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COMPUTATIONAL STUDIES OF TRIAZOLE DERIVATIVE

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Abstract – *The use of quantum chemical techniques to make virtual determinations in corrosion inhibition investigations has become standard practise. The electronic density and quantum chemical characteristics, including the highest occupied molecular orbital (HOMO), lowest unoccupied molecular orbital (LUMO), and HOMO-LUMO energy gap, are virtually identified. It is simple to screen the structure and activity of compound, even ones that have not yet been using computational methodology and a set of mathematical equations that can precisely reflect the chemical phenomenon under investigation. This study explains the theoretical justification and exploratory intent behind the specific evidence of nuclear structure, HOMO–LUMO gap, the molecular electrostatic potential, and mulliken charges utilising a density functional theory (DFT) system with a B3LYP/6-311++ basis set and the calculated Fukui and Parr functions have been used to locate the reactive electrophile and nucleophile centers in the molecule.*

Key Words: **Density Functional Theory, HOMO-LUMO Energy Band Gap, Chemical Potential, Electrophilicity**

1.INTRODUCTION

Triazoles are heterocyclic compounds with three nitrogen atoms that belong to the nitrogen class. Depending on where the nitrogen is bonded, they can be found in the 1,2,3-triazole and 1,2,4-triazole tautomeric forms Triazole[1] compounds have been employed as pioneer structures in numerous fields for a long time[2]. Numerous biologically active classes, such as those that are antitubercular3, anticancer[3], antiviral[4], anti-inflammatory[5], antiepileptic[6], antidepressant[7], antidiabetic[8], antianxiety[9], antitubercular[10], antibacterial[11], antifungal[12], and antioxidant[13], have triazole nuclei in their structures. Additionally, several triazole compounds are sold as medicines. Triazole 1,2,4 Three nitrogen atoms make up the ring, which can act as a hydrogen bond acceptor or donor at the receptors' active site and control the activity of the receptors accordingly. Due to its polar nature, the triazole nucleus can improve pharmacokinetic and pharmacodynamic properties and boost the solubility of the ligands. The study of 1, 2, and 4 triazole medicines has increased during the past few decades. Among them, 3-amino-1,2,4-triazoles derivatives have drawn particular interest due to their wide range of bioactivities, which include prospective uses against thrombotic disorders, fibrotic, auto-immune diseases, and central nervous system disorders. As of right now, research indicates that 1,2,4-triazole is a crucial and more promising ant proliferative impact, but as more and more studies come to Heterocyclic chemistry serves as an illustration for the lack of clear boundaries because it permeates many of the other chemical fields. Triazole 1,2,4 Three nitrogen atoms make up the ring, which can act as a hydrogen bond acceptor or donor at the receptors' active site and control the activity of the receptors accordingly. Due to its polar nature, the triazole nucleus can improve pharmacokinetic and pharmacodynamic properties and boost the solubility of the ligands. The study of 1, 2, and 4 triazole medicines has increased during the past few decades. Among them, 3-amino-1,2,4-triazoles derivatives have drawn particular interest due to their wide range of bioactivities, which include prospective uses against thrombotic disorders, fibrotic, auto-immune diseases, and central nervous system disorders. As of of novel medications contain heterocycles. fibrotic, auto-immune diseases, and central nervous system disorders. As of right now, research indicates that 1,2,4-triazole is a crucial and more promising ant proliferative impact, but as more and more studies come to light, 1,2,3-triazole will also emerge as a crucial component.The most potent heterocycles with notable biological effects, such as antifungal, anti-inflammatory, antibacterial, anticonvulsant, antiallergic, herbicidal, and anticancer activity, are covered in this review article.

It is now well established that theoretical calculations, such as the Density Functional Theory approach (DFT), are a useful method for assessing the structural and spectral properties of organic molecules. Several published DFT tests have documented a wide range.

2. COMPUTATIONAL DETAILS

Using the usual geometric parameters, geometry optimization was performed as the first task in density functional theory calculation without using any constraints. The optimized ground state structure is as shown in Fig.1. Molecular geometry is a sensitive indicator of intra and intermolecular interactions. The accurate determination of geometrical deformation in

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substituted benzimidazole rings is an important tool for investigating the nature of the interactions between the ring and the substituent's .The geometry of N-((1H-benzo[d] imidazol-2-yl) methyl)-4H-1,2,4-triazol-4-amine was optimized at DFT (B3LYP) levels using 6-311++G (d,p) basis set. All DFT calculations of the 1A[14] compound were carried out using Gaussian 09[15] program package using default thresholds and parameters.

It is observed that most of the optimized bond lengths and bond angles are slightly shorter, as well as longer than the experimental value in B3LYP method. As a result of partial protonation of both nitrogen atoms C1-N2 and C3-N2 bond lengths in benzimidazole moiety is 1.3767 & 1.3724 Å.

For the 1A compound, Triazole ring attached to second position of benzimidazole were found to be planar with the ring. This result was supported by the fact that the computed dihedral angles for N5-C1-C10-N16 and N2-C1-C10-N16 are 0° or 180°.

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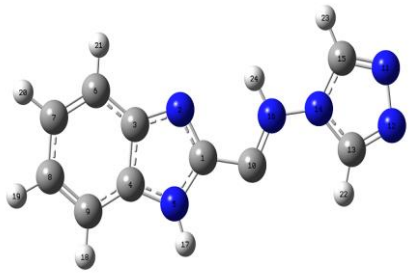


Fig -1: Optimized molecular geometries and atomic numbering of 1A

2.1 HOMO–LUMO Analysis:

Molecular orbitals include HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital). For chemists and physicists, these electronic characteristics were crucial. The inner-maximum orbital known as the LUMO contains free sites to merely take electrons. The HOMO stands for the ability to give an electron, while the LUMO, which is an electron acceptor, stands for the ability to receive an electron. The kinetic stability, chemical reactivity, optical polarizability, and chemical hardness-softness of a molecule are all governed by the energy difference between HOMO and LUMO. HOMO-LUMO energy gap has been estimated at the DFT level. The chemical activity of the molecule is reflected in the Eigen values of the LUMO-HOMO energy gap. Figure 2 illustrates the molecular orbitals atomic orbital compositions The atomic orbital compositions of the molecular orbitals are sketched in Fig.2. The calculated energies and the energy gap is

HOMO energy = −4.6885eV,
LUMO energy = −2.1660eV,
HOMO—LUMO energy gap = −2.5224eV.

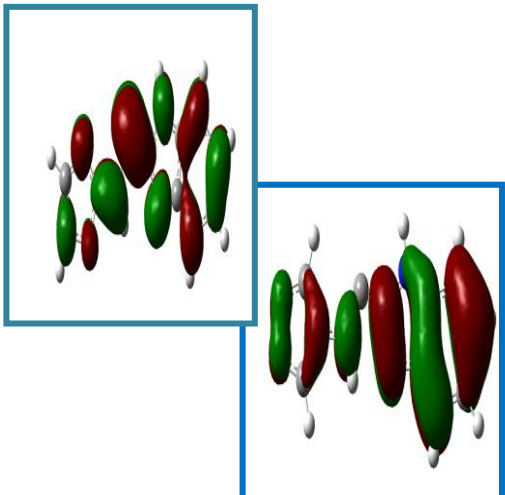
The lower with inside in the HOMO and LUMO energy gap explains the eventual charge transfer interaction taking place within the molecule, due to the strong electron-accepting ability of the electron acceptor group. The strong charge transfer interaction is responsible for the bioactivity of the molecule.

2.2. LOCAL REACTIVE DESCRIPTORS

All the calculated values of ionization potential, electron affinity, hardness, potential, softness and electrophilicity index are shown in Table 1. Compound 1A with higher energy E_{HOMO} = −4.6885eV allows it to be the best electron donor and the lowest LUMO energy E_{LUMO} = −2.1660eV which signifies that it can be the best electron acceptor. The two properties like I (potential ionization) and A (affinity) are so important, the determination of these two properties allow us to calculate the absolute electro negativity (χ) and the absolute hardness (η). These two parameters are related to the one-electron orbital energies of the HOMO and LUMO respectively.

TABLE-1

Parameters	1A
E_{HOMO} (eV)	−4.6885
E_{LUMO} (eV)	−2.1660
ΔE_{gap} (eV)	−2.5224
Ionization potential IE (eV)	4.6885
Electron affinity A (eV)	2.1660
Electro negativity χ (eV)	-3.4272
Global hardness η (eV)	3.4272
Chemical potential μ (eV)	1.2612
Chemical softness α(eV)	0.1982
Global electrophilicity index ω (eV)	2.3282



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HOMO **LUMO**

Fig -2: HOMO-LUMO pictures of compound 1A

2.3. Molecular electrostatic potential map (MEP)

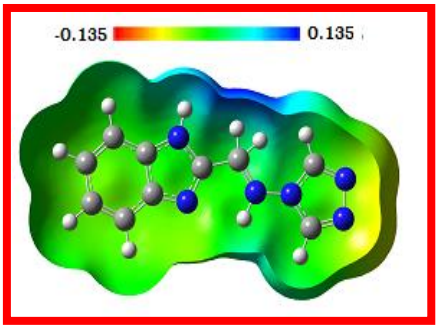

Fig -3: MEP pictures of compound 1A

The electrostatic potential surface (MEP) displays electrostatic potential (electron+ nuclei) distribution, molecular shape, size of the molecule and it provides a visual method to understand the relative polarity of the compounds. Electrostatic potential maps illustrate the charge distribution of molecules three dimensionally. These maps allow us to visualize the different polar regions of a molecule. Knowledge of the charge distributions can be used to determine how molecules interact with one another. The total electron density and MEP surfaces of of N-((1H-benzo[d] imidazol-2-yl) methyl)-4H-1,2,4-triazol-4-amine are constructed by using B3LYP/6-311G (d,p) method. The total electron density surface mapped with electrostatic potential is given in Fig.3.The negative electrostatic potentials are shown in red, the intensity of which is proportional to the absolute value of the potential energy, and positive electrostatic potentials are shown in blue while green indicated surface areas where the potentials are close to zero. Local negative electrostatic potentials (red) nitrogen atoms with lone pair of electrons whereas local positive electrostatic potentials (blue) signal hydrogen's in C-H.

3. CONCLUSION

In this work, we have performed the theoretical DFT analysis of a pharmaceutically important heterocyclic aromatic molecule, N-((1H-benzo[d] imidazol-2-yl) methyl)-4H-1,2,4-triazol-4-amine for the first time. The optimized molecular geometry, energy gap between HOMO-LUMO and Molecular electrostatic potential of the N-((1H-benzo[d] imidazol-2-yl) methyl)-4H-1,2,4-triazol-4-amine in the ground state have been calculated by using DFT (B3LYP) methods with 6–311++G (d, p) basis set. Furthermore, the absolute electro negativity (χ) , the absolute hardness (η) ionization potential, electron affinity, hardness, potential, softness and electrophilicity index of the compound have been calculated in order to get insight into molecular structure of the compound. The greatest and least maximum and minimum observed total electron density of the (1A) particle is $\pm 0.135e^{0}$.The calculated frontier molecular orbitals and related parameters shows that eventual charge transfers takes place within the molecule and the molecule is chemically reactive.

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