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DFT STUDIES OF OXAZOLE DERIVATIVE

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Abstract – *The theoretical calculations of the oxazole derivative has been carried out using the more popular density functional theory method, Becke-3-Parameter-Lee-Yang-Parr (B3LYP) in 6-311G++(d,p) basis set.. In this work we employed the Density Functional Theory (DFT) in our calculations to predict the optimized structure, HOMO-LUMO energies, and chemical reactivity parameters including chemical potential, global chemical hardness, electrophilicity index and polarizability revealing that the compound is highly reactive.*

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

1.INTRODUCTION

Heterocyclic chemistry serves as an illustration for the lack of clear boundaries because it permeates many of the other chemical fields. The processes of life are intricately linked with heterocycles. The crucial importance of heterocycles to the pharmaceutical and agrochemical industries is frequently linked to their existence in nature. Many heterocyclic systems are available thanks to synthetic chemistry. The boundary between chemistry and biology, where so much new scientific understanding, discovery, and application is taking place, is spanned by heterocyclic molecules, and more than 90% of novel medications contain heterocycles. 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.

A member of the azole family of heterocyclic compounds, oxazole is a five-member heterocycle with two significant hetero atoms—nitrogen and oxygen—included in its cyclic structure. One of the best scaffolds for the discovery of new drugs is oxazole[1-10]. The distinctive characteristics of the oxazole moiety's structure give its derivatives the ability to exert a variety of supramolecular interactions, including van der Waals forces, hydrophobic effects, hydrogen bonds, coordination bonds, ion-dipole interactions, and cation-p and p-p stacking interactions. As a result, molecules based on oxazoles have a wide range of potential uses, including those in medicine, agriculture, and chemicals. activity with antibacterial, anticonvulsant, allergenic, herbicidal, and anticancer properties Exhibiting extensive biological activities , such as antibacterial, antifungal, antiviral, antitubercular, anticancer, and antiinflammatory properties, oxazole compounds in medicinal chemistry could easily bond with a range of enzymes in biological systems.

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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

All DFT calculations of the 1A[11] compound were carried out using Gaussian 09[12] program package using default thresholds and parameters]. The ground state structural geometries were fully optimized at the B3LYP method along with the standard 6-311g basis sets . In the DFT calculations the Lee, Yang and Parr correlation functional is used together with Beck's three parameters exchange functional B3LYP The molecular geometry has not been limited and all the calculations (optimized geometric parameters and other molecular properties) have been performed using the Gauss View[13] molecular visualization program and the Gaussian 09W program package. Structural parameter like bond distance, length or radius is the

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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 .The oxazole ring N15–C16–O12 and O12–C13–C14 bond angles are 114.1 and 107.4°, oxazole to benzimidazole ring [O12–C16–N11] is 117.1-124.0°, respectively. Also the predominant oxazole *via* C10 benzimidazole ring dihedral angle O12–C16–N11–C10 is found to be 170-180.0° for B3LYP/6-31 G (d,p) method. The above explanation obviously indicates that 1A has almost same geometrical parameters and which is reveals that the C10 benzimidazole ring and oxazole ring are in same plane.

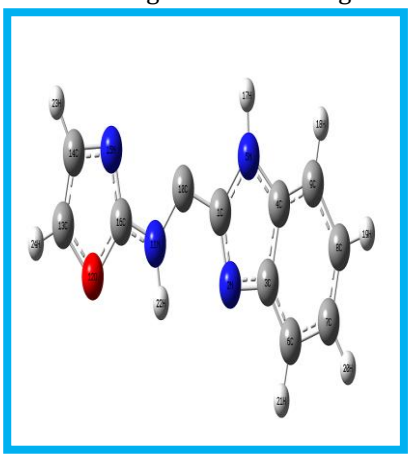


Fig -1: Optimized molecular geometries and atomic numbering of 1A

2.1. FRONTIER MOLECULAR ORBITALS:

The energy gap measures the kinetic energy stability of the molecules. Considering the chemical hardness, large HOMO-LUMO gap means a hard molecule and small HOMO-LUMO gap means a soft molecule and also can relate the stability of the molecule to hardness, which means that increase of the HOMO-LUMO energy gap decreases reactivity of the compound that leads to increase in the stability of the molecule . The frontier molecules orbital, HOMO and LUMO and frontier molecular energy gap helping the reactivity and kinetic stability of molecules are essential parameters in the electronic studies . The energy values of HOMO (EHOMO) and LUMO (ELUMO) are 5.6518 and 0.8083 for 631-G , 4.8435eV respectively. In the studied compound the HOMO-LUMO energy gap (ΔE) is 4.8435eV that reflects the chemical reactivity of the molecule.

2.2. LOCAL REACTIVE DESCRIPTORS

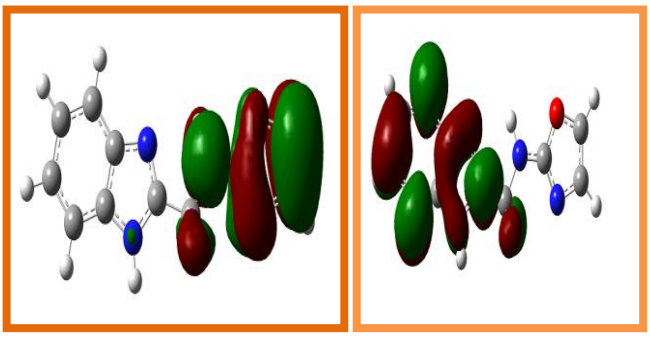
The molecule with highest E_{HOMO} value has highest tendency to donate electrons to appropriate acceptor molecule of low empty molecular orbital energy. From results of quantum chemical calculations, it was evident that 1A(Fig.2) had highest value of E_{HOMO} -5.6518 (eV) and would be better adsorbed on metal surface and be a best corrosion inhibitor. Energy gap (ΔE) provides information about overall reactivity of a molecule. As ΔE decreases, reactivity of molecule increases leading to increase in inhibition efficiency of molecule. Low values of ΔE gap will render good inhibition efficiencies since energy to remove an electron from last occupied orbital will be minimized . From the quantum chemical study, tendency for (ΔE) value which suggests that 1A was good reactivity and would therefore likely interact strongly with metal surface and act as good inhibitor.

High ionization energy indicates high stability and chemical inertness and small ionization energy indicates high reactivity of the atoms and molecules .Absolute hardness and softness are important properties to measure molecular stability and reactivity. A hard molecule has a large energy gap and a soft molecule has a small energy gap .For simplest transfer of electron, adsorption could occur at part of molecule where softness (S), which is a local

TABLE-1

Parameters	1A
E_{HOMO} (eV)	-5.6518
E_{LUMO} (eV)	-0.8083
ΔE_{gap} (eV)	-4.8435
Ionization potential IE (eV)	5.6518
Electron affinity A (eV)	0.8083
Electro negativity χ (eV)	-3.2300
Global hardness η (eV)	2.4217
Chemical potential μ (eV)	3.2300
Chemical softness α(eV)	0.2064
Global electrophilicity index ω (eV)	2.1540

property, has a highest value 1A with softness value of 0.2128 has highest inhibition efficiency. 1A with low hardness value 0.2064 (eV) have a low energy gap. Normally, inhibitor with least value of global hardness can be expected to have highest inhibition efficiency .



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HOMO **LUMO**

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

2.2. Molecular electrostatic potential map (MEP)

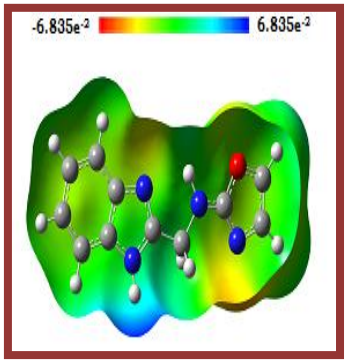

Fig -3: MEP pictures of compound 1A

The MEP surface displays the molecular shape, size and electrostatic potential value. The color scheme for the MEP surface is partially negative charge or red-electron rich; partially positive charge or blue-electron deficient; yellow slightly electron rich region; light green-slightly electron deficient region, respectively. Potential increases in the order red < orange < yellow < green < blue. The MEP diagram of 1A is shown in Fig. 3.

The molecule must present atoms either with positive potential isosurface and atoms with negative potential isosurface. MEP is very helpful for the qualitative elucidation of electrophilic and nucleophilic reactions for the study of biological discovery process and hydrogen bonding interactions . An electron density iso-surface mapped with electrostatic potential surface depicts the size, shape, charge density and site of chemical reactivity of the molecule From the MEP picture, oxygen has higher electronegativity value than hydrogen and carbon.

These surfaces are accustomed compare different inhibitors with substrates or transition states of the reaction. Electrostatic potential surfaces are either displayed as iso contour surfaces or mapped onto the molecular electron density

3. CONCLUSION

In this study work, we have performed the theoretical DFT analysis of a pharmaceutically important heterocyclic aromatic molecule, N-((1H-benzo[d] imidazol-2-yl) methyl) oxazol-2-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) oxazol-2-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 $\pm 6.835e^{-2}$. The calculated frontier molecular orbitals and related parameters shows that eventual charge transfers takes place within the molecule and the molecule is chemically reactive.

REFERENCES

1. Smith, A. L.; Nicolaou, K. C., J. Med. Chem., 1996, 39, 2103.
2. Gringauz, A. Introduction to medicinal chemistry, Wiley-VHC, 1997
3. Matsuda, H.; Morikawa, T.; Ando, S.; Iwao, T.; Masyuki, Y., Bioorg. Med. Chem., 2003, 11, 1995.
4. Zhen Z,; Zhi-Long Z,; Cheng-He Z,; Eur. J. Med. Chem., 2018, 144, 444
5. Shriram P, Kumar D, Sudhir I, et al. Study on Synthesis and Different Biological Activities of Oxazole Based Derivatives. Unique Res. J. Chem. 2013;1:16–29.
6. Turchi IJ, Dewar MJ. Chemistry of oxazoles. Chem Rev. 1975;75(4):389–437.
7. Kharb R, Sharma J, Sharma AK. Vistas of Novel Oxazole Derivatives as Potent Antimicrobial Agents. Int J Adv Pharm Bio Chem. 2013;2(2):390–404.
8. Zhang HZ, Zhao ZL, Zhou CH. Recent advance in oxazole-based medicinal chemistry. Eur J Med Chem. 2018;20(144):444–492.
9. Kakkar S, Narasimhan B. A comprehensive review on biological activities of oxazole derivatives. BMC Chem. 2019;13(1):1–24.
10. Rymbai EM, Chakraborty A, Choudhury R, et al. Review on chemistry and therapeutic activity of the derivatives of furan and oxazole: the oxygen containing heterocycles. Der Pharma Chemica. 2019;11(1):20–41
11. C.M. Mahalakshmi and V. Chidambaranathan, "Synthesis, Spectral Characterization And Antimicrobial Studies Of Novel Benzimidazole Derivatives," *Int. J. Chem. Sci.*: 13(1), 2015, 205-212.
12. Frisch, M.J., et al. (2009) Gaussian 09, Revision B. 01. Gaussian, Inc., Wallingford.
13. Dennington, R.D., Keith, T.A. and Millam, J.M. (2008) GaussView 5.0.8, Gaussian