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STRUCTURAL HOMO-LUMO,MEP ANALYSIS AND MULLIKEN CHARGES OF THIAZOLE DERIVATIVE

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Abstract –

The present investigation informs a descriptive study of N-((1H-benzo[d] imidazol-2-yl) methyl) thiazol-2-amine compound, by using density functional theory at B3LYP method with 6-311++G (d,p) basis set.. To determine the energy gap and probable sites of electrophilic and nucleophilic reactivity in the 6-311++G (d,p) basis set, the HOMO-LUMO energies and MEP map were computed. This research used the electrostatic molecular potential (MEP) and electrostatic contour to understand the regions of reactivity of the this molecule.

Key Words: **DFT, HOMO-LUMO, MEP, Mulliken charges,**

1.INTRODUCTION

A stable heterocyclic molecule is produced by thiazole by using both an electron-donating group (-S-) and an electron-accepting group (C=N)[1] . One significant class of heterocycles with numerous biological features is the thiazole and its equivalent, the oxazole[2]. The azole chemical isothiazole, which has the same atoms (nitrogen and sulphur) but in a different location, is isomeric with the thiazole substance. Thiazole is a transparent, pale yellow liquid. Boiling between 116 and 118 degrees Celsius soluble in ether and alcohol but only marginally so in water[3]. Thiazole is a heterocyclic compound that contains a delocalization of six electrons from the sulphide atom's lone pair of electrons, according to Huckel's rule[4]. Due to their planar, aromatic structure and greater -electron delocalization than oxazoles, thiazole derivatives are appealing model molecules for chemistry research.

It has become clear that theoretical calculations, like the Density Functional Theory method (DFT), are an effective way for evaluating the structural and spectral characteristics of organic molecules. A wide variety of thiazole attributes have been described in numerous DFT experiments that have been published [5-9] DFT was also used to characterise newly synthesised thiazole by substitution groups in their derivative structure.

2. QUANTUM CHEMICAL STUDY

The geometry of N-((1H-benzo[d] imidazol-2-yl) methyl) thiazol-2-amine was optimized at DFT (B3LYP) levels using 6-311++G (d,p) basis set. At the optimized geometry for the title molecule no imaginary frequency modes were obtained, so there is a true minimum on the potential energy surface. The optimized molecular structure with symbols and numbering of the title molecule is obtained from Gaussian 09W [10]and Gauss View programs as shown in the Fig. (1).

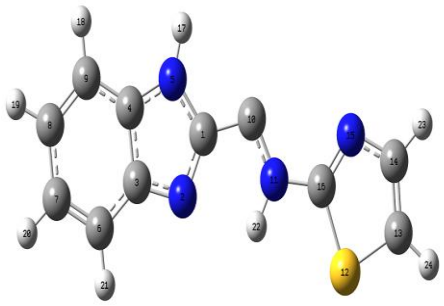

Fig -1: **Optimized molecular geometries and atomic numbering of 1A**

2.1. Structural Parameters

The common distance between the nuclear of two bonded atoms in a molecule is known as a structural parameter, and its values are normally in the range of less than 1 to 2. 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 .

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. In the geometrical parameter of compound **1A**, the thiazole ring C14–N15 (1.378–1.388 Å) bond lengths are greater than the C16–N15 (1.284–1.304 Å), because both are in chemically different environments, which also indicate that the C16–N15 bond has double bond character. Besides, the C16–S12 (1.774-1.798 Å) bond lengths are slightly higher rather than C13–S12 (1.754-1.778 Å). The thiazole ring S12–C16–N15, S12–C13–C14 and N15–C14–C13 bond angles are 114.2 – 113.8°, 109.6 – 108.3° and 117.0°, respectively. Also the prominent thiazole ring *via* benzimidazole dihedral angles C10–N11–C16–N15 is (0)°. The above observations clearly indicate that all the compound 1A are having almost same geometrical parameters and which is reveals that the both benzimidazole rings and thiazole ring are in same plane.

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2.2. HO MO–LUMO Analysis

The highest occupied molecular orbital, HOMO, and the lowest unoccupied molecular orbital, LUMO, of a molecule are called the frontier orbitals. It was Fukui who first noticed the prominent role played by HOMO and LUMO in governing chemical reactions. The positive phase is represented in red colour and the negative phase is represented in green colour. The energy gap of HOMO–LUMO explains the charge transfer interaction within the molecule The HOMO–LUMO analysis for 1A was conducted B3LYP/6-311G (d,p) level of theory is shown in Fig-1.

The calculated energies and the energy gap is

HOMO energy = −5.5293eV,

LUMO energy = −0.8302eV,

HOMO—LUMO energy gap = −4.6991eV.

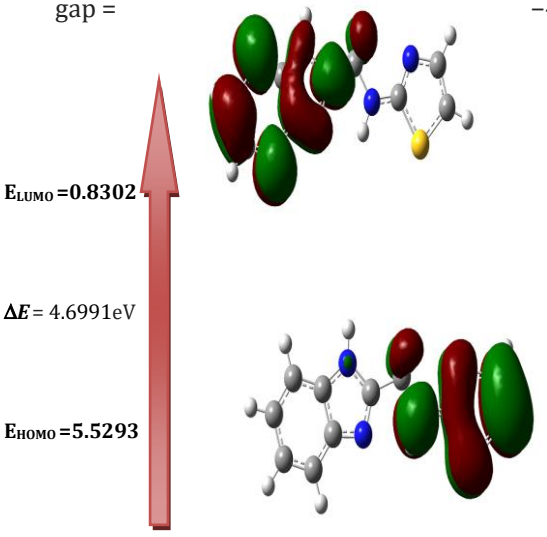


Fig -1: HOMO-LUMO pictures of compound 1A

2.2. . Mulliken charge distribution

Mulliken charge distribution of 1A is presented in Table .1 More negative the atomic charges of adsorbed centre, more easily the atom donates its electron to unoccupied orbital of the metal . Inhibition efficiency of inhibitors under study depends on presence of electronegative atoms in their molecular structure. 1A has more electronegative N5, C13 and N2 with charges -0.428, -0.344 and -0.371 that shows due to more electron-donating nature of the atoms. S12 and C1 in 1A are the most liable sites for nucleophilic attacks with highest positive charge. Therefore, 1A can accept electrons from metal through these atoms and hence could serve as good corrosion inhibitor against metal surface protection.

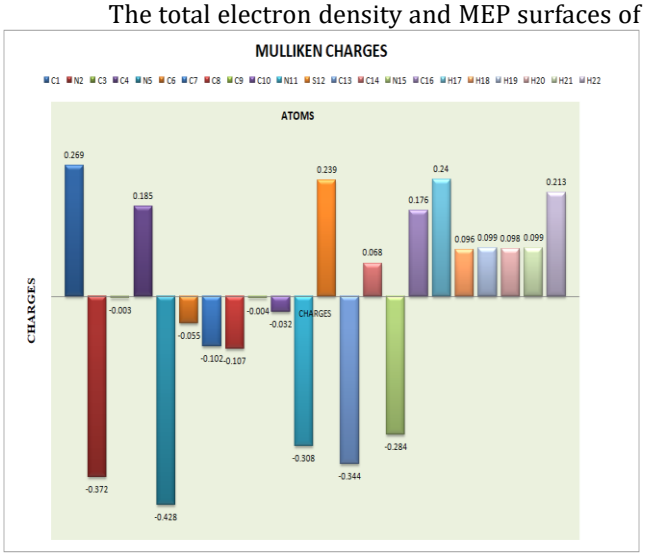
Table:1 Mulliken charges of compound 1A

ATOMS	CHARGES	ATOMS	CHARGES
C1	0.269	C13	-0.344
N2	-0.372	C14	0.068
C3	-0.003	N15	-0.284
C4	0.185	C16	0.176
N5	-0.428	H17	0.240
C6	-0.055	H18	0.096
C7	-0.102	H19	0.099
C8	-0.107	H20	0.098
C9	-0.004	H21	0.099
C10	-0.032	H22	0.213
N11	-0.308	H23	0.119
S12	0.239	H24	0.145

Fig -2 Mulliken charges of compound 1A

2.3. MEP ANALYSIS

The total electron density and MEP surfaces of N-



((1H-benzo[d] imidazol-2-yl) methyl) thiazol-2-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.

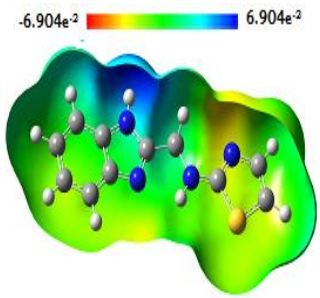


Fig -3.: MEP diagram of compound 1A

3. CONCLUSIONS

In this paper, we have performed the theoretical DFT analysis of a pharmaceutically important heterocyclic aromatic molecule, N-((1H-benzo[d] imidazol-2-yl) methyl) thiazol-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) thiazol-2-amine in the ground state have been calculated by using DFT B3LYP/6-311G (d,p)basis set.. The greatest and least maximum and minimum observed total electron density of the (1A) particle is $\pm 6.904e^{-2}$. The calculated frontier molecular orbitals and related parameters shows that eventual charge transfers takes place within the molecule and the molecule is chemically reactive.

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BIOGRAPHIES

Dr.C.M.MAHALAKSHMI working as an Assistant professor and she has known the knowledge of synthetic organic chemistry ,DFT and Molecular docking studies.