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ELECTRONIC PARAMETERS AND DFT STUDIES OF METHYLPHENYLTHIAZOLYLNAPHTHYLMETHANONE

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ABSTRACT: The antibacterial, antiviral, antioxidant, analgetic, anticonvulsant, antidiabetic, anticancer, and antimalarial effects of methylphenylthiazolylnaphthylmethanone scaffolds can be found in a wide range of natural and synthesised biomolecules, according to a literature review. The mulliken charges, the values of the molecule's electrical dipole moment, vibrational spectral analysis were computed using DFT calculations obtained from Gaussian 09 software. For the resulting compounds, total energy, dipole moment, electron affinity, electronegativity, hardness, softness and energy difference are determined. The calculated HOMO and LUMO energies reveal the molecule's chemical interest and this energy gap is a essential for the balancing index.

Key words: - Mulliken charge, Dipole moment, DFT, Gaussian, HOMO – LUMO.

INTRODUCTION :

The shape of naphthalene is a fused pair of benzene rings. It's the most basic and important member of the arene family, consisting of two benzene rings joined in ortho positions[1]. Because of their wide range of uses in drug development, naphthalene derivatives have gotten a lot of attention in the field of medicinal chemistry[2]. Naphthalene is a chemical compound that is used to dyes, explosives, polymers, and lubricants[3]. Naphthalene-containing drugs include nafacillin[4], naftifine[5], tolnaftate[6], terbinafine[7] and others[1]. They are essential in the control of microbial infection. Thiazole is a five-membered, unsaturated, planar heteroaromatic with one sulphur atom and one pyridine-kind nitrogen atom at position 3 of the cyclic ring system. It's also known as 1,3-thiazole[8]. Many natural chemicals, such as vitamin B1-thiamine, alkaloids, anabolic steroids, and flavones, contain thiazoles as a fundamental scaffold[9]. Thiazoles have antifungal, antibacterial, anti-inflammatory, anthelmintic, antiretroviral, sedative, hypnotic, and other pharmacological effects[10].

The main purpose of this study is to use the DFT/B3LYP technique to present more precise bond lengths, bond angles, atomic charges, and HOMO-LUMO of methylphenylthiazolylnaphthylmethanone. The experimental data were compared to the estimated molecule geometry. Theoretical calculations were performed on electronic parameters such as total energy, softness, hardness, dipole moments, and electronegativity[11].

Computational details:

DFT statistics of methylphenylthiazolylnaphthylmethanone use the Gaussian 09 system package at B3LYP level (Becke-3Lee-Yang-Parr) with a basic set of 3-21G[12]. A precise report on vibrational spectra and structure of the compound is done. The electronic components of a molecule are

determined by the activation of electron density through close contact with the free electron gas. All theoretical statistics were researched in the Gaussian 09 program package and the calculated results were visualized using Gauss View 5.0. The method is very accurate for small calculation costs. Electronic parameters and geometric enhancements for naphthyl outflow were performed using DFT (B3LYP) with a base set of 6-31G.

RESULTS AND DISCUSSION:

Molecular geometry

The optimized structure of the methylphenylthiazolylnaphthylmethanone molecule of the numerical system given in Figure 1 and the geometric parameters is shown in Tables 1 & 2. Self-Consistent Field (SCF) compounds targeted at B3LYP level on the basis of set 3-21G are available. to be -1471.11, -1549.73, -1540.56 , -1587.83 and -1623.69 and respectively. On atomic size increases bond length and increases. Examples of derived compounds (2-dimethylamino-4-methylphenylthiazol-5-yl-2-naphthyl) methanone containing, bonds C-N, C-C, C-H, C-O and C-S. Bond range C5-S1 is the longest, while C30-H31 is the shortest. The length of the C28-C33 bond is greater compared to the length of the carbon - carbon bond due to the methyl group present in the phenyl ring. Bond length order is C-S> C-C> C-N> C-O> C-H.

Data of methylphenylthiazolylnaphthylmethanone

Abbreviations:

C1 - (2-dimethylamino-4-methylphenylthiazol-5-yl-2-naphthyl)methanone

C2 - (2-diethylamino-4-methylphenylthiazol-5-yl-2-naphthyl)methanone

C3 - (4-methylphenyl-2-pyrrolidin-1-ylthiazol-5-yl-2-naphthyl)methanone

C4 - (4-methylphenyl-2-piperidin-1-ylthiazol-5-yl-2-naphthyl)methanone

C5 - (4-methylphenyl-2-morpholin-1-ylthiazol-5-yl-2-naphthyl)methanone

Frontier molecular orbital studies:

The series of methylphenylthiazolylnaphthylmethanone, HOMO and LUMO is shown in Figure 2. The difference between HOMO (Highest Occupied Molecular Orbital) and LUMO (Lowest Unoccupied Molecular Orbital) is called Energy gap (ΔE).

Koopmans' eqn, the orbital frontier molecular orbital energies is given below

$-\varepsilon_{HOMO} = I - \varepsilon_{LUMO} = A$ 1

There, I = ionization potential;

A = electron affinity.

The absolute electro negativity (χ), total hardness (H) and softness (S) can be calculated using the HOMO energy and LUMO energies of electronic parameters given in Table -3.

$(x) = (I+A)/2$; $\eta = (I-A)/2$ and

$S = 1/(2\times\eta)$ 2

The eqn 2 is used to calculate electro negativity(x), hardness (η) and softness (S) are listed in Table -3.

Mulliken charge distribution:

Mulliken charge distribution is calculated at the B3LYP level on the basis of the 3-21G set given in Figure 3. It was an important role for bond structure, molecular conformation and electronic atomic charge, according to the chemical quandam calculations of the dipole moment effort, electronic structure, molecular polarizability etc. Values indicate N3 (-0.459), N39 (-0.542), O17 (-0.436), S1 (0.425) etc. Mulliken's atomic charge of all hydrogen atoms is positive, all nitrogen and oxygen is negatively charged and sulphur positive. The literature reveals that mulliken charge calculations provided important features in the use of

chemical calculations in the molecular system because of charges, dipole moment, molecular polarizability, electronic structure, acidity-basicity behavior and a wide range of molecular system structures.

Assigning vibrations

Frequency calculation analysis is used to determine the spectroscopic assignments of the substances. Theoretical vibrational frequencies are calculated using a scaling factor of 0.962. The calculated results and the theoretical vibrational spectra of the compound (2-dimethylamino-4-methylphenylthiazol-5-yl-2-naphthyl)methanone are displayed in **Fig 4**. Theoretically, the phenyl ring's C-H stretching modes are detected at 3068 cm^{-1}. The C-N stretching modes are potentially observed at 1339 cm^{-1}. At 1531 cm^{-1} the stretching mode of C=O may be seen. The C-C aromatic stretching vibration is detected in the 1506 cm^{-1} region. The aliphatic C-H stretching vibration of 2920 cm^{-1}. Theoretically, the C-S stretching modes are seen at 696 cm^{-1}.

CONCLUSION:

The investigation of the paper is vibrational assignments of (2-dimethylamino-4-methylphenylthiazol-5-yl-2-naphthyl)methanone utilizing DFT technique (B3LYP) with 3-21G premise set. Improved molecular geometry, bond length, bond angles, dihedral angles and atomic charges are calculated in the ground state. The distribution of nuclear charge was determined by determining the number of electrons in a molecule. The strengths of the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) have clarified the energy gap of the particle. The full parameters of the improved geometric structure of the compound are found in ab initio and DFT calculations.

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Table: 1 Bond length data

Position	Parameter	C1	C2	C3	C4	C5
Thiazole	C-S	1.827	1.830	1.829	1.831	1.830
Thiazole	C=N	1.314	1.316	1.317	1.313	1.319
Thiazole	C-N	1.392	1.392	1.395	1.393	1.395
Naphthalene	C-C	1.438	1.437	1.437	1.434	1.433
Naphthalene	C-H	1.086	1.086	1.085	1.087	1.084
Phenyl	C-C	1.413	1.411	1.413	1.415	1.417
Phenyl	C-H	1.086	1.085	1.083	1.082	1.085
Chain	C=O	1.261	1.260	1.259	1.262	1.261
Chain	N-C	1.469	1.482	1.489	1.480	1.479
Chain	C-H	1.098	1.096	1.097	1.101	1.099
Chain	C-C	1.511	1.511	1.517	1.511	1.511
Chain	C-O	-	-	-	-	1.462

Table: 2 Bond angle data

Position	Parameter	C1	C2	C3	C4	C5
Thiazole	S-C-N	113.8	113.6	113.3	113.7	113.9
Thiazole	N-C-C	115.2	115.2	115.4	115.5	115.7
Thiazole	C-N-C	114.4	114.5	114.3	114.2	114.5
Naphthalene	C-C-C	120.7	121.4	121.6	121.5	121.7
Naphthalene	C-C-H	118.8	118.7	118.6	118.6	118.7
Phenyl	C-C-C	121.1	120.8	120.3	120.1	120.5
Phenyl	C-C-H	120.1	120.3	120.1	120.3	120.2
Chain	C-N-C	121.5	118.1	113.3	123.8	124.0
Chain	H-C-H	109.7	109.3	109.1	109.4	109.7
Chain	N-C-H	112.0	112.3	112.8	112.6	112.8
Chain	C-C-H	-	109.9	110.1	110.3	110.3
Chain	C-O-C	-	-	-	-	111.1

Table: 3 Calculated electronic parameters

Parameters (a.u)	C1	C2	C3	C4	C5
Total Energy (a.u)	-1471.11	-1549.73	-1540.56	-1587.83	-1623.69
Dipole Moment (Debye)	5.1841	5.2227	5.8705	5.5231	3.3596
HOMO	-0.2258	-0.2255	-0.2268	-0.2251	-0.2287
LUMO	-0.0250	-0.0244	-0.0228	-0.0234	-0.0287
HOMO-LUMO (ΔE)	0.2008	0.2011	0.2040	0.2017	0.2000
Ionisation potential (I)	0.2258	0.2255	0.2268	0.2251	0.2287
Electron affinity (A)	0.0250	0.0244	0.0228	0.0234	0.0287
Electronegativity (x)	0.1254	0.1249	0.1248	0.1242	0.1287
Hardness (Ƞ)	0.1004	0.1005	0.1020	0.1008	0.1000
Softness (S)	4.9800	4.9751	4.9019	4.9603	5.0000

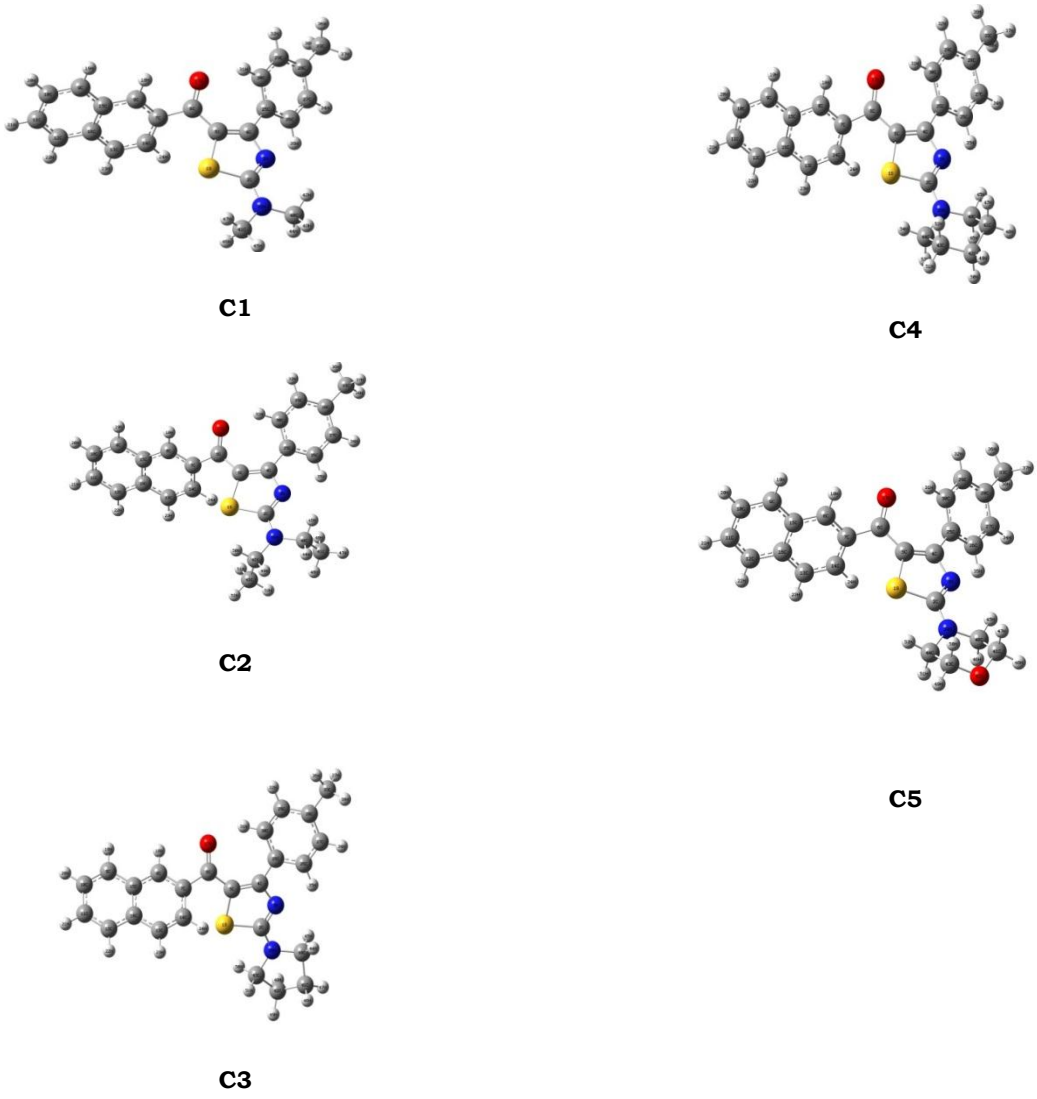
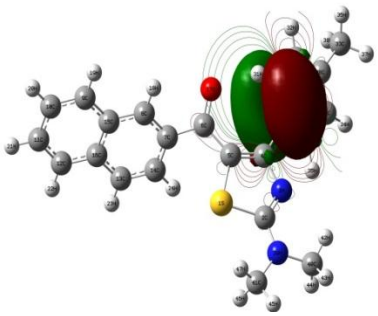
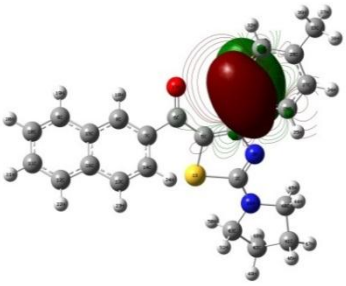


Figure: 1 Optimized structure of methylphenylthiazolylnaphthylmethanone derivatives



Homo (C1)



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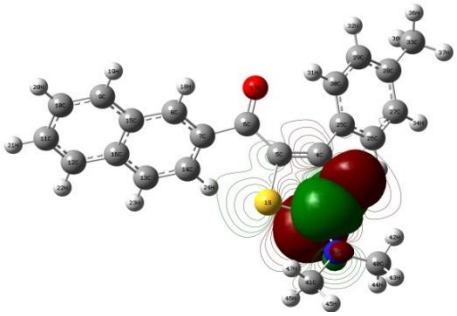
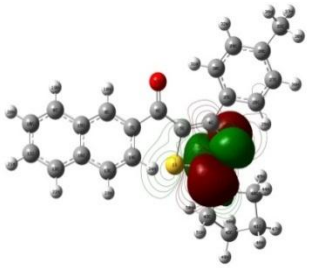
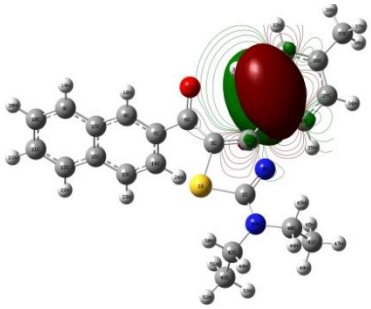


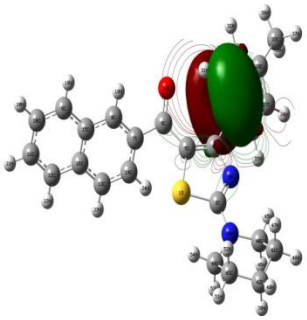
Lumo (C1)



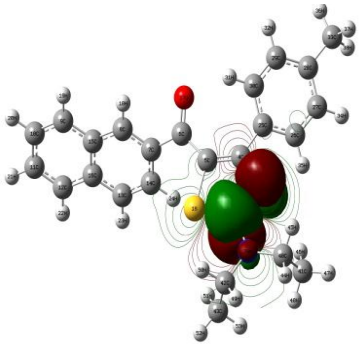
Lumo (C3)



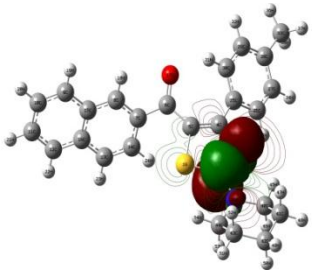
Homo (C2)



Homo (C4)



Lumo (C2)



Lumo (C4)

Homo (C5)

Lumo (C5)

Figure: 2 Homo-Lumo of methylphenylthiazolylnaphthylmethanone

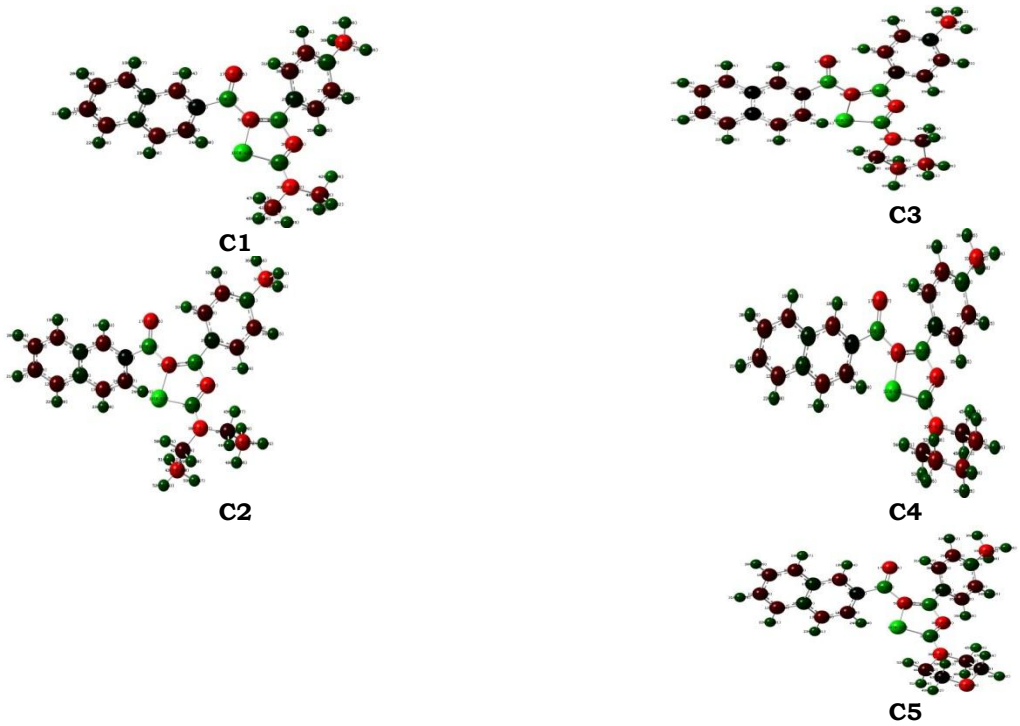


Figure: 3 Mulliken charge of methylphenylthiazolylnaphthylmethanone

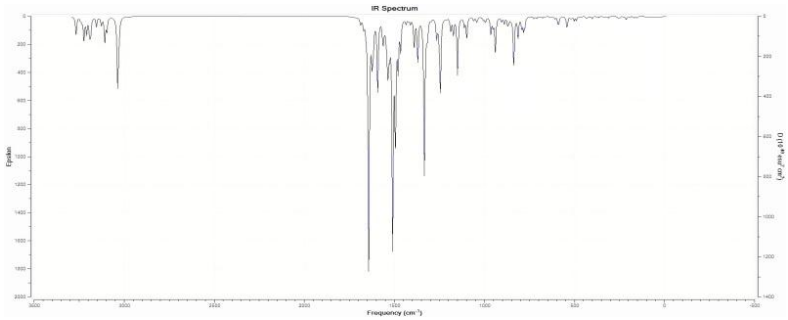


Figure: 4 Theoretical FT-IR spectrum of (2-dimethylamino-4-methylphenylthiazol-5-yl-2-naphthyl)methanone