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ACADEMIC YEAR

2022-2023

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S.No	Name of the Faculty and Designation	Conducted By	Month & Year	Theme of the Conference	Amount Paid	Mode of Payment	Signature
1	Dr.(Mrs) G.Nirmala, Principal, KCSAMW	National Institute of Educational Planning and Administration, New Delhi	Nov- Dec 2022	National Workshop on Leadership Development for College principals	Rs. 5000	Cash	
2	Mrs.G.Packialakshmi, Assistant Professor,Department of commerce, KCSAMW	Journal of the asiatic society of Mumbai ISSN: 0972-0766	Jun-22	Consumer awarness towards features of durable goods special reference to cuddalore district	Rs. 2500	Cash	
3	Dr(Mrs) M.Sivasakthi, Assistant Professor, Department of maths, KCSAMW	International journal of mathamatics trends and technologyIssn: 2234 -5373	Jul-22	Some corona product of root square mean labeling of graphs	Rs. 2500	Cash	
4	Dr(Mrs)N.Vennila, Associate Professor,Department of Tamil, KCSAMW	UGC sponsored webinar orgniseed by Bharathidasan University, Thrichirappali	Aug-22	Changing role of teacher NEP 2020 prospectives	Rs. 1000	Cash	
5	Dr(Mrs)N.Vennila, Associate Professor,Department of Tamil, KCSAMW	shanlax, International Journal of Tamil Research : P-ISSN:2454-3993, E-ISSN : 2582-2810	Oct-22	Goddess Worship of Mu Thinaikudi Muma	Rs. 1500	Cash	
6	Dr(Mrs) M.Sivasakthi, Assistant Professor, Department of maths, KCSAMW	Research and reflections on Education ISSN 0974-648X(P)	Oct-22	Some results on harmonic mean graphs	Rs. 2500	Cash	
7	Dr(Mrs)N.Vennila, Associate Professor,Department of Tamil, KCSAMW	Maayan International Jounal of Tamil Rearch ISSN: 2583-0449	Dec-22	Innakkuzh samugangalin samanisam	Rs. 1500	Cash	
8	Mrs.G.Packialakshmi, Assistant Professor,Department of commerce, KCSAMW	Journal fundamental & comparative research , Mumbai ISSN 2277 7067	July - Dce 2022	Consumer satisfaction on features of durable goods special reference to cuddalore district	Rs. 2500	Cash	

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9	Dr(Mrs)N.Vennila, Associate Professor,Department of Tamil, KCSAMW	Ilakkiyasudar, International Archeotogy Art, Literature, Cultural Journal	Jan-23	Thinai kudigalin pennirmaium pen theiva vazhipadum	Rs. 1500	Cash	
10	Dr(Mrs)N.Vennila, Associate Professor,Department of Tamil, KCSAMW	shanlax, Journals E-ISSN :2582-2810	Jan-23	Sanga ilakiyangal kattum thinai manthargal	Rs. 1500	Cash	
11	Dr(Mrs)N.Vennila, Associate Professor,Department of Tamil, KCSAMW	Maayan International Jounal of Tamil Rearch ISSN: 2583-0449	Oct-22	Inakkuzh samugamum arasu uruvakkamum	Rs. 1500	Cash	
12	Dr(Mrs) C.M.Mahalakshmi, Associate Professor, Department of chemistry, KCSAMW	International journal of education and technology ISSN 2581-7795	Aug-23	Structural homo-lumo-MEP analysis and mulliken charges of thiazole derivative	Rs. 3000	Cash	C.M. Mahal
13	Dr(Mrs) C.M.Mahalakshmi, Associate Professor, Department of chemistry, KCSAMW	International journal of education and technology ISSN 2581-7795	Aug-23	DFT caluculations on molecular structure, homo, Lumo study reactivity descriptors of triazine derivative	Rs. 3000	Cash	C.M. Mahal
14	Dr(Mrs) C.M.Mahalakshmi, Associate Professor, Department of chemistry, KCSAMW	International journal of education and technology ISSN 2581-7795	Aug-23	Computational studies of triazole derivative	Rs. 3000	Cash	C.M. Mahal
15	Dr(Mrs) C.M.Mahalakshmi, Associate Professor, Department of chemistry, KCSAMW	International journal of education and technologyISSN 2581-7795	Aug-23	Homo lumo study, reactivity descriptors and mulliken chargs of imidazole derivative	Rs. 3000	Cash	C.M. Mahal
16	Dr(Mrs) C.M.Mahalakshmi, Associate Professor, Department of chemistry, KCSAMW	International journal of education and technology ISSN 2581-7795	Aug-23	Molecular geometry, , homo, Lumo analysis and docking studies of pyrimidine derivative	Rs. 3000	Cash	C.M. Mahal
17	Dr(Mrs) C.M.Mahalakshmi, Associate Professor, Department of chemistry, KCSAMW	International journal of education and technology, ISSN 2581-7795	Aug-23	DPT studies of Oxazole derivative	Rs. 3000	Cash	C.M. Mahal

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VOUCHER

Date : 25.11.2022

Paid to	Dr.G.Nirmala, Principal	
Debit A/c		**5,000.00**
Towards	Remuneration for National workshop on Leadership development for college Principals in New Delhi, November & December -2022	
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[G. NIRMALA]

National Institute of Educational Planning and Administration

Certificate

This is to certify that Dr G Nirmala, Principal
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participated in the **National Workshop on Leadership Development for College Principals** organized by Department of Higher and Professional Education, National Institute of Educational Planning and Administration during 28 November - 02 December, 2022 at NIEPA, New Delhi.

(Prof. Neeru Snehi)
Programme Coordinator

December 02, 2022
New Delhi

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Authored By

G.PACKIALAKSHMI,

Ph.D. Research Scholar (Part time - External), Department of Commerce, Annamalai University, Annamalainagar, Tamilnadu

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Original Article

Some Corona Product of Root Square Mean Labeling of Graphs

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Abstract *- A graph G= (V,E) with p vertices and q edges is said to be a Root Square Mean graph if it is possible to label the vertices x∈V with distinct elements f(x) from 1,2,....,q+1 in such a way that when each edge e=uv is labelled with* $f(e=uv)=\left\lfloor\sqrt{\frac{f(u)^2+f(v)^2}{2}}\right\rfloor$ *or* $\left\lceil\sqrt{\frac{f(u)^2+f(v)^2}{2}}\right\rceil$*, then the resulting edge labels are distinct. In this case f is called a Root Square Mean labeling of G. In this paper we prove that some corona product of Root Square Mean labeling of graphs, such as* $L_n\odot K_1, Q_n\odot K_1$*.* $T_n\odot K_1$ *are Root Square Mean labeling of graphs.*

Keywords *- Graph, Root Square Mean graph,* $L_n\odot K_1, Q_n\odot K_1$*,* $T_n\odot K_1$

AMS subject classification *- 05078.*

1. Introduction

The graph considered here will be finite, undirected and simple. The vertex set is denoted by V(G) and the edge set is denoted by E(G). The concept of graph labeling was introduced by Rosa [6]. For all detailed survey of graph labeling we refer to Gallian[1]. For all other standard terminology and notations we follow Harary [2]. The concept of mean labeling has been introduced by S.Somasundaram and R. Ponraj in 2004 [5]. S.S.Sandhya, S.Somasundaram and S.Anusa introduced the concept of Root Square Mean labeling of graphs. The definitions and other informations which are useful for the present investigation are given below. The following definitions are useful for present investigation.

Definition 1.1:

A graph G= (V,E) with p vertices and q edges is said to be a Root Square Mean graph if it is possible to label the vertices x∈V with distinct elements f(x) from 1,2,...,q+1 in such a way that when each edge e=uv is labelled with $f(e=uv)=\left\lfloor\sqrt{\frac{f(u)^2+f(v)^2}{2}}\right\rfloor$ or $\left\lceil\sqrt{\frac{f(u)^2+f(v)^2}{2}}\right\rceil$, then the resulting edge labels are distinct. In this case f is called a Root Square Mean labeling of G.

Definition 1.2:

The Corona of two graphs G_1 and G_2 is the graph $G=G_1\odot G_2$ formed by one copy of G_1 and $|G_1|$ copies of G_2 where the i^{th} vertex of G_1 is adjacent to every vertex in the i^{th} copy of G_2.

Definition 1.3:

The product graph $p_2 \times p_n$ is called a ladder and it is denoted by L_n.

Definition 1.4:

A Triangular Snake T_n is obtained from a path $u_1u_2.....u_n$ by joining u_i and u_{i+1} to a new vertex v_i for $1\leq i \leq n-1$. That is every edge of a path is replaced by a triangle C_3.

Definition 1.5:

A Quadrilateral Snake Q_n is obtained from a path $u_1u_2.....u_n$ by joining u_i and u_{i+1} to two new vertices v_i and w_i respectively and then joining v_i and w_i. That is every edge of a path is replaced by a cycle C_4.

In this paper we prove that $L_n\odot K_1, Q_n\odot K_1$, $T_n\odot K_1$ are Root Square mean graph.

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Goddess Worship of Mu Thinaikudi Muma

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Abstract
In the worship of thinaikudis, the names of the deities and the rituels are set up to honor the feminine. In a different environment from the ancient tamis who wore afraid of nature, natural products,trees and bodies of water not to be fecered and running, running was to be feared and. That natural enargy that gives fear is called sur, Anangu and sur mean suffering and fear. Anangu means suffering she who brings great suffering. The word surara daughter gives fear Goddess is meaning. In the beginning surum and Anang were tought formless. And then those to speak gracefuldy and at the same time without taunting.

Key Words:
Anangu, Muruku, Pazhaiyol, Katalkezhu Selvi, Kadukezhu Selvi, Amman, Seematti, Surmakal, Kotravai, Perukattukkotravai, Kamar Selvi, Kadu Kizhar, Kadukizhavol, Kataikataul, Kollippavai

References

1. U.V.saminatha Iyar-Kurunthogai .Thenninthiya Saiva Sithantha Pathippu. Chennai
2. .....1949 ingurunooru,
3. S.v .Suppiramaniyan Sanga Ellakkiyam Moolamum Uraium, Manivasagar Pathippagam-Chennai
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16. Sanmugam Pillai Sangathamizharin Vazhipadum Satangukalum- Ulagathamizh Araichi Niruvanam.
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SOME RESULTS ON HARMONIC MEAN GRAPHS

ABSTRACT

A graph G with p vertices and q edges is called a harmonic mean graph if it is possible to label the vertices $x \in V$ with distinct labels f(x) from {1,2,.....q+1} in such a way that each edge e = uv is labeled with $f(uv) = \left\lfloor \frac{2f(u)f(v)}{f(u)+f(v)} \right\rfloor$ *(or)* $\left\lceil \frac{2f(u)f(v)}{f(u)+f(v)} \right\rceil$ *then the edge labels are distinct. In this case f is called Harmonic mean labeling of G. In this paper we prove that some families of graphs such as Toad pole T (n,t) , T (n,t)* $\odot K_1$, *T (n,t)* $\odot \overline{K_2}$, *T (n,t)* $\odot K_2$ *are harmonic mean graphs.*

Keywords: *Harmonic mean graph, Toad pole T (n,t) , T (n,t)* $\odot K_1$, *T (n,t)* $\odot \overline{K_2}$, *T (n,t)* $\odot K_2$.

1. Introduction:

Let G=(V,E) be a (p,q) graph with p = |V(G)| vertices and q =|E(G)| edges, where V(G) and E(G) respectively denote the vertex set and edge set of the graph G. In this paper, we consider the graphs which are simple, finite and undirected. For graph theoretic terminology and notations we refer to Harary [4]

The concept of graph labeling was introduced by Rosa [1] in 1967. A detailed survey of graph labeling is available in Gallian[6].The concept of Harmonic mean labeling of graph was introduced by S.Somasundaram, R.Ponraj and S.S.Sandhya and they investigated the existence of harmonic mean labeling of several family of graphs such as path, comb, cycle C_n, in [10,11]. The following definitions are useful for the present investigation.

Definition: 1.1

A Graph G = (V, E) with p vertices and q edges is called a Harmonic mean graph if it is possible to label the vertices $x \in V$ with distinct labels f(x) from {1,2,....,q+1} in such a way that when each edge e = uv is labeled with $f(uv) = \left\lfloor \frac{2f(u)f(v)}{f(u)+f(v)} \right\rfloor$ (or)

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3ஆம் ஆண்டில் நமது இலக்கியச்சுடர்

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திணைக்குடிகளின் பெண்ணீர்மையும் பெண்தெய்வ வழிபாடும் – முனைவர்.ந.வெண்ணிலா

திணைக்குடிகளின் பெண்ணீர்மையும் பெண்தெய்வ வழிபாடும்

முனைவர்.ந.வெண்ணிலா
இணைப்பேராசிரியர், தமிழ்த்துறை
கிருஷ்ணசாமி மகளிர் அறிவியல் கலை மற்றும்
மேலாண்மையியல் கல்லூரி – கடலூர்

ஆய்வுச்சுருக்கம்

திணைக்குடிகளின் பாலினப் பாகுபாட்டில் ஆண் பெண் இருவரும் உயர்நிலை பண்புகளோடு பண்டைக் காலத்தில் வாழ்ந்தனர். அறம், பொருள், இன்பம் என்னும் பொருண்மையைப் போற்றி வாழ்ந்திருந்தனர். அக வாழ்வியலை நோக்குங்கால் களவு, கற்பு என்னும் இருநிலைக் கோட்பாட்டின் வழியே பயணித்திருக்கின்றனர். அறநோக்கோடு பொருள் தேடலும், அறத்தின் வழி பொருளீட்டலும் உயர் நோக்காக கொண்ட பண்டைத் தமிழர்கள் ஒத்த அன்புடையவராகஇல்லற வாழ்க்கை யினை இயம்பினர். அன்பின் ஐந்திணை வழி தொன்மையுடைய வாழ்வியலை மேற்கொண்டவர்கள்.சமூக ஏற்றத்தாழ்வற்ற சமநிலைச் சமுதாயத்திற்கு வழி கோலியவர் களானவர். தொழில் வழி, தொழில் செய்பவர்களை வகைப்பிரித்தனர். இவ்வகைப்பிரிப்பு நிலத்திற்கேற்ற தொழிலும், தொழிலின் இயல்பு தன்மையும் கொண்டே பிரிக்கப்பட்டன. தொழில் சார்புடைய ஐந்திணை மாந்தர்கள் உயர்ந்தோர், தாழ்ந்தோர் என்றும் வேறுபடுத்தியிருந்தனர் என்பதற்கானச் சான்றுகள் சங்க இலக்கியங்களில் காணக்கிடைக்கின்றன. பாணன், பறையன், கூத்தர், விறலி, கணிதன், உழவன், உழத்தி, இடையன், இடைச்சி, குறவன்,

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வெளியீட்டுச் சான்றிதழ்

முனைவர். **ந. வெண்ணிலா**

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

J.PRIYAVADHANA[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

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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).

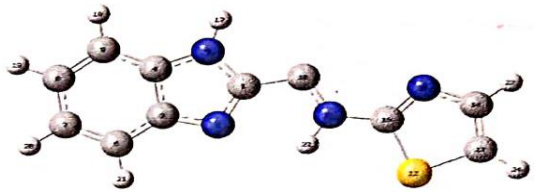

Fig -1: Optimized molecular geometries and atomic numbering of 1A

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

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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°.

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COMPUTATIONAL STUDIES OF TRIAZOLE DĒRIVATIVE

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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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HOMO LUMO STUDY , REACTIVITY DESCRIPTORS AND MULLIKEN CHARGES OF IMIDAZOLE DERIVATIVE

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Abstract – *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. The HOMO-LUMO essentialness levels' uniqueness chooses the molecule's engine steadfastness, substance reactivity, compound nonabrasiveness, and hardness. The molecular electrostatic potential (MEP) is a critical mechanical assembly in electrophilic and nucleophilic goals affirmation.*

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

1.INTRODUCTION

Debus[1] made the initial discovery of the imidazole nucleus in the year 1859 by reacting glyoxal and ammonia to indicate its source, for which he offered the name glyoxalin. Hantzsch[2] coined the name "imidazole," which refers to a five-membered heterocyclic ring structure with an imino group and a tertiary nitrogen atom at positions 1 and 3, respectively. The extensive presence of imidazole and imidazolium compounds in biological and chemical systems has sparked interest in imidazole chemistry. A five-membered ring of three carbons and two nitrogens, with the nitrogens placed in the 1 and 3 positions, makes up the cyclic, planar molecule imidazole [3,4,5,6]. The nitrogen at the first position is of the "pyrrole" kind.

Nucleobases and the hydrogen bonds between them in the Watson and Cricks model of DNA are actually responsible for the transmission of genetic information from generation to generation. In addition mononucleotides such as ATP and GTP are also important in regulating the cellular processes. Hence, more number of purines and pyrimidine compounds has been screened for a wide variety of biological targets than other heterocycles.[7-9]

Pyrimidines (cytosine, thymine and uracil) and their derivatives were found to possess a broad spectrum of pharmacological activities. In recent years, considerable attention has been directed towards synthesis of nucleic acid analogues in the hope of discovering new and more effective antisense compounds. Many N-substituted uracil derivatives possess biological activity. The most prominent representatives are 5-fluorouracil, 5-thiouracil and their derivatives.

2. Ground State Structure Analysis[10,11]

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 1,1'-(5-bromo-1H-imidazole-2,4-diyl)dipyrimidine-2,4(1H,3H)-dione)[12]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 are presented in Table 4.1. 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.

For disubstitued derivative **1A**, pyrimidine ring attached to second position of imidazole were coplanar with the imidazole ring. This result was confirmed by following torsional angles N2-C1-N9-C10 (-179.9) in **1A**. But the pyrimidine ring substituted at the 4[th] position of the imidazole ring were non-planar with the ring, because the high electronegativity of the bromine atom induces polarization both in σ — and π-frameworks of the imidazole moiety. In these compounds, due to interaction between bromogroup in imidazole and carbonyl group in pyrimidine ring, the pyrimidine ring (4[th] position of imidazole) is rotated out of the imidazole plane, making dihedral angles of 43.3° in **1A**.

2.1.Frontier Molecular Orbitals

The highest occupied molecular orbital, HOMO, and the lowest unoccupied molecular orbital, LUMO, of a molecule are called the frontier orbitals. It was Fukui[13]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 byB3LYP/6-311G (d, p) level of theory. Highly occupied molecular orbital (HOMO) and Lowest unoccupied molecular orbital (LUMO) are the main orbital that take part

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MOLECULAR GEOMETRY, HOMO AND LUMO ANALYSIS AND DOCKING STUDIES OF PYRIMIDINE DERIVATIVE

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Abstract – *The theoretical calculations of the N-((1H-benzo[d]imidazol-2-yl)methyl) pyrimidin-4-amine 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.. Moreover, the highest occupied molecular orbital, the lowest unoccupied molecular orbital, molecular electrostatic potential, chemical reactivity parameters and natural bond orbital of the optimized structure have been evaluated at the same level of theory. Besides, the molecular docking simulation of the mentioned molecule with target protein was also investigated. 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, Molecular docking.**

1.INTRODUCTION

The majority of chemical entities, which are found in numerous natural goods, fine chemicals, and physiologically active medications essential for improving the quality of life[1], contain heterocyclic compounds that contain nitrogen. Due to the diversity of their structural makeup and connections to a wide range of biological activities, synthetic studies of fused pyrimidines have been widely published. Due to their anti-inflammatory, psychopharmacological, bactericidal, anticancer, antitubercular, antioxidant, anticonvulsant, antibacterial, antiplasmodial, antifungal, anticancer [2-4], antimicrobial, antibiotic, antiviral activity as HIV-1 reverse transcriptase inhibitors, antifolates [5] and antihismatic activity [6] properties, pyrimidines are also of pharmacological interest.

Pyrimidines are heterocyclic aromatic compounds with two nitrogen atoms at positions 1 and 3 of the six-membered rings, analogous to benzene and pyridine. Pyrimidine has a molecular weight of 80 and the chemical formula $C_4H_4N_2$. It is isomeric with two more diazene forms[7]. It is the source of a large group of heterocyclic compounds and is essential to many biological processes, as evidenced by the presence of nucleic acids, a number of vitamins, co-enzymes, and purines. Although the pyrimidine ring itself does not occur in nature, substituted pyrimidines and compounds that include it do. Additionally, pyrimidine[8] and its derivatives, such as fused pyrimidines, are among the most prominent structures in nucleic acids, including uracil, thymine, cytosine, adenine, and guanine, which are essential components of both DNA and RNA20.

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 of pyrimidine characteristics. The antioxidant, anticonvulsant, antibacterial, antiplasmodial, antifungal, anticancer, antimicrobial, antibiotic, antiviral activity as inhibitors of HIV-1 reverse transcriptase, antifolates, and antihismatic activity were also used to characterise newly synthesised pyrimidine by substitution groups in their derivative structure.

2. OPTIMIZED GEOMETRIES

Molecular geometry is a sensitive indicator of intra and intermolecular interactions. The accurate determination of geometrical deformation in 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) pyrimidin-4-amine[9] 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[11] as shown in the Fig. (1). 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. Selected geometrical parameters like bond length, bond angle and dihedral angle are listed in Table 4.1. As a result of partial protonation of both nitrogen atoms C1-N2 and C3-N2 bond lengths in benzimidazole moiety is 1.3747 and 1.3897.

For the 1A compound, pyrimidine ring attached to second position of benzimidazole were found to be planar with the ring. This result was shown by the fact that the dihedral angles for C10-N11-C14-N13 and C10-N11-C14-C15 in 1A are 0° and 180° respectively.

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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.

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 oxiazole. 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

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