International Research Journal of Education and Technology
Peer Reviewed Journal
ISSN 2581-7795

DFT CALCULATIONS ON MOLECULAR STRUCTURE, HOMO LUMO STUDY REACTIVITY DESCRIPTORS OF TRIAZINE DERIVATIVE

M.LAVANYA [1], Dr.C.M.MAHALAKSHMI[2]

[1]Student, Krishnasamy College of Science, Arts And Management For Women, Cuddalore,India
[2]Assistant professor, Krishnasamy College of Science, Arts and Management for Women, Cuddalore, India

---

Abstract – *Triazine chemistry offers a wide range of uses, from commercial applications like melamine resins to academic research on dendritic structures that could one day lead to molecules with potential for use in medicine. For practical purposes, organic synthesis utilising the 2,4,6-Trichlorotriazine derivative of 1,3,5-triazine, cyanuric chloride, was studied. It is possible to synthesise a wide range of targets, from tiny molecules to giant dendrimers, by taking advantage of the specific reactivity of cyanuric chloride. The synthesis of simazine, a popular herbicide, in an undergraduate laboratory required the adaptation of triazine chemistry for teaching purposes. The laboratory was created to promote an understanding of how chemistry is used in everyday life throughout the world and how it affects society and the environmentThis study explains the theoretical justification and exploratory intent behind the specific evidence of nuclear structure, HOMO–LUMO gap and reactivity descriptors of N-(1H-benzo[d] imidazol-2-yl) methyl)-1,2,4-triazin-3-amine 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. The HOMO-LUMO essentialness levels' uniqueness chooses the molecule's engine steadfastness, substance reactivity, compound nonabrasiveness, and hardness.*

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

1.INTRODUCTION

Triazine is thermally stable up to a point where it decomposes into hydrogen cyanide at temperatures exceeding 600 °C. Electrophilic substitution is largely resisted by the triazine ring. It is, nevertheless, particularly vulnerable to hydrolysis by water and other hydroxyl compounds to a lesser extent, and may rapidly undergo ring cleavage with nucleophiles. By treating 1,3,5-triazine with bifunctional amines or similar substances, a variety of heterocycles can be produced, and it can be utilised in processes in place of HCN.

The most popular triazine derivatives are melamine, cyanuric chloride and cyanuric acid used to create triazines during their initial synthetic process. Triazines can be divided into three classes: 1,2,3-triazine, 1,3,5-triazine, and 1,2,4-triazine. A key role in medicinal chemistry is played by 1,2,4-triazine and its derivatives due to its significant potential for pharmacological actions. Among the activities are those against cancer[1-3], analgesic and anti-inflammatory[4-6], anti–HIV[7,8], anti–microbial [9-11], and anti–malarial [12-15]

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. GROUND STATE STRUCTURE ANALYSIS

The minimum energy configuration of the 1A molecule was again optimized at B3LYP/6-311G++ (d, p) level. The optimized stable geometry and the scheme of atom numbering of the compound of N-(1H-benzo[d] imidazol-2-yl) methyl)-1,2,4-triazin-3-amine[16] is represented in Fig.1. The optimized structural parameters bond length, bond angle and the dihedral angle for the more stable geometry of the title compound is determined at B3LYP with 6-311g basis sets[17,18] are presented in Table 1. 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.

As a result of partial protonation of both nitrogen atoms C1-N2 and C3-N2 bond lengths in benzimidazole moiety are 1.3751 & 1.3897 Å in 1A . From the geometry of compound 1A triazine ring attached to second position of benzimidazole were coplanar with the Benzimidazole ring. This result was confirmed by following torsional angles C10-N11-C14-N13 in 152 and C10-N11-C14-N15 in 153 are 0° and 180°.

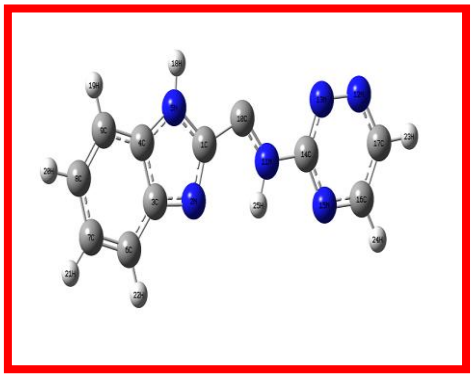
International Research Journal of Education and Technology
Peer Reviewed Journal
ISSN 2581-7795

Table.1. Optimized geometrical parameter compound of 1A

Atom numbering	1A
Bond lengths (Å)	
C1- N10	1.4989
C10-N11	1.4438
C1- N5	1.3751
C3-N2	1.3897
N11-C14	1.3488
N13-N12	1.3233
Bond angles °	
N2-C1-N5	112.9
N2-C1-C10	124.7
C4-N5-C1	107.0
C3-N2-C1	105.4
C1-C10-N11	108.7
N11-C14-N15	117.0
C14-N13-N12	118.1
C14-N15-C16	114.4
Dihedral angles°	
N5-C1-C10-N11	180
N2-C1-C10-N11	0
C14-N15-C16-C17	0

.

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 (E_{HOMO}) and LUMO (E_{LUMO}) are 6.2967 and 1.8096 for 631-G respectively. In the studied compound the HOMO-LUMO energy gap (ΔE) is 4.4871eV that reflects the chemical reactivity of the molecule.

2.2. GLOBAL REACTIVE DESCRIPTORS

Highest occupied molecular orbital (E_{HOMO}), energy of lowest unoccupied molecular orbital (E_{LUMO}), global reactivity parameters such as chemical hardness (η), chemical potential (μ) and electrophilicity index (ω) were obtained to analyse reactivity of inhibitor molecules. Chemical potential is negative of electronegativity (Parr, 1989). Electronegativity is measure of power of an electron or group of atoms to attract electrons towards it.

$$\mu = -\chi \quad \text{--------Eqn.1}$$

Molecular properties related to reactivity and selectivity of inhibitors like ionization potential (I), electron affinity (A), electronegativity (χ), global hardness (η) and softness (σ), were estimated according to Koopman's theorem which relates to energy of HOMO and LUMO. Ionization potential is the amount of energy required to remove an electron from a molecule. Lower the ionization potential, easier is to remove an electron from a molecule. High Ionization energy indicates high stability and chemical inertness and small ionization energy indicates high reactivity of atoms and molecules . Ionization potential (I) can be related to energy of E_{HOMO} through the equation

$$I = -E_{HOMO} \quad \text{--------Eqn.2}$$

Electron affinity (A) can be related to ELUMO through the equation:

$$A = -E_{LUMO} \quad \text{--------Eqn.3}$$

Electronegativity (χ) and global hardness (η) can be determined from the values of I and A. Chemical hardness fundamentally signifies the resistance towards deformation or polarization of electro cloud of the atoms, ions or molecules under small perturbation of chemical reaction. A hard molecule has least tendency to react while a soft molecule has high tendency to react. A hard molecule has a large energy gap and soft molecule has a small energy .

Absolute electronegativity (χ) and absolute chemical hardness (η) of the inhibitor molecule can be given as,

$$\chi = (I + A)/2 \quad \text{--------Eqn.4}$$

$$\eta = (I - A)/2 \quad \text{--------Eqn.5}$$

International Research Journal of Education and Technology
Peer Reviewed Journal
ISSN 2581-7795

TABLE-2

Parameters	1A
E_{HOMO} (eV)	-6.2967
E_{LUMO} (eV)	-1.8096
ΔE_{gap} (eV)	-4.4871
Ionization potential IE (eV)	6.2967
Electron affinity A (eV)	1.8096
Electro negativity χ (eV)	-4.0531
Global hardness η (eV)	2.2435
Chemical potential μ (eV)	-4.0531
Chemical softness α(eV)	0.2228
Global electrophilicity index ω (eV)	3.6611

Electron polarizability, also called as chemical softness (σ) is a measure of capacity of an atom or group of atoms to receive electrons , was estimated by using the equation:

$$\sigma = 1/2\eta \qquad \text{--------Eqn.6}$$

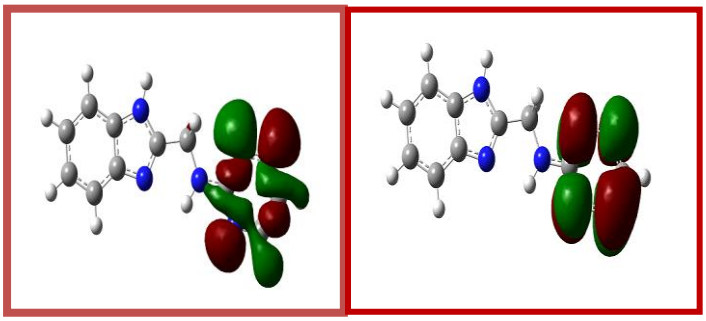
Electrophilicity values gives information on nucleophilic or electrophilic nature of molecule. A high electrophilic value informs that the molecule has a high tendency to act as an electrophile while a low value of electrophilicity informs that the molecule has a high tendency to act as a nucleophile.

The absolute electrophilicity index (ω) can be calculated by the equation

$$\omega = \mu^2 / 2\eta \qquad \text{--------Eqn.7}$$

According to the definition, this index measures the propensity of chemical species to accept electrons. All the calculated values of ionization potential, electron affinity, hardness, potential, softness and electrophilicity index are shown in **Table 2**

Electro negativity (**A**), hardness (**η**), softness (**α**), electrophilicity index (**ω**) are ordinarily utilized as worldwide reactivity parameters inside density functional theory. In the present examination, the HOMO and LUMO energies gap, absolute electronegativity, absolute hardness and electrophilicity index of the 1A molecule WASregistered by B3LYP/6-311+G(d,P)., It has been found from the examination of the responsive descriptors that the chemical hardness of the title molecule was observed to be 2.2435eV which is similarly high. While its electro negativity value is nearly high uncovering that the compound is equipped for showing certain organic movement.



HOMO **LUMO**

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

3. CONCLUSION

In this study, we have performed the theoretical DFT analysis of a pharmaceutically important heterocyclic aromatic molecule, N-(1H-benzo[d] imidazol-2-yl) methyl)-1,2,4-triazin-3-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)-1,2,4-triazin-3-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 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, 2 Kumar R, Sirohi TS, Singh H, Yadav R, Roy RK, Chaudhary A, et al. 1,2,4-Triazine analogs as novel class of therapeutic agents. Mini Rev Med Chem. 2014;14:168–207.
2. Salih NA. Synthesis and characterization of novel azole heterocycles based on 2,5-disubstituted thiadiazole. Turkish J Chem. 2008; 32:229–35.

3. El Massry AM, Asal AM, Khattab SN, Haiba NS, Awney HA, Helmy M, et al. Synthesis and structure elucidation of novel fused 1,2,4-triazine derivatives as potent inhibitors targeting CYP1A1 activity. Bioorg Med Chem. 2012;20:2624–37.
4. Wittman MD, Carboni JM, Yang Z, Lee FY, Antman M, Attar R, et al. Discovery of a 2,4-disubstituted pyrrolo-[1,2-f][1,2,4]triazine inhibitor (BMS-754807) of insulin-like growth factor receptor (IGF-1R) kinase in clinical development. J Med Chem. 2009;52:7360–3
5. Abdel-Aziem A, El-Gendy MS, Abdelhamid AO. Synthesis and antimicrobial activities of pyrido[2,3d]pyrimidine, pyridotriazolopyrimidine, triazolopyrimidine, and pyrido[2,3-d:6,5d']dipyrimidine derivatives. Eur J Chem. 2012;3:455–60.
6. Amin KM, Hanna MM, Abo-Youssef HE, George RF. Synthesis, analgesic and anti-inflammatory activities evaluation of some bi-, tri- and tetracyclic condensed pyrimidines. Eur J Med Chem. 2009;44:4572–84.
7. Hynes J, Dyckman AJ, Lin S, Wrobleski ST, Wu H, Gillooly KM, et al. Design, synthesis and anti-inflammatory properties of orally active 4-(phenylamino)-pyrrolo[2,1-f][1,2,4]triazine p38 mitogen-activated protein kinase inhibitors. J Med Chem. 2008;51:4–16.
8. Wrobleski ST, Lin S, Hynes J, Wu H, Pitt S, Shen DR, et al. Synthesis and SAR of new pyrrolo[2,1-f][1,2,4]triazines as potent p38α MAP kinase inhibitors. Bioorganic Med Chem Lett. 2008;18:2739–44.
9. Makki MSI, Abdel-rahman RM, Khan KA. Fluorine substituted 1,2,4-triazinones as potential anti-HIV-1 and CDK2 inhibitors. J Chem. 2014;2:1–14.
10. Rusinov VL, Egorov IN, Chupakhin ON, Belanov EF, Bormotov NI, Serova OA. The search for new drugs: synthesis and antiviral activity of 1,2,4-triazine derivatives. Pharm Chem J. 2012;45:655–9.
11. Bondock S, Rabie R, Etman HA, Fadda AA. Synthesis and antimicrobial activity of some new heterocycles incorporating antipyrine moiety. Eur J Med Chem. 2008;43:2122–9.
12. Arshad M, Bhat AR, Hoi KK, Choi I, Athar F. Synthesis, characterization, and antibacterial screening of some novel 1,2,4-triazine derivatives. Chin Chem Lett. 2017;28:1559–65.
13. Hashem HE, Abo-Bakr AM. Synthesis of some new 1,2,4-triazine and 1,2,5-oxadiazine derivatives with antimicrobial activity. Heteroat Chem. 2019;12:1–7.
14. Kaiser A, Kusch P, Deininger S, Specht S, Maniako R, Haubrich S, et al. In vitro and in vivo antimalarial activity assays of seeds from Balanites aegyptiaca: compounds of the extract show growth inhibition and activity against plasmodial aminopeptidase. J Parasitol Res. 2011;2011:368692
15. March LC, Bajwa GS, Lee J, Wasti K, Joullié MM. Antimalarials. 3. 1,2,4-triazines. J Med Chem. 1976;19:845–8
16. 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.
17. Frisch, M.J., et al. (2009) Gaussian 09, Revision B. 01. Gaussian, Inc., Wallingford.
18. Dennington, R.D., Keith, T.A. and Millam, J.M. (2008) GaussView 5.0.8, Gaussian