Analysis on biological importance of antiseptic drug, O-Benzyl hydroxylamine, by the application of spectroscopic and theoretical tools

A. Abbas Manthiri a, b, Gene George a, S. Ramalingam c, *, R. Aarthi d

a Department of Physics, T.B.M.L. College, Porayar, Tamilnadu, India
b Department of Physics, Jamal Mohamed College, Tiruchirappalli, Tamilnadu, India
c Department of Physics, A.V.C. College, Mayiladuthurai, Tamilnadu, India
d Department of Physics, ST. Theresa’s Arts and Science College, Tharangambadi, Tamilnadu, India

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ABSTRACT

Biological importance of antiseptic drug; O-Benzyl hydroxylamine was explored using QSAR studies for ultimate usage for treating fungal infections. In this research work, the molecular spectroscopic tool and theoretical calculation method of analysis. The data acquired from both tools were evaluated and compared to validate structural and vibrational characteristics. Mulliken charge displacement around molecular site in order for exploring electronic properties to find out the cause of inducement of drug potential. The Lipinski rule of five was evaluated for the measurement of biological importance of the drug compound. The lipophilicity and topological surface area of the drug was monitored for determining biological process activity. The partial involvement of compositional bonds of the molecule was appraised for influential vibrational characteristics. The chemical environment for making chemical property was monitored from the uniform and asymmetrical chemical shift of core and allied carbons. The resultant oscillating potential orientation in the molecular site was identified and the residing zones were recognized to find out the origin of drug potential. The occurrence of CT complex process was studied and the CTC was found to be CC and C-N for generating drug activeness. The enhancement of hyper active polarization was measured in first and second order from which the charge level pulling on different entities were observed for ensuring the biological affinity of the compound. The enantiomer characteristics were thoroughly studied to measure the level of toxicity.

1. Introduction

The phenol is basically drug compound and particularly it is widely used as an antiseptic. Normally, the Phenol is medically used as a preservative in special type of vaccines [1]. Here, the phenol is converted in to hydroxyl methyl benzene and it is directly substituted with amine group and formed the O-Benzyl hydroxylamine. Usually, when N–O bonded compound has peculiar structure which is significant type of chemical species due to their special biological activity [2]. In this case, hydroxyl methyl group is protected by amine group which enhances the medical activity and thereby the species has multidimensional pharmaceutical activity [3]. The present compound has attracted many organic scientists for the preparation of pharmaceutical products due to the biological activeness.

Recent days, the hydroxylamine derivatives intermediate are having much attention due to usage of the preparation of Aziridines [4], β-Amino acids and Isoxazolidinones [5]. Since, the present chemical species is powerful inhibitors and have pharmacological and therapeutic effects; it is chemically used for the preparation of antibiotic, antiseptic and anti fungal compounds which provides better results when compared with other similar compounds [6, 7].

By screening the literatures as well as available pharmaceutical resources, it was clear that, the present drug; O-Benzyl hydroxylamine is fundamentally having drug potential and the medical data explained that, the part of the pharmaceutical applications of the compound was only briefed. It is necessary to explore the entire drug potential of the present compound in order to use this chemical species for fabricating new novel multifunctional drug. It is well known that, by examining the drug properties of the chemical species, the application of the drug compound can be determined. In order to expose biological property of the compound, biological as well as structural activity properties are to be studied. In this way, it is an attempt to study the entire physic-
chemical properties making use of molecular spectroscopic and computational tools. Here, the molecular spectroscopic tools have been used in non conventional way to analyze the present compound.

2. Experimental

The present drug compound; O-Benzyl hydroxylamine is obtained from Chemical industry, USA, it is well known that, the compound is under good spectroscopic grade and it can be used for recording the spectra.

- The FT-IR spectral pattern of the compound was recorded using a Bruker IFS 66V with high resolution vib-rot spectrometer with different scanning speed [7].
- The FT-Raman spectral sequence of present compound was recorded using Bruker spectrometer adopted with FTR instrument with Raman module equipped with a Nd:YAG laser source being operated at 1.068 μm line width with 500 mW power.
- The high resolution 1H NMR and 13C NMR spectra were recorded using 300 MHz and 75 MHz NMR spectrometer with high magnetic gradient.
- The UV-Vis spectra were recorded in solid phase in the region of 200 nm-800 nm, with the scanning interval of 0.22 nm, using the UV-1800 series instrument.

2.1. Biological parameter observation

The biological parameters and QSAR values have been experiential from Molinspiration apparatus and it is broad series of cheminformatics fields and also modules for electronic structure calculations at semiempirical and ab-initio levels. The chemical tool is also used for Computing the structure and stability of molecules using MMX method.

3. Calculation

In computational part, all the parameters have been calculated by performing quantum chemical computations on Gaussian 16 D. 01 version software program in IMAC computer [8]. The spectral pattern and optimized geometrical parameters were computed at the true geometry which was found after performing structure stability scan. The associated properties related with electronic spectra; NBO and frontier orbital sequence were calculated by adopting time-dependent SCF method with best fit basis set. The 1H and 13C Nuclear Magnetic Resonance isotropic chemical shifts were calculated by Gauge Independent Atomic Orbital (GIAO) self consistent method using Polarizable Continuum Model (I-PCM model) at B3LYP/6–311++G (2d,p) basis set. The Mullikian charge distortion due to the chemical change of molecular orbitals was mapped and the values were purposedly analyzed for the identification of key role for pharmaceutical functional process of the compound. The DM, linear polarizability and the first order hyper polarizability in different coordinates of the compound have been extracted using B3LYP method with the 6–311++G (d,p) basis set. The enhanced ECD and VCD spectral pattern were drawn and the enantiomer characteristics of the compound were studied to explore the toxicity effect of ligands.

4. Results and discussions

4.1. Structure modification analysis

The structure of present molecule was optimized and the related parameters were calculated and are depicted in Table 1 and the corresponding diagram is presented in Fig. 1. Usually, the base structure is modified with respect to the type of ligand group injected to the ring. The reception of substitutions in the base frame is pronounced by the alteration of bond length and bond angle due to the electronic configuration of atoms in different places of the ring. Once, the changes take place in the electronic arrangement that will change all the respective parametric changes in the molecule like fundamental physical properties. Simultaneously, the physico-chemical properties are altered with respect to the effect of ligand group.

Here, the CHO–NH2 groups were added in the benzene ring and the molecular structure comes in to optimized form. Here, the benzene is the base in which the substitutional groups were injected and the corresponding bond length of C2–C3 and C3–C4 were found to be enlarged by 0.005 Å as in Table 1. This change of bond length showed the disturbance of chemical equilibrium forces existed among the core CC. In the ligand chain, the bond length alternation took place at C12–O15 and O15–N16 as 1.437 Å and 1.440 Å. Due to the higher chemical force of attraction in C12–O15 than O15–N16, the first bond length decreased in first case than second. Usually, the attraction between the atoms C and O is much higher than attraction between O and N since C is more positive than N. By the consequence of stretching of bond length O–N, the asymmetrical enlargement of bond length appeared on N–H by 1.019 Å. This induced the decrement of amino flavor in the chain. As indicated in Table 1, the extraordinary bond length elongation took place over the bond C3–C12 (1.505 Å) due to the repulsive forces arranged due to the forces of attraction between CHO and NH2 entities. This atmosphere is making reduction of chemical intensiveness of aldehyde group. Thus, reduced amino energy with enlarged carbonyl energy blended with benzene ring by injecting ligand group, the antiseptic chemical potential was produced.

4.2. Mulliken charge decomposition analysis

The Mulliken partial charge distribution diagram is depicted in Fig. 2. Once the optimized structure is obtained, it is not necessary to look at the position of the nuclei (bond distances and angles) but the electronic density to be account on charge displacement as well. The molecular orbital interaction theory provides more specific and comprehensive information regarding the electronic interactions taking place in a molecule in the form of Mulliken charge population distribution called patrician of electron density [8]. The Energy Partitioning is nothing but electronic structure interaction energy which relates function of ligand groups on the functional pattern of base compound [9]. Here, the Mulliken charge assignment was investigated to explore the restoring chemical kinetics for manipulating drug property.

In this case, except, C3, all the core CC of the benzene ring was looking as red, the electrostatic component was appeared and this was due to the electron density pulling by the ring for electronic interaction to make sufficient potential to prepare the drug property. Even though, usually, the repulsive chemical forces arrived between C and C in the ring, due to the reconfiguration of charge density, the electrostatic interaction was observed on the bond C3–C12. This was mainly due to the charge pulling by the amino group from O and O was found to be neutral atom from which the chemical potential was exchanged between ring and amino group via O. The Pauli repulsion component was existed between core CC and O & N and it was purely by the reorientation of electron density against protonic region (nucleolus). From the electrostatic interaction and Pauli repulsion among the electronic configuration of molecule described that, the required chemical potential for the molecule to induce the drug potential from such type of successful
Table 1
Optimized geometrical parameters for O-Benzyl Hydroxyflamine.

| Geometrical parameters | HF       | B3LYP    | B3PW91   |
|------------------------|----------|----------|----------|
| Bond length (Å)         |          |          |          |
| C1-C2                  | 1.385    | 1.393    | 1.393    |
| C1-C3                  | 1.397    | 1.394    | 1.392    |
| C1-H7                  | 1.086    | 1.084    | 1.086    |
| C2-C3                  | 1.401    | 1.397    | 1.400    |
| C2-H8                  | 1.085    | 1.085    | 1.087    |
| C3-C4                  | 1.398    | 1.398    | 1.398    |
| C3-C12                 | 1.507    | 1.507    | 1.501    |
| C4-C5                  | 1.396    | 1.393    | 1.394    |
| C4-C9                  | 1.087    | 1.085    | 1.087    |
| C5-C6                  | 1.394    | 1.394    | 1.394    |
| C5-H10                 | 1.086    | 1.084    | 1.086    |
| C6-H11                 | 1.086    | 1.084    | 1.086    |
| C12-H13                | 1.085    | 1.095    | 1.094    |
| C12-H14                | 1.085    | 1.095    | 1.096    |
| C12-O15                | 1.406    | 1.437    | 1.444    |
| O15-N16                | 1.391    | 1.440    | 1.433    |
| N16-H17                | 1.001    | 1.019    | 1.022    |
| N16-H18                | 1.001    | 1.018    | 1.018    |
| N16-C20                | 3.652    | 3.318    | 3.558    |
| H19-C20                | 1.270    | 1.287    | 1.325    |
| Bond angle (°)         |          |          |          |
| C2-C1-C3               | 120.03   | 120.20   | 119.99   |
| C2-C1-H7               | 119.89   | 119.80   | 119.91   |
| C6-C1-C7               | 120.08   | 120.01   | 120.10   |
| C1-C2-C3               | 120.72   | 120.53   | 120.54   |
| C2-C3-H8               | 119.71   | 119.90   | 119.98   |
| C2-C2-H8               | 119.57   | 115.17   | 119.48   |
| C2-C3-C4               | 118.77   | 118.88   | 119.05   |
| C2-C3-C12              | 120.67   | 120.41   | 120.29   |
| C4-C3-C12              | 120.55   | 120.70   | 120.66   |
| C3-C4-C5               | 120.75   | 120.70   | 120.56   |
| C3-C4-C9               | 119.57   | 119.49   | 119.60   |
| C5-C4-C9               | 119.67   | 119.81   | 119.84   |
| C1-C5-C6               | 120.02   | 120.03   | 119.98   |
| C4-C5-C6               | 119.89   | 119.82   | 119.86   |
| C5-C6-C7               | 120.10   | 120.15   | 120.16   |
| C5-C6-C11              | 119.70   | 119.66   | 119.89   |
| C1-C6-H11              | 120.15   | 120.16   | 120.03   |
| C6-C7-C12              | 120.14   | 120.18   | 120.08   |
| C3-C12-H13             | 110.83   | 111.06   | 112.04   |
| C3-C12-C14             | 110.68   | 110.67   | 111.47   |
| C3-C12-O15             | 108.37   | 108.19   | 108.00   |
| H13-C12-H14            | 108.02   | 107.23   | 108.61   |
| H13-C12-O15            | 109.48   | 109.13   | 107.57   |
| H14-C12-O15            | 109.46   | 110.56   | 109.03   |
| C15-O15-N16            | 105.28   | 108.38   | 108.99   |
| O15-N16-H18            | 110.84   | 104.17   | 104.96   |
| O15-N16-C20            | 105.76   | 103.42   | 103.27   |
| H17-N16-H18            | 180.00   | 144.99   | 56.17    |
| H17-N16-C20            | 107.00   | 105.43   | 106.41   |
| H16-N17-C20            | 74.16    | 100.14   | 102.35   |
| H18-N16-C20            | 74.24    | 94.22    | 104.38   |
| N16-C20-H19            | 146.23   | 169.68   | 31.83    |
| Dihedral angle (°)     |          |          |          |
| C6-C1-C2-C3            | 0.05     | 0.39     | -0.04    |
| C6-C1-C2-H8            | -179.99  | -179.58  | -179.99  |
| H7-C1-C2-C3            | 179.89   | 179.73   | 179.77   |
| H7-C1-C2-H8            | -0.15    | -0.54    | -0.17    |
| C2-C1-C6-C5            | -0.04    | -0.39    | -0.06    |
| C2-C1-C6-H11           | 179.82   | 179.82   | 179.85   |
| H7-C1-C6-C5            | -179.88  | -179.73  | -179.87  |
| H7-C1-C6-H11           | -0.02    | -0.05    | 0.00     |
| C1-C2-C3-C4            | -0.06    | 0.15     | 0.14     |
| C1-C2-C3-C12           | 179.10   | -178.38  | 179.07   |
| H8-C2-C3-C4            | 179.99   | -179.05  | 179.94   |
| H8-C2-C3-C12           | -0.85    | 2.42     | -0.70    |
| C2-C3-C4-C5            | 0.05     | -0.68    | -0.14    |
| C2-C3-C4-H9            | -179.99  | 179.29   | 179.77   |
| C12-C3-C4-C5           | -179.11  | 177.84   | -179.07  |
| C12-C3-C4-H9           | 0.85     | -2.19    | 0.97     |

(continued on next page)
### Table 1 (continued)

| Geometrical parameters | Methods
|------------------------|-----------------|
|                        | HF              | B3LYP          | B3PW91         |
|                        | 6-311++G (d, p) | 6-31++G (d, p) | 6-311++G (d, p) |
| C2-C3-C12-H13         | 30.81           | 71.09          | 30.06          | 36.76 | 81.50 |
| C2-C3-C12-H14         | 150.63          | -169.93        | 150.75         | 158.71 | -159.69 |
| C2-C3-C12-O15         | -89.34          | -48.65         | -89.57         | -81.53 | -38.40 |
| C4-C3-C12-H13         | -150.05         | -107.41        | -151.03        | -143.89 | -96.77 |
| C4-C3-C12-H14         | -30.23          | 11.58          | -30.34         | -21.94 | 22.04 |
| C4-C3-C12-O15         | 89.80           | 132.85         | 89.33          | 97.81 | 143.33 |
| C3-C4-C5-C6           | -0.03           | 0.68           | 0.04           | 0.03 | 0.76 |
| C3-C4-C5-H10          | -179.88         | -179.84        | -179.78        | 179.95 | -179.88 |
| H9-C4-C5-C6           | -179.99         | -179.29        | -180.00        | -179.74 | -179.13 |
| H9-C4-C5-H10          | 0.16            | 0.19           | 0.18           | 0.18 | 0.24 |
| C4-C5-C6-C1           | 0.03            | 0.14           | 0.06           | 0.00 | -0.12 |
| C4-C5-C6-H11          | -179.83         | 179.65         | -179.82        | -179.90 | 179.54 |
| H10-C5-C6-C1          | 179.88          | -179.61        | 179.88         | -179.92 | -179.48 |
| H10-C5-C6-H11         | 0.02            | 0.17           | 0.01           | 0.18 | 0.18 |
| C3-C12-O15-N16        | -179.91         | 173.38         | -179.97        | 174.76 | 172.89 |
| H13-C12-O15-N16       | 59.11           | 52.43          | 59.18          | 53.65 | 52.06 |
| H14-C12-O15-N16       | -59.12          | -65.28         | -59.06         | -63.95 | -65.86 |
| C12-O15-N16-H17       | 123.29          | 119.95         | 124.70         | 112.97 | 119.84 |
| C12-O15-N16-H18       | -123.40         | -130.14        | -124.17        | -135.71 | -129.23 |
| C12-O15-N16-C20       | -82.69          | -11.94         | 5.69           | 125.72 | -14.38 |

Fig. 1. (A) Bond type and (B) Tube structures of O-Benzyl Hydroxylamine.
electronic configuration. Here, the accepted electronic configuration in
terms of mulliken charge assignment for this case elucidate that, the
chemical potential which was extracted from amino group was mainly
used for incrementing antiseptic kinetics in the molecule. Thereby, the
antiseptic property was stimulated as in the required rate in the molecule.

The centre of symmetry point of chemical equivalent forces was
papered on C12 on which the exchange of chemical potential was found
to be oscillated between ring and amino group and finally, in the ground
state structure (Optimized), the mulliken charge orientation favour for
the inducement of drug property. The resultant drug energy gained from
the fragmentation of orbitals in base and ligand groups are able to relax
into an optimal form at the point of O in the molecular complex.

4.3. Biological importance investigation

The biological parameters were observed from Molinspiration pro-
gram, are presented in Table 2 and the lipophilicity diagram is illustrated
in Fig. 3. Usually the Molecular mono isotopic mass of the drug com-
pound decides transport properties of molecules, such as blood-brain
barrier penetration (BBB) which is most important molecular-ligand
properties of drug. The drug molecules do not cross BBB in order to
choose the non-CNS targets [10]. The molar Volume of this compound

| Parameters                        | values |
|-----------------------------------|--------|
| Hydrogen bond donor count         | 2      |
| Hydrogen bond acceptor count      | 2      |
| Rotatable bond count              | 2      |
| Topological Polar Surface Area    | 32.5 Å² |
| Mono isotopic Mass                | 159.045 g/mol |
| Exact Mass                        | 159.045 g/mol |
| Heavy Atom Count                  | 10     |
| Covalently-Bonded Unit Count      | 2      |
| LogP                              | 1.28   |
| N atoms                           | 9      |
| MW                                | 123.16 |
| nON                               | 2      |
| nOHNH                             | 2      |
| volume                            | 121.12 |
| GPCR ligand                       | 2.14   |
| Ion channel modulator             | 1.38   |
| Kinase inhibitor                  | 2.28   |
| Nuclear receptor ligand           | 2.35   |
| Protease inhibitor                | 1.80   |
| Enzyme inhibitor                  | 1.19   |

Fig. 2. (A) Plane vertical (B) plane horizontal; Mulliken charge level diagram of O-Benzyl Hydroxylamine.
was found to be 121.12 which is the limited coefficient that will choose the right target to avoid the side effects. The logP is nothing but Octanol-water partition coefficient and is a measure of molecular hydrophobicity which ensure the drug absorption and bioavailability of the chemical compound. Here, the logP was found to be 1.28 and was very low value. In addition to that, the present molecule able to have additive ligand groups for the improvement of the drug properties.

The topological surface area is the passive molecular transport properties of the drug molecule which enable the good transport properties for the targeting molecules [10]. For the present drug, the TPSA was determined to be 32.5 Å² and this value is measured to be very low when compared with allowed rate and the molecule can be added with more number of ligand groups in order to stabilize the drug ability further. According to the Lipinski five rule, the Hydrogen bond donor (HBD) count, Hydrogen bond acceptor (HBA) count, Topological Polar Surface Area, logP and Rotatable bond count are to be within the expected value such as 5:5:140:10:5. For this drug case, all were determined to be 2:2:32:2:1.28:2 respectively and these parameters value was ensured to be within the allowed limit which satisfied the RO5 [11, 12].

The GPCR ligand is a 7-T integral membrane protein and sensory signal mediator protein which was found to be 2.14 for the present compound. From the observed value, it was found that, it was optimized value that transduces extracellular stimuli into intracellular signals usefully. The ion channel modulator is pore like membrane protein which permit ion to pass via the channel pore which transduce the signal to generate the action potential across the cell membrane. For the present case, it was calculated to be 1.38, is enough to modulate the signal proportionate to the drug action. Kinase inhibitor is the drug substance that blocks a kind of enzyme called kinase that controls the function the cell signaling and metabolism. The present case is already antiseptic compound and has the calculated value of kinase inhibitor been 2.28 which are enough to inhibit the action of the blood vessels to help the unusual growth of cells. The nuclear receptor is the protein that has ability to directly interact with DNA and control the expression of genomic DNA. Here, the related value of the same was determined to be 2.35 which is trace value of the expected limit. So the present molecule has the ability to interact with corresponding protein and isolate the function of organ. The Protease and enzyme inhibitor coefficient were found to be 1.80 and 1.19 respectively. Here, these values are moderate and both the inhibitors are ligand-molecules which can hold back the function of proteases and enzymes which were supported by the literature [13].

![CPK 3D view](image1)

![Molecular Lipophilicity Potential](image2)

**O-Benzyl Hydroxylamine Hydrochloride**

![Topological Polar Surface Area](image3)

![CPK Polar Surface Area](image4)

**Fig. 3.** (A) CPK view, (B) MLP view, (C) TPS view and (D) PSA view of O-Benzyl Hydroxylamine.
4.4. Vibrational analysis

4.4.1. Vibrational assignments

The optimized molecular structure was composed by 18 atoms in terms of base and ligand groups. In order to study the vibrational characteristics, the IR and Raman peaks are to be assigned to compositional bands on the vibrational pattern and the respective values along with calculated values are depicted in Table 3. The assigned frequencies with respect to fundamental and group frequency rules for cyclic compound (Vib. = 3n-6). The in plane and out of plane vibrations of compositional bands are classified and represented by μ and γ. According to the mutual exclusion principle [14], the total number of vibrations was found to be 48 in which 18 stretching, 15 in plane bending and 15 out of plane bending were assigned and their related FT-IR and FT-Raman spectral pattern are displayed in Figs. 4 and 5 respectively.

$\Gamma_{vib} = 3\mu^2 + 15\mu^2$

### Table 3

| Symmetry species $C_s$ | Observed frequency (cm$^{-1}$) | Methods | Vibrational assignments |
|------------------------|-------------------------------|---------|------------------------|
|                        | FT-IR (G, d, p) | FT-Raman | HF | B3LYP | B3PW91 | 6-31+G(d) | 6-31+G(d, p) | 6-31G(d) | 6-31G(d,p) | 6-31G(d, p) | 6-31G(d, p) |
| $\mu^1$ | 3450m | 3455 | 3440 | 3439 | 3442 | 3455 | (N-H) ν |
| $\mu^1$ | - | 3350vw | 3351 | 3351 | 3354 | 3343 | (N-H) ν |
| $\mu^1$ | - | 3030vw | 3028 | 3029 | 3044 | 3033 | (C-H) ν |
| $\mu^1$ | - | 3020vw | 3019 | 3022 | 3009 | 3023 | (C-H) ν |
| $\mu^1$ | - | 3010vw | 3010 | 3012 | 3000 | 3015 | (C-H) ν |
| $\mu^1$ | - | 3005vw | 2973 | 2974 | 2992 | 2976 | 2971 | (C-H) ν |
| $\mu^1$ | - | 2980vs | 2907 | 2996 | 3015 | 3003 | 2995 | (C-H) ν |
| $\mu^1$ | - | 2970vw | 2914 | 2913 | 2893 | 2904 | 2909 | (C-H) ν |
| $\mu^1$ | - | 2880vs | 2878 | 2879 | 2879 | 2877 | 2874 | (C-H) ν |
| $\mu^1$ | - | 1610m | 1611 | 1654 | 1640 | 2850 | 1609 | (C=O) ν |
| $\mu^1$ | - | 1605m | 1608 | 1602 | 1608 | 1647 | 1665 | (C=O) ν |
| $\mu^1$ | - | 1590s | 1597 | 1588 | 1587 | 1607 | 1587 | (C=O) ν |
| $\mu^1$ | - | 1480vw | 1481 | 1476 | 1479 | 1590 | 1481 | (C=O) ν |
| $\mu^1$ | - | 1470vw | 1479 | 1476 | 1470 | 1484 | 1470 | (C=O) ν |
| $\mu^1$ | - | 1460m | 1446 | 1445 | 1449 | 1473 | 1448 | (C=O) ν |
| $\mu^1$ | - | 1400m | 1401 | 1400 | 1431 | 1450 | 1394 | (C=O) ν |
| $\mu^1$ | - | 1330vw | 1328 | 1329 | 1333 | 1408 | 1326 | (N-D) ν |
| $\mu^1$ | - | 1320vw | 1317 | 1323 | 1320 | 1334 | 1315 | (N-D) ν |
| $\mu^1$ | - | 1230m | 1227 | 1240 | 1237 | 1316 | 1230 | (N-H) ν |
| $\mu^1$ | - | 1220m | 1217 | 1222 | 1213 | 1294 | 1223 | (N-H) ν |
| $\mu^1$ | - | 1180m | 1181 | 1180 | 1176 | 1224 | 1180 | (C-H) ν |
| $\mu^1$ | - | 1175vw | 1182 | 1175 | 1174 | 1180 | 1173 | (C-H) ν |
| $\mu^1$ | - | 1160m | 1163 | 1166 | 1162 | 1174 | 1158 | (C-H) ν |
| $\mu^1$ | - | 1100vw | 1102 | 1100 | 1104 | 1163 | 1103 | (C-H) ν |
| $\mu^1$ | - | 1050vw | 1054 | 1052 | 1050 | 1100 | 1049 | (C-H) ν |
| $\mu^1$ | - | 1030vw | 1037 | 1036 | 1031 | 1050 | 1029 | (C-H) ν |
| $\mu^1$ | - | 1010vw | 1012 | 1010 | 1013 | 1028 | 1007 | (C-H) ν |
| $\mu^1$ | - | 1005vs | 1001 | 1005 | 1023 | 1010 | 1006 | (N-H) γ |
| $\mu^1$ | - | 1000vs | 1003 | 1004 | 1018 | 1008 | 999 | (N-H) γ |
| $\mu^1$ | - | 995vs | 990 | 1000 | 1012 | 1006 | 997 | (C-H) γ |
| $\mu^1$ | - | 985vw | 981 | 988 | 1005 | 1000 | 995 | (C-H) γ |
| $\mu^1$ | - | 970vw | 967 | 944 | 958 | 991 | 970 | (C=O) γ |
| $\mu^1$ | - | 930vw | 930 | 924 | 936 | 959 | 931 | (C-H) γ |
| $\mu^1$ | - | 880s | 880 | 864 | 875 | 933 | 870 | (C-H) γ |
| $\mu^1$ | - | 820vw | 821 | 820 | 822 | 864 | 819 | (C-H) γ |
| $\mu^1$ | - | 750vs | 753 | 750 | 751 | 818 | 759 | (C-H) γ |
| $\mu^1$ | - | 700vs | 700 | 701 | 697 | 749 | 702 | (C-H) γ |
| $\mu^1$ | - | 610m | 608 | 612 | 607 | 703 | 611 | (C=O-N) δ |
| $\mu^1$ | - | 600vw | 599 | 601 | 599 | 610 | 603 | (CCC) δ |
| $\mu^1$ | - | 500vw | 500 | 500 | 501 | 599 | 494 | (CCC) δ |
| $\mu^1$ | - | 410vw | 409 | 410 | 411 | 501 | 410 | (CCC) δ |
| $\mu^1$ | - | 350vw | 350 | 350 | 351 | 410 | 350 | (CCC) δ |
| $\mu^1$ | - | 300vw | 300 | 300 | 300 | 350 | 300 | (C-O-N) γ |
| $\mu^1$ | - | 290vw | 290 | 290 | 289 | 300 | 284 | (C-O-N) γ |
| $\mu^1$ | - | 180ow | 180 | 179 | 180 | 290 | 181 | (CCC) γ |
| $\mu^1$ | - | 140m | 139 | 141 | 140 | 180 | 140 | (CCC) γ |
| $\mu^1$ | - | 120v | 120 | 120 | 120 | 120 | 120 | (CCC) γ |
| $\mu^1$ | - | 105s | 105 | 105 | 105 | 105 | 105 | (C-C) γ |

VS - Very strong; S - Strong; m - Medium; w - weak; As - Asymmetric; s - symmetric; ν - stretching.

α - deformation, δ - In plane bending; γ - out plane bending; τ - Twisting.
Such observed view showed that, some of the vibrational energy related to the chemical potential was consumed by the substitutional groups. So that, equivalent chemical potential of the ring was altered with respect to the ligand groups and the chemical property was definitely rehabilitated in to the chemical assistance provided by the ligand groups. Here, in such a way, the antiseptic property of the present compound was found to be prepared by the ligand potential blended with benzene ring.

4.4.3. Core ring vibrations

The aromatic ring core vibrations called CC stretching, in plane and out of plane ring breathing modes for benzene and its derivative chemical species are observed in the region 1600-1430 cm\(^{-1}\), 630-605 cm\(^{-1}\) and 560-415 cm\(^{-1}\) respectively \cite{17, 18, 19}. The present case was mono substituted benzene derivative and the respected CC stretching bands were identified at 1610, 1605 & 1590(C=C) cm\(^{-1}\), 1480, 1470 & 1450 (C–C) cm\(^{-1}\) as in Table 3. The in plane and out of plane ring breathing vibrational modes have been observed in the IR and Raman spectra at 600, 500 & 410 cm\(^{-1}\) and 180, 140 & 120 cm\(^{-1}\) respectively. Since the core CC stretching bands were found at top end of the expected limit, there was no chemical energy related to such vibrations taken by the substitutional groups. Instead of that, the ring breathing modes have been observed to be suppressed much due to chemical energy suction by the taken up ligand groups. Only low order bond energy was absorbed by the substitutional groups and thereby that energy was consumed for blending of property of benzene and ligand groups.

4.4.4. Amino group and ethyl group vibrations

The amino group in the base compound always dominates the vibrational characteristics as well as chemical property organizer. If it is substituted directly, it will be dominated straight and affect the molecular property rationally. If it is substituted along with the passive and active substitutional groups, it will inject the bound ligand property into the base compound. So, the methoxy enthalpy energy is transferred to the ring by amino group via ethyl group. Since the energy transferred from amino group, the chemical energy may be affected little bit. As per Table 3, vibrations of N–H group was found to be 3450 and 3350 cm\(^{-1}\) (stretching), 1230 & 1220 cm\(^{-1}\) (in plane bending) and 1005 & 1000 cm\(^{-1}\) (out of plane bending) respectively to pronounce the amino group in the ring. Generally, in the case of hydroxylamine, the stretching, in plane and out of plane bending vibrational bands are assigned in the region 3255-3235 cm\(^{-1}\), 1450-1200 cm\(^{-1}\) and 895-650 cm\(^{-1}\) respectively \cite{20}. Actually, instead of suppression of vibrational energy of amino group due to the conjugation of methoxy group, the vibrational bands have elevated to the higher vibrational region when compared with expected limit. The dominated character and endothermic property of the amino group was proved in this case also.

4.4.5. C–O–N and C–O vibrations

The hydroxylamine compound has finite wavenumber in the region 855-840 cm\(^{-1}\) for C–O–N stretching band, 510-420 cm\(^{-1}\) for C–O–N in plane bending and below 300 cm\(^{-1}\) for C–O–N out of plane bending modes. In this case, the stretching, in plane and out of plane bending modes were observed at 1330, 610 and 300 cm\(^{-1}\) correspondingly for the methoxylamine group. From this vibrational process, it was traced that, the bridge bond of C–O–N was intensively pronounced in the wavenumber assignment for the present compound. The C–O stretching signals are normally denoted around the region 1050 cm\(^{-1}\) whereas in this case, it was observed at 1320 cm\(^{-1}\) and the in plane and out of plane bending bands were recognized at 700 and 350 cm\(^{-1}\) respectively. All the vibrational enthalpy energy in the chain bonds were found to be active.

Fig. 4. (A) Experimental and Calculated (B) HF, (C) B3LYP, (D) B3PW91 FT-IR spectra of O-Benzyl Hydroxylamine.
and energized to send the chemical energy to the chain to provide the specific drug kinetics.

4.5. NMR chemical interpretation

The chemical reactivity mechanism of the chemical compound is formulated with respect to the chemical shift regulated in the core as well as ligand merged carbons and their related hydrogens [21]. Usually, the chemical reaction path can be identified through the core carbons due to the charge dislocation take place around the ligand groups are added to the appropriate places in the compound [22]. The chemical mechanism for generating the useful drug activity in the chemical species is setup by the adopting atoms or molecules with the base compound. The charge domain displacement from atom to atom in the molecular entities is achieved by chemical equivalent molecular kinetic forces in the form of coagulation of diamagnetic shield breaking which leading asymmetric charge gradient. The NMR chemical shift representation was presented in Table 4 and its graphical spectra are depicted in Fig. 6.

In this case, this was observed as usual that, the core carbon C3 has shifted more than other carbons in the ring which was the substitutional place. But, the chemical shift core carbons C5, C6 and C1 have unusually shifted (Cal. = 133, 132 and 134 ppm) (Expt. = 128, 127 and 134 ppm). This view showed the extension of reaction path in the core carbons and abruptly the same chemical environment was observed. In the case of C2 and C4, the chemical shift (Cal. = 130 ppm) was found to be lower than C1, C5 and C6, and from which the nodal point of core carbons were identified. This impact was felt in the uniform chemical shift of allied

| Atom position | Chemical shift - TMS-B3LYP/6-311 + G (2d,p) (ppm) | Experimental shift (ppm) |
|---------------|--------------------------------------------------|--------------------------|
|               | Gas Solvent phase                                 |                          |
|               | DMSO CCl₄                                         |                          |
| C1            | 134.25 134.62 134.65 134.0                        |                          |
| C2            | 131.92 130.95 131.61 127.0                        |                          |
| C3            | 145.25 146.28 145.69 135.0                        |                          |
| C4            | 129.21 130.33 129.60 126.5                        |                          |
| C5            | 132.08 131.77 131.30 128.0                        |                          |
| C6            | 132.78 132.91 132.80 127.5                        |                          |
| C12           | 71.87 71.87 71.86 75.0                            |                          |
| H7            | 7.424 7.558 7.480 7.30                            |                          |
| H8            | 7.722 7.714 7.727 7.35                            |                          |
| H9            | 7.101 7.351 7.195 7.3                            |                          |
| H10           | 7.298 7.479 7.368 7.3                            |                          |
| H11           | 7.242 7.392 7.301 7.3                            |                          |
| H13           | 5.426 5.325 5.395 5.15                            |                          |
| H14           | 5.426 5.325 3.549 5.10                            |                          |
| H17           | 2.105 2.256 2.537 -                               |                          |
| H18           | 2.073 2.615 2.294 -                               |                          |
| H19           | 6.534 6.641 6.568 -                               |                          |

Table 4
Experimental and calculated $^1$H and $^{13}$C NMR chemical shift in O-Benzyl Hydroxylamine.

![Fig. 5. (A) Experimental and Calculated (B) HF, (C) B3LYP, (D) B3PW91 FT-Raman spectra of O-Benzyl Hydroxylamine.](image-url)
hydrogens; H7, H9, H10 and H11 (ranged from 7.1 ppm to 7.7 ppm). From this chemical shift of core carbons, it was clear that, the acquired or oriented resultant chemical potential from the chain was restored over the carbons which were identified as chemical shift.

The chemical shift of nodal point carbon; C12 was found to be 71(Cal.) and 75 (Expt.) ppm for ligand chain. This is very low and was due to the refilling of electron domain at the breaking shield of carbonC12 which was gained from the O–NH2 group. The C12 was ensured to be oscillating nodal point about which the chemical potential is oscillated back and forth to facilitate the antiseptic drug potential. Simultaneously, endothermic enthalpy energy was transited from the amino group which was accumulated in O. As the partial charge domain favor for regulating reaction path to charge chemical flavor, the desired chemical potential was attained in the molecular site.

4.6. Molecular interaction profile

The bonding MOs primarily hold base as well as ligand character to interact with each other and the degenerative orbitals communicated in terms of chemical energy accumulated in the form of nucleophilic and electrophilic to explain the structure and reactivity of molecules [23]. The molecular reactivity for the formation of useful application is represented by sensitive types of bonding and is shown in Fig. 7 and the energy levels shown in Table 5. Accordingly, the 6-nucleophilic bonding interaction (HOMO) appeared on the semicircle of the benzene ring which is isolated from the ligand group and small ligand interactive overlapping was found on the ligand group separately. Here, two discrete orbital interactions take place for generating individual chemical characteristics and they found to be ready to donate the electron domain for enabling reactivity. In first order electrophilic orbital interaction (LUMO) called unfilled interfacial space orbital system. Here, the σ-bonding overlapping was found and among them, the diagonal cross interaction was appeared. One of the σ-bond of core carbon was interlinked with C12 of ligand group which is able to blend the obtained electron cloud character with benzene ring. In the case of HOMO, the interconnected bond orbitals opened to nucleophilic interaction in which the degenerate orbitals overlapped with one another and making group interaction domain cloud. In the case of LUMO, the σ-interactive orbitals overlapped with one another formed electrophilic affinity orbital array by which the electronic domain with restricted chemical energy of 2.95 eV can be established.

In second order nucleophilic interactive orbitals, π-bond interactive zones were found in semicircle of benzene ring and which are appeared to be interlinked with degenerate orbitals of CH2O and NH2. Here, the space interaction orbital lobe was seen in H with N and it was shown in Figure. In the second order LUMO orbital interaction, there was no electrophilic zone observed to enhance the remaining molecular property. In this case, all the property making process was occurred in first order only and it was clearly showed the molecular direct drug property. From this observation, it was inferred that, this molecule is able to have additional ligand group for preservative drug potential.

Fig. 6. (A) 13C, (B) 1H Experimental and (C) 1H, (D) 13C Calculated NMR spectra of O-Benzyl Hydroxylamine.
4.7. UV-visible spectra-CT complex

Usually, the UV-Visible spectra represented the electronic absorption process take place inside the electronic configuration of molecular system [24]. UV-Visible joint spectral pattern clearly showed the vibrational energy exchange between the molecular entities via bonds made from the incorporation of base and ligand groups [25]. By the accumulated electronic transitions in the form of absorptive peak in the respective electronic region of spectrum, the formation of CT complex in the molecular system is viewed. Though, there are many background causes to describe the formation of CT complex and it is very difficult to explain the CT mechanism structure [26].

Here, the CT complex spectral peak was observed at 590 nm along with supplementary peaks at 470 and 480 nm as shown in Fig. 8. The calculated spectral values are depicted in Table 6 and according to which the peaks at 609, 484 and 473 (Cal.) at oscillator strength of 0.04, 0.005 and 0.01 with the energy gap of 2.03, 2.55 and 2.62 eV respectively. These absorption peaks were assigned to n-π* transition which belongs to R-Band (German, radikalartig) and especially, these electronic signals situated at higher wavelength region (Visible-red region). If the electronic spectral peak is observed at visible region for the chemical species and it will be very active with visible light (Photo catalytic excitation).

Here, the entire spectral pattern appeared in visible red and blue regions which showed that, the present chemical is photo-active and produce photo-catalytic process in chemical reaction. All the transitional modes were displayed in spectrum by obtaining the chemical energy from HOMO to LUMO-1 and second order orbital sequence. Here, from the
nucleophilic and electrophilic interaction arrangement and electronic absorption peaks showed that, the C–C and O–N were found to be CT complex by which the antiseptic as well as antibiotic properties in the compound was induced.

4.8. Physico-chemical parameters

For the optimized structure, the molecule should have very low vibrational energy at zero state. Here, the molecular structure without cis and trans formation, has the zero point vibrational energy of 863 and 862 Hartree in IR and UV-Visible region respectively. So it was concluded that, the structure was comfortably making fundamental property with low amount of energy in UV-Visible region than IR. The resultant dipole moment of the molecule was 1.18 and 2.09 dyne in both regions respectively. This was comparatively low which is due to the molecule situated in restricted planes and occupies very low 3D space view. All the physico-chemical parameters are illustrated in Table 7.

The electron affinity and ionization potential were 6.9 & 3.7 and 0.63

Table 6
Theoretical electronic absorption spectral values of O-Benzyl Hydroxylamine.

| λ (nm) | E (eV) | f | Transition level | Major contribution | Assignment | Region | Bands |
|--------|--------|---|-----------------|-------------------|------------|--------|-------|
| Gas    | 609.47 | 2.0343 | 0.0488 | H→L (69%) | H→L | n→π⁺ | Visible-red | R-band (German, radikalartig) |
|        | 484.67 | 2.5581 | 0.0052 | H→L-2 (58%) | H→L-1 | | Visible-blue |
|        | 473.03 | 2.6210 | 0.0159 | H→L-1 (59%) | H+1→L | | Visible-blue |
| DMSO   | 556.25 | 2.2289 | 0.0588 | H→L (53%) | H→L | n→π⁺ | Visible-blue | R-band (German, radikalartig) |
|        | 488.11 | 2.5401 | 0.0154 | H→L-2 (42%) | H→L-1 | | Visible-blue |
|        | 484.01 | 2.5616 | 0.0140 | H→L-1 (52%) | H+1→L | | Visible-blue |
| CCl₄   | 594.42 | 2.0858 | 0.0604 | H→L (64%) | H→L | n→π⁺ | Visible | R-band (German, radikalartig) |
|        | 486.80 | 2.5469 | 0.0068 | H→L-2 (57%) | H→L-1 | | Visible-blue |
|        | 478.37 | 2.5918 | 0.0173 | H→L-1 (61%) | H+1→L | | Visible-blue |

H: HOMO; L: LUMO.

Fig. 8. (A) Experimental and (B) Calculated UV-Visible spectra of O-Benzyl Hydroxylamine.
more than UV region. The aromatic species are always structurally as different physico-chemical properties. The chemical potential of the present compound is able to receive more ligand groups to explore the chemical inertness was so high and compliance was so poor and the interaction was found to be taking place between ring and ligand groups and these exchanges of energy was very high when compared with bonding system. The important transition was found to be taking place between ring structure and ligand groups. From the lone pair of O15 the considerable amount of energy was transferred between the non bonding orbitals of transitional exchange of chemical potential, 20.78 and 20.61 kcal/mol. Here, the moderate number of transitions was taken place by the present compound.

3.11. NBMO electronic transition analysis

According to Huckel's Molecular Orbital Theory, some of higher the non bonding molecular orbitals are filled with paired electrons (donor) and low level non bonding MO was completely unfilled (Acceptor) and according to the LCO arrangements, the interaction was induced by equilibrium interactive forces enhanced among the molecular sites [29]. Among the interactive filled and unfilled orbitals, the important chemical energy exchanged to oscillate the chemical potential to generate the source of chemical properties [30]. The energy exchange transition of title molecule is depicted in Table 9.

In this case, the interaction was found to be taking place between ring and ligand groups and these exchanges of energy was very high when compared with bonding system. The important transition was observed from C1 – C6 to C2 – C3 and C4 – C5 by intake of energy of 20.35 and 19.77 kcal/mol. in terms of \( \pi^* \) and \( \sigma^* \) interactive system within the ring. Similarly, the significant exchange of energy of 20.64 and 20.58 kcal/mol were identified from C2 – C3 to C1 – C6 and C4 – C5 respectively and these transitions were assigned to \( \pi^* \).

In the reversible interaction of non bonding, the same transition was found between C4 – C5 and C1 – C 6 & C2-C3 in the ring itself. For that transitional exchange of chemical potential, 20.78 and 20.61 kcal/mol. amount of energy was transferred between the non bonding orbitals of bonding species. From the lone pair of O15 the considerable amount of chemical energy was exchanged to C12–H13 and C12–H14 by taking the energy of 5.52 and 5.48 kcal/mol. which was assigned by L-\( \sigma^* \) interactive system. Here, the moderate number of transitions was taken place by which the substantial amount of energy was exchanged in another phase to arrange the antiseptic potential. In addition to that, according to the

4.10. Hyperactive biological activity

The molecular bonds arrangements inside the limited iso volume of the molecule produced the hyper polarization which causing the molecular components depletion multiple moments [28]. The hyperactive parameters are presented in Table 8. The active bond polarization atmosphere produced net molecular moments from which net and average polarizability were measured and are to be 144 × 10^{-3} esu and 194 × 10^{-3} esu respectively. These were extracted from intensive dipole bonds and these values so high to produce sensitive biological activity. In addition to that, the hyper active polarization also produced in the molecular site which showed the enhancement of biological involvement of the molecule. Here, it was calculated to be 294.21 × 10^{-3} esu and this was achieved from the resultant dipole moment of the molecule. It was considerably strong and the definite biological support can be provided by the present compound.

Table 8
The Polarisability (a.u.) and the first Hyperpolarizability (\( \beta \) (esu)) of O-Benzyl Hydroxylamine.

| Parameters         | B3LYP/6-311++G (d,p) | Parameters         | B3LYP/6-311++G (d,p) |
|--------------------|----------------------|--------------------|----------------------|
| \( \alpha_{\text{ax}} \) | -53.8786             | \( \beta_{\text{ax}} \) | 72.1308              |
| \( \alpha_{\text{ay}} \) | 1.0559               | \( \beta_{\text{ay}} \) | 25.1519              |
| \( \alpha_{\text{az}} \) | -64.3972             | \( \beta_{\text{ay}} \) | 32.4619              |
| \( \alpha_{\text{xy}} \) | 0.0757               | \( \beta_{\text{yy}} \) | -11.0358             |
| \( \alpha_{\text{xz}} \) | 2.1437               | \( \beta_{\text{zz}} \) | -14.5590             |
| \( \alpha_{\text{yz}} \) | -64.6896             | \( \beta_{\text{yz}} \) | -22.9781             |
| \( \alpha_{\text{zt}} \) | 144.833              | \( \beta_{\text{zt}} \) | 2.5713               |
| \( \Delta \alpha \) | 194.028              | \( \beta_{\text{ax}} \) | 19.4169              |
| \( \mu_{\text{x}} \) | 1.1149               | \( \beta_{\text{yx}} \) | -3.6523              |
| \( \mu_{\text{y}} \) | 0.3059               | \( \beta_{\text{xy}} \) | 8.5432               |
| \( \mu_{\text{z}} \) | -0.1941              | \( \beta_{\text{zz}} \) | 294.21               |
| \( \rho_{\text{elu}} \) | 1.1894               |                     |                      |
previous case \[31\] which dealt antibiotic properties, almost same amount of chemical potential exchange was observed. According which, in this case also, the antibiotic equivalent potential exchange was observed. So, it was concluded that, this present case, having antibiotic characteristics along with antiseptic property.

4.12. VCD graph analysis

The VCD spectra of drug aromatics are much sensitive to measure the asymmetrical sequence of vibrations of compositional parts in dichroic form which is used to characterize drug toxicity \[32, 33\]. The Asymmetrical displacement of absorption and transmission sequence pattern of present molecule was presented in Fig. 10. According to the figure, the asymmetrical sequence was found to be far infrared region which showed the low level wavenumber ligand vibrations. This may be due to the atomic placement in multiple planes and it will not produce any adverse effect. At mid IR region, the strong peak was represented the important ligand characteristics which showed the clear enantiomer property. Such type of strong intensive dichroic peak holds the mirror characteristics of chemical species. In the case of near IR region, the transmission peak was administrated the vibrational dichroism which showed the vibrational property of amino group. Usually, the chemical characteristics are

| Donor NBO (i) | Acceptor NBO (j) | Transitions | E (2) kcal/mol | E(j)-E(i) a.u. | F(i,j) a.u. |
|---------------|------------------|-------------|----------------|----------------|-------------|
| C1 – C2       | C2 – C3          | σ-σ*        | 3.28           | 1.28           | 0.058       |
| C1 – C2       | C3 – C12         | σ-σ*        | 3.54           | 1.12           | 0.056       |
| C1 – C4       | C1 – C2          | π-π*        | 2.74           | 1.28           | 0.053       |
| C1 – C4       | C5 – C6          | π-π*        | 2.68           | 1.28           | 0.052       |
| C1 – H7       | C2 – C3          | σ-σ*        | 20.35          | 0.29           | 0.069       |
| C1 – H7       | C5 – C6          | σ-σ*        | 19.77          | 0.28           | 0.067       |
| C2 – C3       | C1 – C2          | σ-σ*        | 3.54           | 1.12           | 0.056       |
| C2 – C3       | C3 – C4          | π-π*        | 3.52           | 1.27           | 0.060       |
| C2 – C3       | C1 – C6          | π-π*        | 20.64          | 0.28           | 0.068       |
| C2 – C3       | C4 – C5          | π-π*        | 20.58          | 0.28           | 0.068       |
| C3 – C4       | C2 – C3          | π-π*        | 20.78          | 0.28           | 0.068       |
| C4 – C5       | C4 – C5          | π-π*        | 20.61          | 0.28           | 0.069       |
| C4 – C5       | C2 – C3          | π-π*        | 5.52           | 0.70           | 0.056       |

Fig. 9. (A) Filed view, (B) Depletion view and (C) vector depleted view; MEP view of O-Benzyl Hydroxylamine.
dominated by amino group present in the molecule and similarly, this
group dominates in this case also. But, here, the end position of amino
group, the vibrational dichroism showed contradictory enantiomer
characteristics.

5. Conclusion

The aromatic drug species; O-Benzyl hydroxylamine was analyzed to
explore drug, biological properties and hereby the antiseptic property
was evaluated and validated. The molecular spectroscopic and theoret-
cal tools with efficient method were used to carry out the investigation
on molecular structural and vibrational characteristics. The atomic
displacement on molecular site was monitored in order to explore the
physical parameters evaluation to explain the physical characteristics.
Asymmetrical dislocation of charge levels on ligand verses base com-
pound was measured and the asymmetry of Mulliken molecular elec-
tronics arrangement was monitored in order to find the cause of drug
activity configuration. All the biological parameters were checked to
expose the biological involvement of the present molecule. The Lipinski
core rule validates the drug potential and enzyme inhibitor coefficient
was tested to antiseptic intensiveness of the drug. The ligand group and
base core participation in the structural properties in terms of vibrations
were tested in different wavenumber region. The chemical reaction path
was identified in the core carbo-bonds and the oscillation of the chemical
potential around the molecule was monitored with the stipulations of
chemical shift. The interconnected bond orbitals opened the nucleophilic
and electrophilic interaction from which the degenerate orbital profile
was studied to explore exact interactive bonding energy to induce drug
activity. The non bonding partial energy exchange was measured for
important molecular site and reason for inducement of antiseptic nature.
The hyperactive pressure produced by the molecular multipole moments
of the molecule for biological endurance was evaluated.

Declarations

Author contribution statement

S Ramalingam: Conceived and designed the experiments.
A A. Abbas Manthiri: Analyzed and interpreted the data; Wrote the
paper.
Gene George: Contributed reagents, materials, analysis tools or data.
R Aarthi: Performed the experiments.

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Additional information

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