greatly increased its effectiveness and attractiveness as an emerging adjunct to experimental chemistry but also as an independent research field. This work studied some basic bonding Parameters, geometry, Uv-Visible spectra, HOMO-LUMO and harmonic vibrational frequencies of Quinoline were investigated by using density functional theory (DFT/6-31+ (d, p)) methods. The calculated wave numbers (B3LYP) agree properly with the determined wave numbers. The results obtained are then as compared with experimental statistics in which available. The structural parameters; thermochemistry, rotational constants, IR spectra and frequencies, bond distances, angles and dipole moment were obtained from the optimized stable geometries of the compound. The computed optimized geometric bond lengths and bond angles show good agreement with experimental data of the title compound. The calculated HOMO and LUMO energies indicate that charge transfer occurs within the molecule.

## Keywords

Computational Chemistry, Quinoline, Gaussian Software, Thermochemistry

## 1. Introduction

Computational chemistry is a branch of chemistry that overlaps between computer, chemistry and physics [1]. It involves solving chemical problems via the computer based on the fundamental laws of physics [2]. Computational chemistry is a set of techniques for investigating chemical problems by using the ap-

proaches of theoretical Chemistry combined with efficient computer programs in order to determine molecular geometry, spectroscopic properties, chemical reactivity, interaction of a substrate with an enzyme, chemical and physical properties of molecules [3].

The most important computational techniques are the ab-initio is a set of approaches in which molecular structures are calculated with Schrodinger equations, Semi-empirical techniques uses approximations from experimental data to provide inputs into mathematical models and lastly the Molecular Mechanics uses classical physics and semi-empirical force field to explain and interpret the behavior of atoms or molecules. But in this study the best method to do this paper is Density functional theory because DFT methods give information about the structural parameters, orbital interactions and vibrational frequencies [3].

Quinoline is a heterocyclic aromatic organic compound with the chemical formula $C_9H_7N$. Quinoline 1 or 1-azanaphthalene or benzo[*b*]pyridine is aromatic nitrogen containing trocyclic compound (**Figure 1**). Quinoline is a colourless liquid with an unpleasant odour and boiling point 237˚C. It is miscible with water, ethanol and ether [4]. Quinoline moiety commonly exists in various natural compounds (*Cinchona* alkaloids), and pharmacological studies have shown that the quinoline ring system is present in many compounds exhibiting a broad range of biological activities. Quinoline has been found to have antibacterial, antifungal, antimalarial, anthelmintic, anticonvulsant, cardiotonic, anti-inflammatory, and analgesic activities [4] [5].

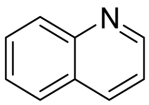
## 1.1. Synthesis of Quinoline

In different literature, a number of established protocols have been reported for the synthesis of quinoline ring, which can be changed to produce a number of differently substituted quinolines [5]. The quinoline ring has been generally synthesized by Skraup synthesis **Figure 2**.

## 1.2. Biological Activities of Quinoline

### 1.2.1. Antimicrobial Activity

The dramatically rising prevalence of multi-drug resistant microbial infections in the past few decades has become a serious health care problem. The search for new antimicrobial agents will consequently always remain as an important and challenging task for medicinal chemists Quinolines [2] [4] is a special structural class of quinoline antimicrobial agents. It is characterized by 1, 4-dihydro-4-oxo-3-pyridine carboxylic acid and a fused benzene ring moiety. Extensive SAR have been established on this nucleus and resulted in number of currently




quinoline

**Figure 1.** Molecular structure of quinoline [4].

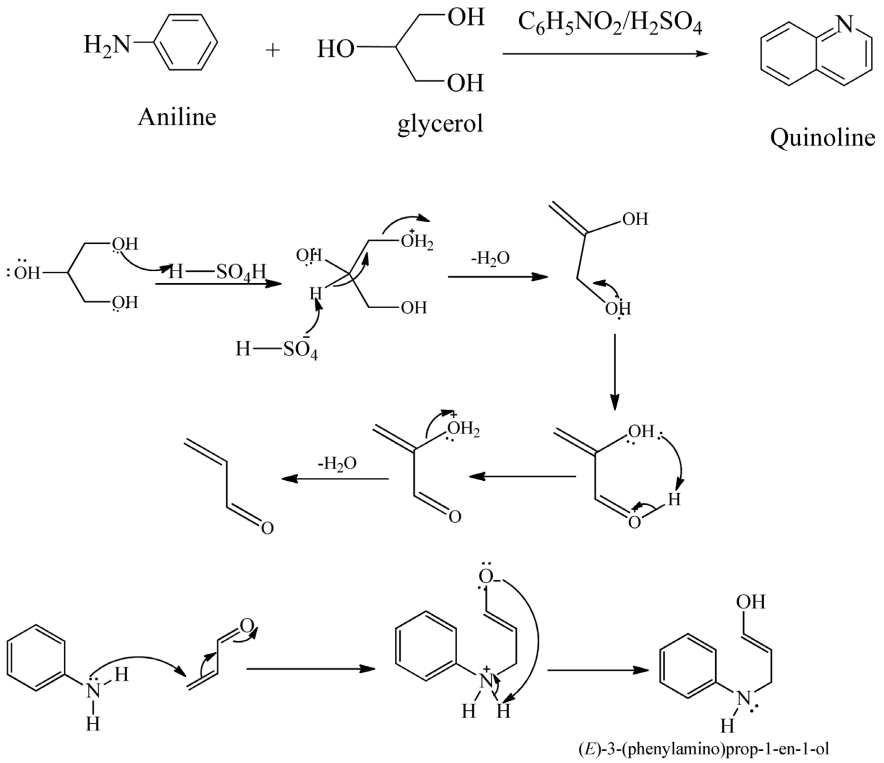



**Figure 2.** Mechanism of synthesis of quinolines [4].

marketed synthetic antimicrobial agent like ciprofloxacin [6].

### 1.2.2. Anticonvulsant Activity

Epilepsy is a common neurological disorder and a collective term given to a group of syndromes that involve spontaneous, intermittent, abnormal electrical activity in the brain. The maximal electroshock (MES) test and the subcutaneous pentylenetetrazole (scPTZ) test are the most widely used animal models of epilepsy to characterize the anticonvulsant activity of new compounds. In recent years various molecular modifications of quinoline derivatives have been reported with promising anticonvulsant results [3] [7].

### 1.2.3. Anti-Inflammatory Activity

Non-steroidal anti-inflammatory drugs (NSAIDs) have a wide clinical use for the treatment of inflammatory and painful conditions including rheumatoid arthiritis, soft tissue and oral cavity lesions, respiratory tract infections and fever. Generally aryl or heteroaryl acetic acid derivatives have been exploited for this activity like indomethacin, tolmetin etc. Later on selective legend for COX-2 were developed with low gastrointestinal injury, suppression of TXA2 formation and platelet aggregation [2] [4] [6].

Computational chemistry has the gain of treating those set of molecules no matter their stability. The purpose of this study was to study the molecular structure, vibrational wavenumbers, thermochemistry and the electronic absorption band theoretically. The molecular structure, harmonic vibrational wave-

numbers and IR absorption intensities have been calculated through density functional theory (DFT) the usage of Gaussian 09 software package deal using B3LYP/6-31+G (d, p) basis set.

## 2. Computational Details

The quantum chemical calculations reported in this work were carried out using the Gaussian 09 suite of programs and DFT computational methods. In view of this, three different computational methods like, Density Functional Theory (DFT), Hartree Fock (HF) and semi-empirical method) were selected for the study of the compounds. HF does not take into account into this study because it is less computationally expensive [6]. DFT takes into account a part of correlation and it has been reported to provide fairly good results for the description of various molecular properties such as the energy of the Highest Occupied Molecular Orbital (HOMO), the energy of the Lowest Unoccupied Molecular orbital (LUMO), the molecular shape, vibrational frequencies, thermochemistry and energy of optimized geometric structure of the molecule were calculated at B3LYP/6-31+G (d, p) basis set using Gaussian 09 software [7] without any symmetry constraint. In the present study, DFT in combination with the B3LYP were utilized in order to compare the effect of the different functional on the calculated molecular properties for the systems under study.

## 3. Results and Discussion

### 3.1. Molecular Geometry

Using the usual geometric parameters, geometry optimization was performed as the first task in density functional theory calculation without using any constraints. The optimized geometric parameters were used in the vibrational frequency calculations to characterize all the stationary points as minima [7]. The optimized ground state structure is as shown in **Figure 3**.

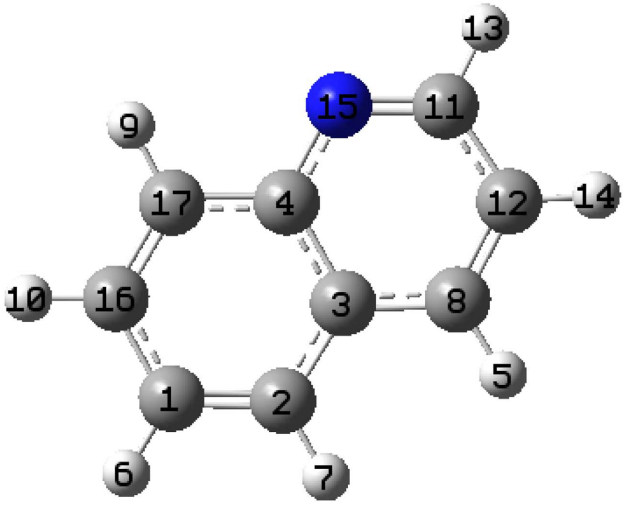



**Figure 3.** Optimized structure of quinoline.

### 3.2. Structural Parameters

Structural parameter like bond distance, length or radius is the common distance between the nuclear of two bonded atoms in a molecule; it has values typically within the range less than 1 to 2 Å. This structural parameter influences the force of attraction binding such a molecule *i.e.* the smaller the bond length between the bonding atoms, the stronger is the force of attraction between them [2]. The bond distances and angle for quinoline are shown in **Table 1** and **Table 2** respectively.

The B3LYP method leads to geometry parameters, which are close to experimental data. A statistical treatment of these shows that for the bond lengths B3LYP/6-31+G (d, p) (**Figure 4**) is slightly better than the bond length (**Figure 5**). The correlation coefficient for bond lengths was 0.97 for B3LYP/6-31+G (d, p) methods. The slight variation with the experimental value is due to the fact that the optimization performed in an isolated condition. Most of the optimized

**Table 1.** Bond distance (Length) of quinoline.

| Selected bond length | Calculated Value (Å) | Experimental Value (Å) | Error | Atom 1 | Atom 2 |
|---|---|---|---|---|---|
| R(C12-C17) | 1.38 | 1.43 | 0.02 | 12 | 15 |
| R(C1-C16) | 1.42 | 1.93 | 0.51 | 1 | 16 |
| R(C1-C2) | 1.38 | 1.45 | 0.07 | 1 | 2 |
| R(C2-C3) | 1.40 | 1.37 | 0.03 | 2 | 3 |
| R(C3-C4) | 1.43 | 1.43 | 0 | 3 | 4 |
| R(C3-C8 | 1.42 | 1.40 | 0.02 | 3 | 8 |
| R(C4-C8) | 1.42 | 1.38 | 0.04 | 4 | 8 |
| R(C8-C12) | 1.38 | 1.42 | 0.04 | 8 | 12 |
| R(N15-C11) | 1.32 | 1.39 | 0.07 | 15 | 11 |
| R(C4-N15) | 1.36 | 1.41 | 0.05 | 4 | 15 |

**Table 2.** Bond angle of quinoline in degree (˚).

| Selected bond angle | Calculated Value | Experimental Value | Error | Connectivity | | |
|---|---|---|---|---|---|---|
| | | | | Atom 1 | Atom 2 | Atom 3 |
| A(C1-C2-H7) | 120.6 | - | | 1 | 2 | 7 |
| A(C2-C3-C8) | 123.4 | 118.5 | 5.4 | 2 | 3 | 8 |
| A(C8-C3-C4) | 117.5 | 121.4 | 3.9 | 8 | 3 | 4 |
| A(C17-C4-N15) | 118.5 | - | | 17 | 4 | 15 |
| A(C3-C4-N15) | 120.4 | 118 | 2.4 | 3 | 4 | 15 |
| A(N15-C11-C12) | 124.2 | 121.6 | 2.6 | 15 | 11 | 12 |
| A(N15-C11-H13) | 116.3 | - | | 15 | 11 | 13 |
| A(H13-C11-C12) | 119.6 | - | | 13 | 11 | 12 |

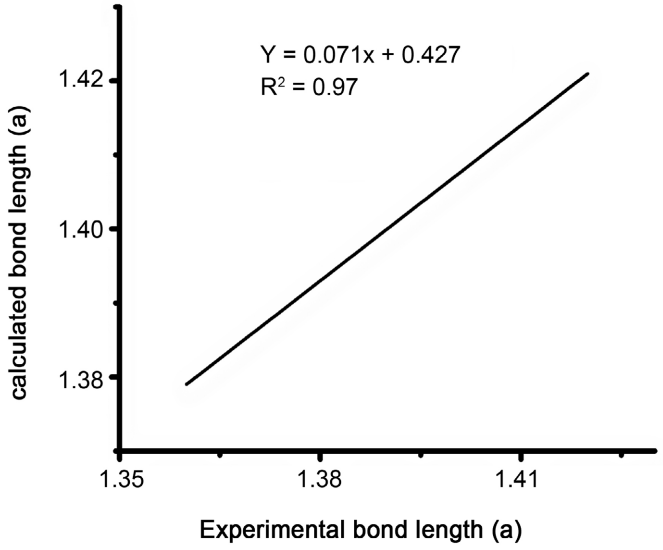



**Figure 4.** Calculated bond lengths in comparison with experimental data.

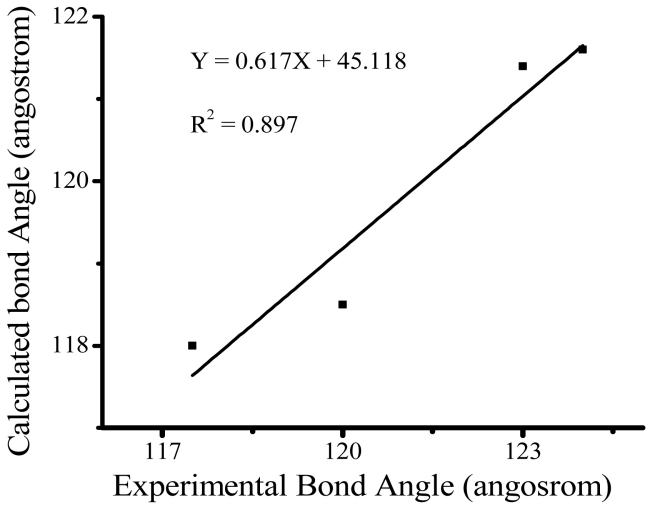



**Figure 5.** Calculated bond angle in comparison with experimental data.

bond lengths are slightly longer than the experimental values and the bond angles are slightly different from the experimental ones, because the molecular states are different in the experimental and theoretical processes [8]. It is observed that the influence of the nitrogen substituent on the molecular parameters.

### 3.3. Thermodynamic Properties

The values of thermodynamic parameters zero point vibrational energy, thermal energy, specific heat capacity, rotational constants, entropy of quinoline at 298.15 K in ground state are listed in Table 3. The variation in zero point vibrational energies (ZPVEs) seems to be significant.

Table 3. The calculated thermodynamical parameter of Quinoline.

| Basis Set | | B3LYP/6-31+G (d, p) | | |
|---|---|---|---|---|
| Zero point energy (Kal/mol) | | 92.94 | | |
| Rotational temperature (Kelvins) | | $T_A$ | $T_B$ | $T_C$ |
| | | 0.149 | 0.058 | 0.042 |
| Energy (E) (kcal/mol) | Translational | 0.889 | | |
| | Rotational | 0.889 | | |
| | Vibrational | 95.605 | | |
| | Total | 97.383 | | |
| Specific heat ($C_V$) (cal/mol-kelvin) | Translational | 2.981 | | |
| | Rotational | 2.981 | | |
| | Vibrational | 23.291 | | |
| | Total | 29.253 | | |
| Entropy (S) (cal/mol-kelvin) | Translational | 40.502 | | |
| | Rotational | 28.966 | | |
| | Vibrational | 13.838 | | |
| | Total Energy | 84.684 | | |

### 3.4. Vibrational Spectroscopy

The vibrational frequency deals with the periodic movement of atoms of a molecule relative to each other and usually range from less than $10^{13}$ Hz to $10^{14}$ Hz, or 300 $cm^{-1}$ 3000 $cm^{-1}$, it is important and necessary because it aids in the elucidation of molecular transition and molecular structure [2]. The calculated wavenumbers and observed IR with relative intensities are shown in (Table 4 and Figure 6).

### 3.5. Rotational Constant

In Table 5, the equilibrium rotational constants for the Quinoline calculated at the G09 level of theory are shown below. The error difference between the calculated and experimental rotational constants data for quinoline reveal that there is consistency and therefore shows high accuracy in our findings. This work gives the rotational constant values of 3.1010, 1.218 and 0.875 are consistent with reported experimental results of -, -, - GHz [1]. Therefore, for the quinoline with no experimental data, it is concluded that the G9 computational method has predicted the parameters with high accuracy.

### 3.6. Dipole Moment

Dipole moment is an important molecular property widely used to probe the infrared spectroscopy of molecule. A molecule is infrared active only when there is a change in dipole moments. Thus, provided that there is a dipole moment change during a normal molecular rotation, vibration or a combination of the

**Table 4.** Calculated and experimental vibrational frequencies of quinoline ($cm^{-1}$) [7] [9].

| Calculated frequency ($cm^{-1}$) | Experimental frequency ($cm^{-1}$) | % error ($cm^{-1}$) | IR Intensity |
|---|---|---|---|
| 144.13 | 155.4 | 7.82 | 4.57 |
| 177.87 | 188.45 | −5.95 | 2.50 |
| 300 | 325 | −8.33 | 0.078 |
| 370.96 | 354 | 4.499 | 1.84 |
| 409.62 | 425 | −3.75 | 71.19 |
| 464.43 | 486.43 | −4.74 | 11.99 |
| 511.76 | 517.34 | −1.09 | 1.11 |
| 517.76 | 536.23 | −3.57 | 0.51 |
| 524.09 | 542.43 | −3.5 | 0.26 |
| 583.14 | 574.32 | 1.51 | 0.13 |
| 611.08 | 599.23 | 1.94 | 0.94 |
| 660.42 | 636.23 | 3.66 | 48.72 |
| 712.46 | 736.34 | −3.35 | 4.03 |
| 749.97 | 764.32 | −1.91 | 95.48 |
| 762.37 | 789.54 | −3.56 | 1.10 |
| 765.27 | 789.43 | −3.16 | 14.81 |
| 812.48 | 836.43 | −2.95 | 2.72 |
| 852.48 | 845.65 | 0.80 | 0.27 |
| 912.55 | 923.67 | −1.21 | 4.31 |
| 965.75 | 989.32 | −2.44 | 0.018 |
| 1035.76 | 1012.34 | 2.26 | 40.13 |
| 1096.79 | 1112.54 | 7.69 | 12.14 |
| 1139.07 | 1154.45 | −1.35 | 8.069 |
| 1196.30 | 1187.32 | 0.75 | 6.677 |
| 1235.38 | 1223.65 | 0.95 | 17.46 |
| 1274.08 | 1239.31 | 2.73 | 12.17 |
| 1290.17 | 1265.98 | 1.87 | 5.39 |
| 1399.65 | 1389.43 | 0.73 | 32.75 |
| 1428.92 | 1412.54 | 1.15 | 35.35 |
| 1507.33 | 1512.43 | −033 | 22.67 |
| 1531.02 | 1523.32 | 0.5 | 0.20 |
| 1605.56 | 1623.45 | −1.11 | 4.43 |
| 1628.56 | 1624.45 | 0.25 | 5.95 |
| 3167.27 | 3138.23 | 0.92 | 13.42 |
| 3178.16 | 3189.21 | −0.35 | 4.72 |
| 3200.13 | 3223.32 | −0.72 | 6.93 |
| 3207.20 | 3224.54 | −0.54 | 20.80 |
| 3243.91 | 3268.9 | −0.77 | 4.42 |
| 3650.53 | 3689.34 | −1.06 | 50.07 |

**Table 5.** Rotational constants (GHz) for quinoline [1] [2] [5].

| Molecules | | Rotational constants (GHz) | | |
|---|---|---|---|---|
| | | A | B | C |
| Quinoline | Calculated value | 3.101 | 1.22 | 0.875 |
| | Experimental value | - | - | - |
| | % Error - | - | - | - |

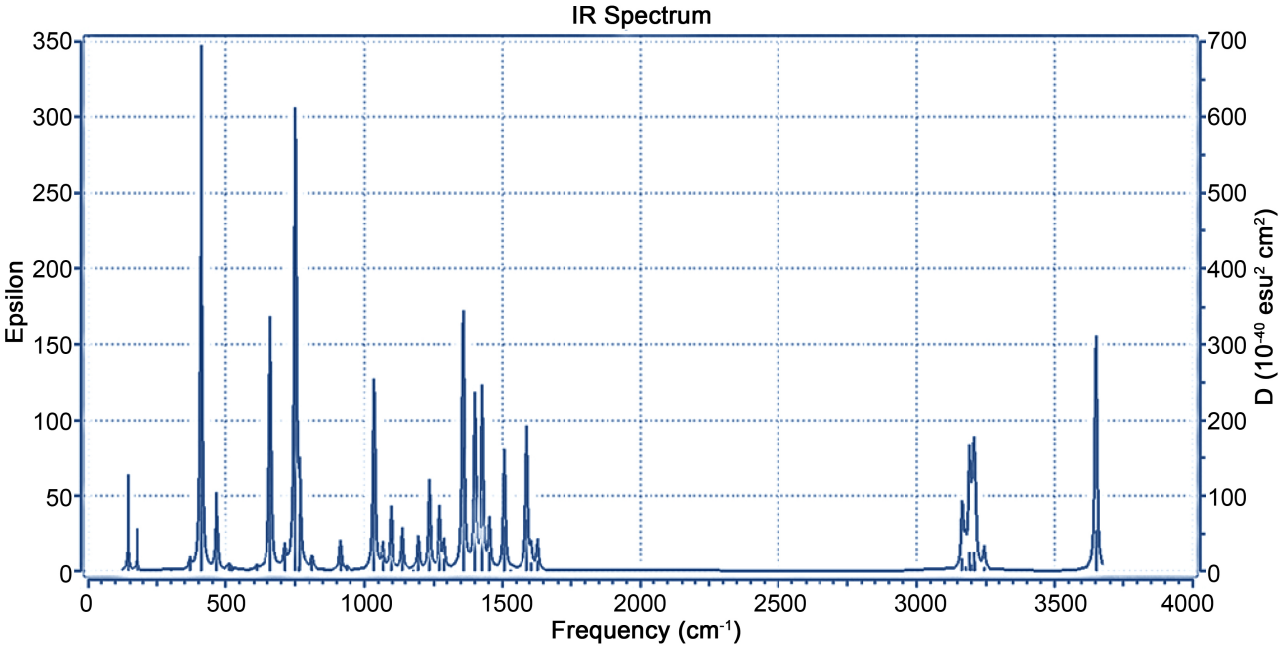



**Figure 6.** Computational IR spectrum of Quinoline at DFT (B3LYP)/6-31+G (d, p) level [7].

two molecular rotation–vibrations, chemical compounds can absorb at the infrared regions and are said to be IR active [1] [2]. For charged systems, its value depends on the choice of origin and molecular orientation [9]. As a result of DFT (B3LYP) calculations, the dipole moment of quinoline (2.004 D) was observed in this study agrees well with the experimental reported literature data was for B3LYP/6-31G+ (d, p).

### 3.7. UV-Visible Spectroscopy

UV-visible spectroscopy offers some valuable information about the nature of electronic transitions between the two prominent frontier molecular orbitals named as; HOMO (characterized with the aid of using maximum occupied molecular orbital) and LUMO (characterized with the aid of using unoccupied molecular orbital) [10]. The nature of electronic transition has been studied with the aid of using the usage of TD-DFT using 6-31+G (d, p) basis set. The theoretical absorption spectra are shown in **Figure 7**. The calculated electronic transitions with excessive oscillator strength are listed in **Table 6**.

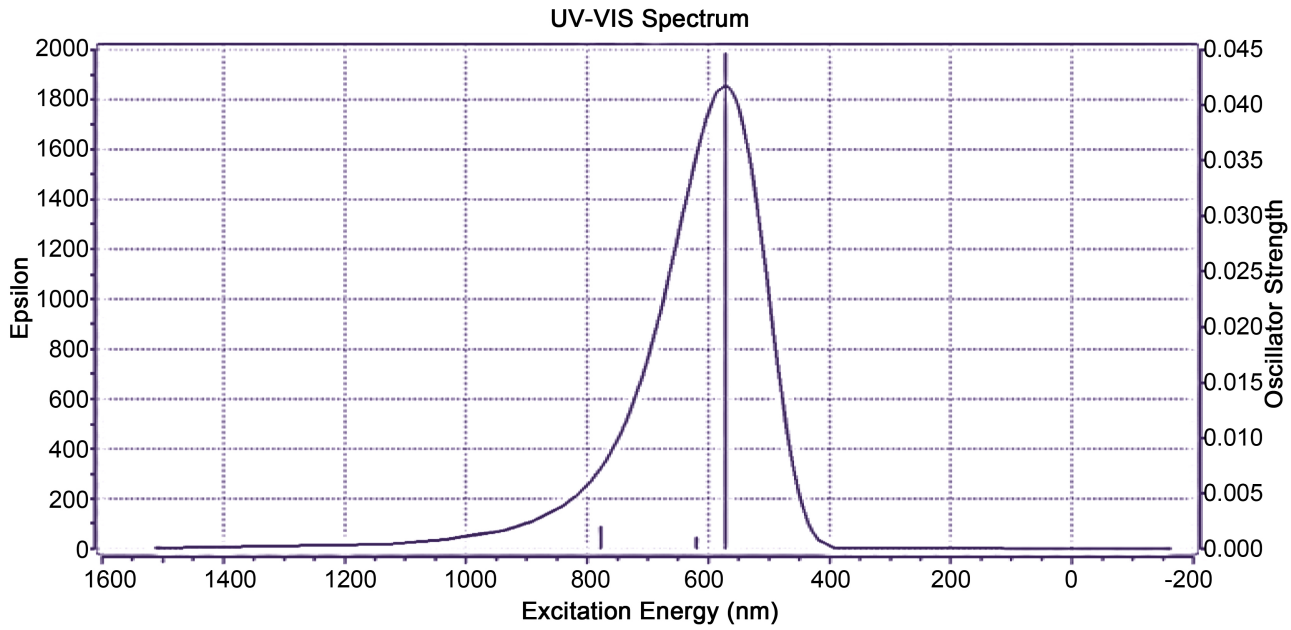



**Figure 7.** UV-VIS spectra of the present compounds [7].

**Table 6.** Calculated absorption wavelength (nm), excitation energies *E* (eV), and oscillator strengths (*f*) of quinoline.

| TD-DFT/6-31+G (d, p) | | |
|---|---|---|
| $\lambda$ (nm) | (*f*) | *E* (eV) |
| 570.76 | 0.045 | 0.333 |

### 3.8. HOMO–LUMO Analysis

HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) are referred to as Molecular orbitals. They were very important electronic parameters for chemist and physicist. The LUMO are referred to as the inner-maximum orbital containing loose locations to simply accept electrons [11]. The HOMO represents the capacity to donate an electron; LUMO as an electron acceptor represents the capacity to obtain an electron. The energy gap between HOMO and LUMO determines the kinetic stability, chemical reactivity, and optical polarizability and chemical hardness-softness of a molecule [9]. The HOMO–LUMO energy gap for quinoline has been calculated DFT level. The Eigen values of LUMO–HOMO energy gap reflect the chemical activity of the molecule [8]. The atomic orbital compositions of the molecular orbitals are sketched in **Figure 8**. The calculated energies and the energy gap is

HOMO energy = −6.646 eV,

LUMO energy = −1.816 eV,

HOMO—LUMO energy gap = −4.83 eV.

The lower with inside in the HOMO and LUMO energy gap explains the eventual charge transfer interaction taking place within the molecule, due to the strong electron-accepting ability of the electron acceptor group. The strong charge transfer interaction is responsible for the bioactivity of the molecule.

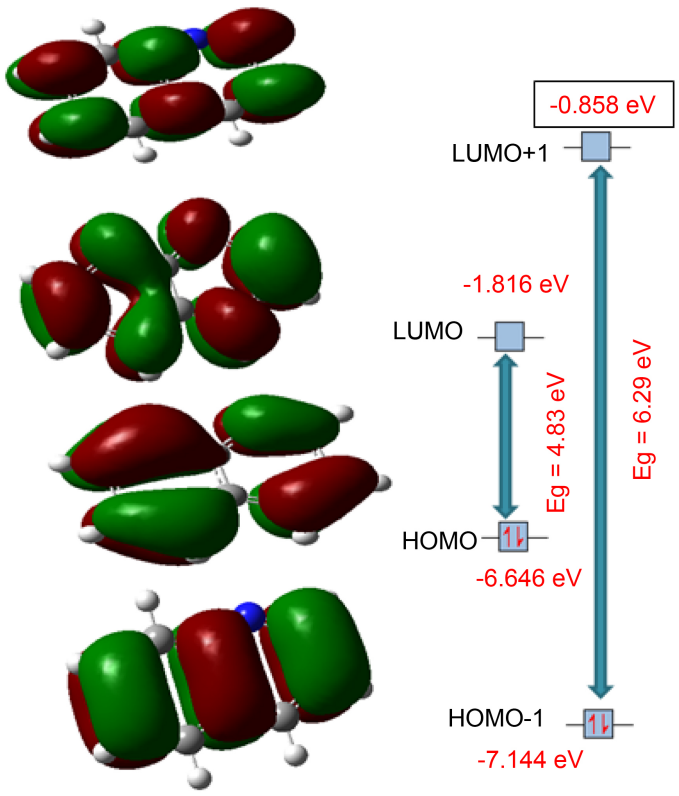



**Figure 8.** The molecular orbitals and energies for the HOMO, HOMO-1, and LUMO and LUMO+1 of quinoline.

Based on the above molecular orbitals composition (HOMO and LUMO) information we can determine the molecular properties, related to the reactivity and selectivity of the compounds, were estimated following the Koopmans's theorem relating the energy of the HOMO and the LUMO (**Table 7**). Electronegativity is estimated using the following the equation:

$$x = -\frac{1}{2}\left(E_{\text{HOMO}} + E_{\text{LUMO}}\right) \tag{1}$$

Chemical hardness ($\eta$) measures the resistance of an atom to a charge transfer [6]. On the basis of frontier molecular orbitals, chemical hardness corresponds to the gap between the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) [12].

Chemical hardness is approximated using the equation.

$$\eta = -\frac{1}{2}\left(E_{\text{HOMO}} - E_{\text{LUMO}}\right) \tag{2}$$

Electron polarizability, also called chemical softness ($\sigma$), describes the capacity of an atom or group of atoms to receive electrons and is estimated by using the equation

$$\sigma = \frac{1}{\eta} = \frac{-2}{E_{\text{HOMO}} - E_{\text{LUMO}}} \tag{3}$$

**Table 7.** Energy of HOMO, LUMO, energy gaps ($\Delta E_{HOMO-LUMO}$), Electron polarizability and Chemical hardness of quinoline (eV) [6].

| Basis set | $E_{HOMO}$ | $E_{LUMO}$ | $\Delta(E_{HOMO-LUMO})$ | Electron polarizability ($\sigma$) | Chemical hardness |
|---|---|---|---|---|---|
| DFT/6-31+G (d, p) | −6.646 | −1.816 | −4.83 | 0.414 | 2.415 |

**Table 8.** Mulliken atomic charges of quinoline.

| Atoms | B3LYP/6-31+G (d, p) |
|---|---|
| C1 | −0.140663 |
| C2 | −0.112599 |
| C3 | −0.028592 |
| C4 | 0.045878 |
| H1 | 0.134316 |
| H2 | 0.131265 |
| C7 | −0.163647 |
| H6 | 0.127712 |
| H8 | 0.131018 |
| C11 | −0.090727 |
| C12 | −0.135540 |
| H13 | 0.148544 |
| N15 | −0.259007 |

### 3.9. Mulliken Atomic Charges

Mulliken atomic charge calculation is a critical device with inside the software the application of quantum chemical calculation to molecular system because atomic charges influence dipole moment, molecular polarizability, electronic structure of molecular systems. The atomic charge depends on basis set presumably occur due to polarization [9]. The calculated Mulliken charge values of N atom is −0.259007 for DFT/6-31+G (d, p) (**Table 8**).

The charge of H1, H2, H6, H8, and H13 is positive in DFT diffuse functions. Hydrogen atom exhibits a positive charge, which is an acceptor atom. Considering DFT methods and basis set used in the atomic charge calculation, the carbon atoms (C1, C2, C3, C7, C11 and C12) exhibit a substantial negative charge, which are donor atoms. But the charge of C4 is exhibit a positive charge, which is an acceptor atom.

## 4. Conclusion

In this study work, we have performed the experimental and theoretical vibrational analysis of a pharmaceutically important heterocyclic aromatic molecule, quinoline for the first time. The optimized molecular geometry, vibrational frequencies, infrared activities, energy gap between HOMO-LUMO and thermodynamics of the molecule in the ground state have been calculated by using DFT

(B3LYP) methods with 6–31+G (d, p) basis set. The vibrational frequencies were calculated and scaled values are compared with the recorded IR spectra of the compound. The observed and the calculated frequencies are found to be in good agreement. Furthermore, the thermodynamic and total dipole moment properties of the compound have been calculated in order to get insight into molecular structure of the compound. These computations are carried out with the main aim that the results will be of assistance in the quest of the experimental and theoretical evidence for the title molecule in biological activity and coordination chemistry.

## Acknowledgements

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## Conflicts of Interest

The author declares that there is no conflict of interest.

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