International Journal of Recent Development in Engineering and Technology
Website: www.ijrdet.com (ISSN 2347-6435 (Online) Volume 15, Issue 04, April 2026)

Geometry, Biochemical, NLO, Vibrational Analysis of 2-Amino-4,6-bis(4-chlorophenylthio) Pyrimidine: A DFT Study

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***Abstract*-- The molecule 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine has attracted attention due to its potential applications in material science and pharmaceuticals. This study investigates its geometry electronic properties, Vibrational analysisNLO and, biological uses through detailed computational analysis. The molecular structure, optimized geometry, vibrational modes, and electronic properties such as HOMO, LUMO, electronegativity, dipole moment, hardness, softness, electrophilicity index, and electron transfer capacity are examined. The findings suggest that this molecule holds promise for applications in organic electronics, photovoltaic devices, and pharmaceuticals, warranting further experimental exploration. The Biological activities of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine molecule are proposed by PASS online server.**

***Keyword*- HOMO, LUMO, DFT, NLO, PASS**

I. INTRODUCTION

The molecule 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine has amass significant interest due to its potentially grand applications in various fields, including material science and pharmaceuticals[1]. This study aims to explore the electronic properties, structural characteristics, and potential applications of this molecule through comprehensive computational analysis[2]. The molecular structure of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine consists of a pyrimidine core substituted with amine and chlorophenylthio groups. This unique arrangement contributes to its distinct electronic and chemical properties. Geometry optimization was performed using density functional theory (DFT) to determine the most stable conformation of the molecule. The optimized geometry revealed key bond lengths and angles, providing insights into the molecular stability and reactivity. Vibrational mode analysis was created to identify the characteristic vibrational modes of the molecule.

The results indicated the presence of specific stretching and bending vibrations associated with the functional groups, which are crucial for understanding the molecular dynamics. The correlation factor between the theoretical and experimental data was calculated to validate the computational methods used. The analysis focused on the electronic properties of the molecule, encompassing the Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO), electronegativity (χ), hardness (η), softness (S), dipole moment (μ), and electrophilicity index (ω). These properties are essential for understanding the molecule's behavior in various chemical environments[3]. The unique electronic properties of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine make it a promising candidate for applications in organic electronics, photovoltaic devices, and as a potential pharmaceutical agent[4]. Further experimental studies are recommended to explore its practical applications. This comprehensive study offers important information regarding the electronic and structural characteristics of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine, paving the way for future research and potential applications in various scientific fields[5].

II. COMPUTATIONAL METHODS

The DFT calculations were carried out using the B3LYP functional, employing the 6-31G(d,p) basis set for all atomic species. The Gaussian 09 software package was employed for the calculations. The optimized geometry was obtained using the Berny algorithm with tight convergence criteria. Vibrational frequencies were calculated using the harmonic oscillator approximation. The optimization of molecular structure of 2-Amino-4, 6-bis(4-chlorophenylthio) pyrimidine was performed using Density Functional Theory (DFT) with the B3LYP functional and 6-31G(d,p) basis set, utilizing the Gaussian 09 software. The optimization was performed without any symmetry constraints.

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III. Results And Discussion

Molecular Geometry Optimization

The chemical formula of title molecule is C32H22Cl4N6S4, (I), includes two sole molecules that distinctly subordinate through a three-centre NH--N/S interaction, two linear one-dimensional (1D) chains are formed, connected by hydrogen bonds. The two phenyl rings and pyrimidine ring are linked with dihedral angles molecule are 82.6 and 89.3, and 83.9 are well matched with observed value.

The compound shows Monoclinic, P21/c with a = 28.4777 (A^0), b = 8.6020 (A^0), c = 14.2055 (A^0) and β = 102.5620^0 [6]. The optimized geometry of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine is shown in Figure 1. Following geometry optimization, a frequency analysis was conducted to confirm that the stationary points corresponded to energy minima, as evidenced by the absence of imaginary frequencies. The total energy of the molecule was calculated to be -3174.2354 Hartree. The computed bond length and bond angle of molecule 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine are listed in table-1.

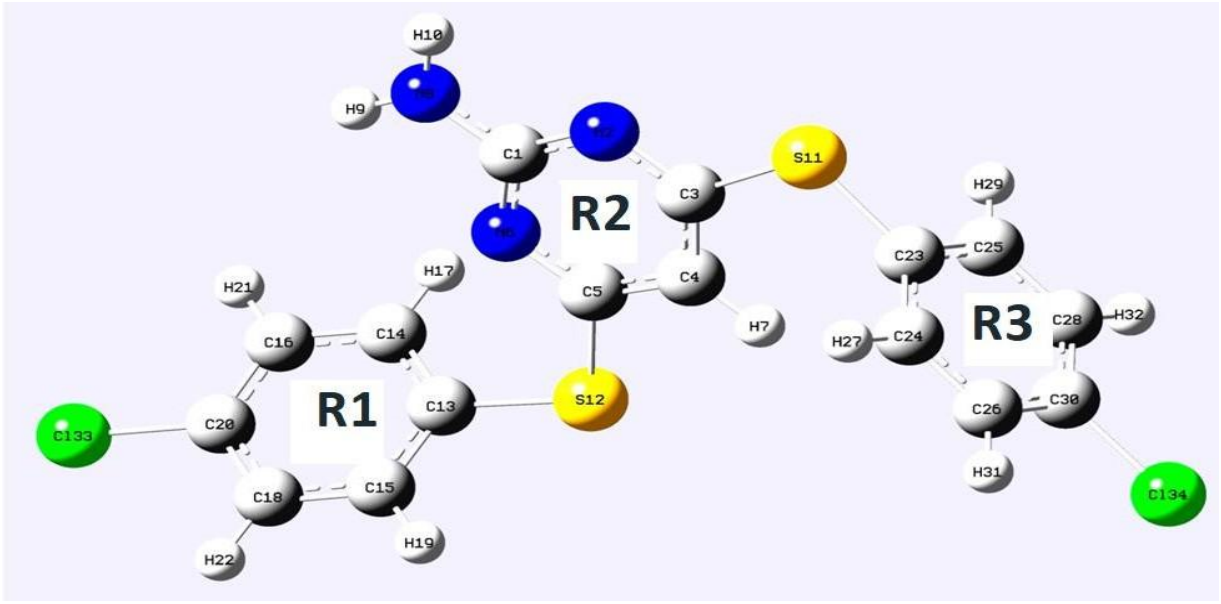

Fig.-1 (a) The optimized geometry of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine

Table- 1
Calculated Bond length (A^0) and Bond angle of molecule-Amino-4,6-bis(4-chlorophenylthio) pyrimidine by using DFT/B3LYP method

S.N	Bonds	BAND LENGTH	Angle	BOND ANGLE
1	$Cl_{33}C_{20}$	1.8322	$Cl_{33}C_{20}C_{16}$	118.6953
2	$C_{20}C_{18}$	1.3862	$C_{20}C_{16}H_{21}$	120.3187
3	$C_{18}H_{22}$	1.0814	$H_{21}C_{16}C_{14}$	120.9821
4	$C_{18}C_{15}$	1.3979	$C_{16}C_{14}H_{17}$	120.3039
5	$C_{15}H_{19}$	1.0801	$H_{17}C_{14}C_{13}$	119.9888
6	$C_{15}C_{13}$	1.3944	$C_{14}C_{13}S_{12}$	120.9441
7	$C_{13}C_{14}$	1.3953	$S_{12}C_{13}C_{15}$	118.3046
8	$C_{14}H_{17}$	1.0801	$C_{14}C_{13}C_{15}$	120.7079
9	$C_{14}C_{16}$	1.3960	$C_{13}C_{15}H_{19}$	119.9406
10	$C_{16}H_{21}$	1.0816	$C_{13}C_{15}C_{18}$	119.9170
11	$C_{16}C_{20}$	1.3882	$H_{19}C_{15}C_{18}$	120.1421
12	$C_{13}S_{12}$	1.8421	$C_{15}C_{18}H_{22}$	121.0179

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13	$S_{12}C_5$	1.8552	$H_{22}C_{18}C_{20}$	120.5235
14	C_5N_6	1.3264	$C_{15}C_{18}C_{20}$	118.4565
15	N_6C_1	1.3628	$Cl_{33}C_{20}C_{18}$	118.7934
16	C_1N_8	1.3495	$C_{18}C_{20}C_{16}$	122.5112
17	N_8H_9	1.0112	$C_{13}S_{12}C_5$	102.0731
18	N_8H_{10}	1.0113	$S_{12}C_5N_6$	119.5259
19	C_1N_2	1.3564	$C_5N_6C_1$	116.4620
20	N_2C_3	1.3347	$N_6C_1N_8$	117.5101
21	C_3C_4	1.3916	$C_1N_8H_9$	119.3736
22	C_4H_7	1.0771	$H_9N_8H_{10}$	121.3096
23	C_4C_5	1.3966	$H_{10}N_8C_1$	119.2862
24	C_3S_{11}	1.8478	$N_8C_1N_2$	117.9013
25	$S_{11}C_{23}$	1.8443	$N_6C_1N_2$	124.5881
26	$C_{23}C_{25}$	1.3959	$C_1N_2C_3$	116.3893
27	$C_{25}H_{29}$	1.0825	$N_2C_3S_{11}$	112.8460
28	$C_{25}C_{28}$	1.3970	$N_2C_3C_4$	123.8794
29	$C_{28}H_{32}$	1.0815	$S_{11}C_3C_4$	123.2736
30	$C_{28}C_{30}$	1.3879	$C_3C_4H_7$	122.7507
31	$C_{30}CL_{34}$	1.8289	$C_3C_4C_5$	114.7410
32	$C_{30}C_{26}$	1.38709	$H_7C_4C_5$	122.5066
33	$C_{26}H_{31}$	1.0815	$C_4C_5S_{12}$	116.5275
34	$C_{26}C_{24}$	1.3970	$C_4C_5C_6$	123.9288
35	$C_{24}H_{27}$	1.0825	$C_3S_{11}C_{23}$	101.5698
36	$C_{24}C_{23}$	1.3959	$C_{25}S_{11}C_{23}$	25.5364

IV. Electronic Structure Calculations Homo-Lumo Gap Calculation

The Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), collectively known as frontier molecular orbitals, play a pivotal role in determining chemical reactivity. Specifically, the HOMO energy level typically acts as an electron donor, whereas the LUMO functions as an electron acceptor. The energy required for electrons to transition from the Highest Occupied Molecular Orbital (HOMO) to the Lowest Unoccupied Molecular Orbital (LUMO) is known as the energy gap or band gap. This energy gap significantly influences the chemical reactivity of a system, with a smaller band gap indicating higher reactivity, and vice versa. When the energy difference between the HOMO and LUMO is smaller, it indicates a higher degree of polarization in the molecules, resulting in reduced kinetic stability[6].

Using the Kohn-Sham Orbitals method the HOMO level of the molecule in question is at -6.20758 eV, while the LUMO level is at -0.95173 eV, with the energy gap being 5.25585 eV, which falls within the range of other organic compounds[7]. All the calculated values are given in Table-2. An energy gap greater than 5 eV suggests that the molecule in question is nonreactive. The HOMO-LUMO Molecular Electrostatic Potential (MESP) plot of the title molecule is illustrated in Figure 2. Notably, the Highest Occupied Molecular Orbital (HOMO) is predominantly localized over the R1 and R2 rings, whereas the Lowest Unoccupied Molecular Orbital (LUMO) is delocalized across the entire molecule. The HOMO primarily acts donor and LUMO acts acceptor so electron transfer from HOMO to LUMO determine nature of reactivity. The MESP plot shows red color centered over S11 and N of ring R2 so acts as negative charge center however blue color centered over NH2 group so acts as electropositive charge center.

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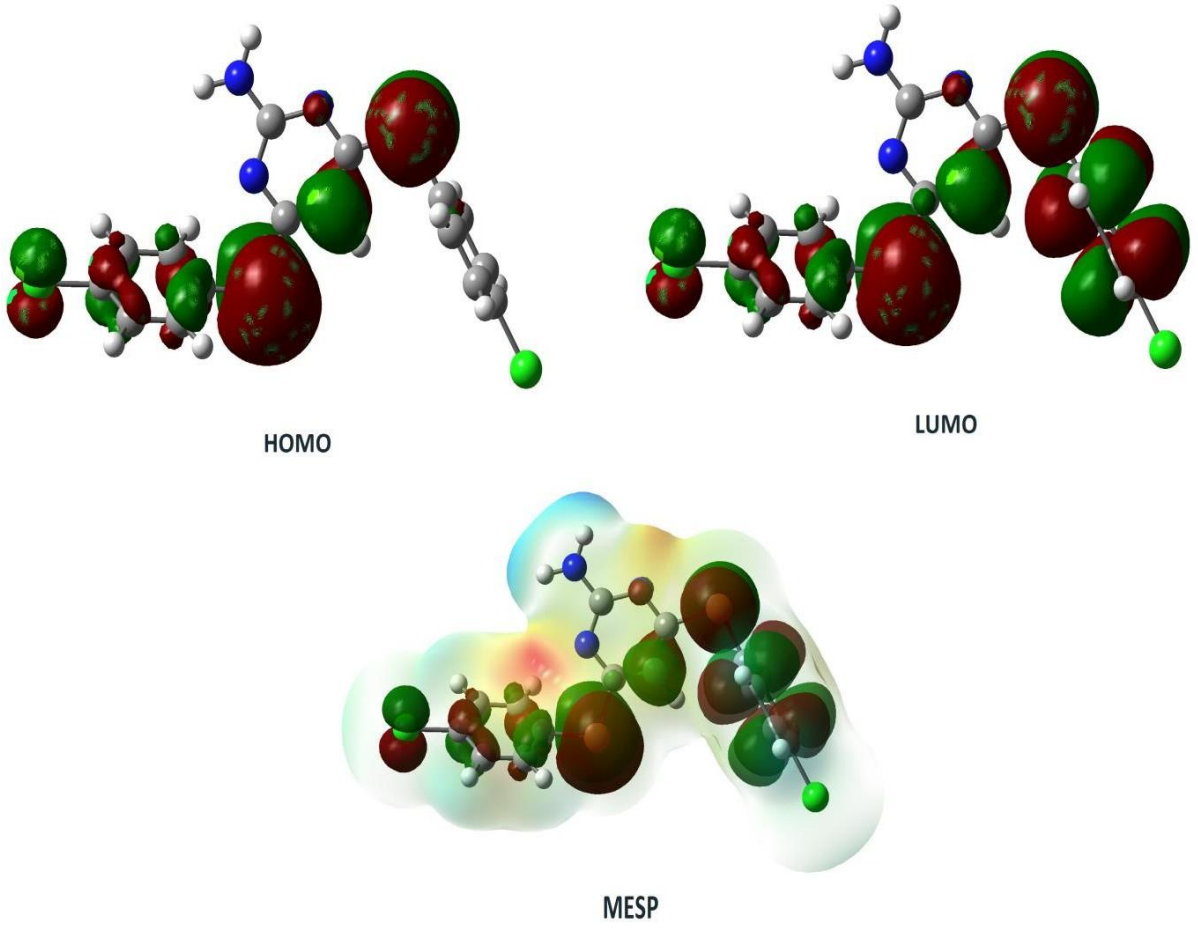

Fig-2 HOMO LUMO MESP Plot of title molecule

Table-2
Several Electronic properties of title molecule is calculated and listed

Name of Properties	Values in au	Values in eV
HOMO	-0.22822	-6.20758
LUMO	-0.03499	-0.95173
χ	3.581064	97.40494
μ	-3.58106	-97.4048
η	2.628962	71.50777
s	0.190189	5.173141
ω	2.43899	66.34053
N_{max}	1.362159	37.05072

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V. Non Linear Optical (NLO) Property Calculations

The 1st order hyperpolarizability (β) of the molecule 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine was calculated using Finite-Field (FF) method with basis set 6-31G(d,p) for all atoms to evaluate its NLO properties. The components of the hyperpolarizability tensor were computed and mentioned in Table-3and the total static hyperpolarizability was derived.

These calculations provide insights into the potential of the molecule for applications in NLO materials. In general, the first hyperpolarizability of urea by calculation is 1.136 x 10^{-30} esu, while that for 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine molecule is 2.82317 x 10^{-30} esu. Similarly in general the dipole moment of water is 1.85D and that for 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine molecule is 0.8957D.

Table- 2
Hyperpolarizability, Polarizability and Dipole Moment of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine molecule

Electronic Properties		Values
Hyper Polarizability	β_{tot} (au)	326.783148
	β_{tot} (esu)= β_{tot} (au)*8.6393*10^{-33}	282318 x 10^{-30}
Mean Polarizabilty	α_{mean} (au)	183.6598
AnistropicPolarizability	α_{aniso} (au)	108.9988
Order of Polarizability	α_{order} (au)	0.254591
Dipole Component	μ (D)	0.8957083

VI. Vibrational Analysis Of 2-Amino-4,6-Bis(4-Chlorophenylthio) Pyrimidine

The potential energy distribution (PED) was used to compute and assign the vibrational frequencies. A computational model was used to construct the theoretical infrared spectra. With 34 atoms, the title molecule has 3N-5 (97) modes of vibration. Thirty-three of the 97 vibration modes are stretching modes, while the remaining modes are bending modes. We have scaled computed frequencies by 0.96 in order to compare them with observed frequencies [8]. Table- 3 have data of calculated frequencies, infrared intensities, and vibrational modes. Below is a discussion of a few chosen scaled modes of vibration for 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine molecule.

-C-H modes of vibration

Vibrational analysis revealed characteristic -CH stretching modes attributed to the -CH group attached to the benzene ring. Typically, C-H stretching vibrations are observed within the 3000-3100 cm^{-1} range. In this study, calculated C-H stretching vibrations occurred between 3222 cm^{-1} and 3152 cm^{-1}. Additionally, several bending modes, combined with -C=C stretching modes, were detected in the mid-spectral region.

Notably, in-plane -CH bending modes exhibited significant intensity at 1114 cm^{-1}, while out-of-plane -CH bending modes appeared at 1003 cm^{-1} in the lower frequency region.

-N-H modes of Vibration

The presence of the -NH2 group in the title molecule gives rise to computed N-H stretching modes of vibration. Typically, -NH stretching vibrations are observed within the 3700-3800 cm^{-1} range. Consistent with this, our calculations reveal -NH stretching modes at 3689 cm^{-1}. Furthermore, mixed bands and -NH bending modes are evident at 1565 cm^{-1} in the lower frequency region. Notably, in-plane -NH bending modes exhibit considerable intensity at 1565 cm^{-1}, while out-of-plane -CH bending modes appear at 505 cm^{-1} in the low-frequency spectral region.

-C=C modes of vibrations

The addition of a heavy substituent tends to shift the absorption band to slightly lower wavenumbers, while the presence of multiple substituents on the ring results in a broader absorption region[9]. The C-C aromatic stretch, characterized by a semi-circular stretching motion, typically occurs within the 1310-1512 cm^{-1} range.

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Although C-C stretching modes may correspond to opposing ring stretching quadrants, the literature conventionally follows the contracting superseding quadrants[9]. Furthermore, out-of-plane CCC bending modes are observed at lower frequencies, involving the coordinated movement of carbon atoms, where all sextant carbons move out of the plane while intervening carbons move in the opposite direction.

Chlorine exhibits distinct vibrational modes, particularly the Cl-C group attached to the benzene ring. Due to the increased reduced mass, the -S-C stretching modes of vibration occur at lower frequencies. Notably, the estimated -Cl-C stretching modes of vibration appear with significant intensity at 1099 cm^{-1}. Additionally, other S-C stretching modes are observed within the range of 786-1099 cm^{-1}. Table 3 provides a comprehensive listing of the various vibrational modes for molecular atoms, as well as the mixing of other vibrational modes.

Table- 3
Vibrational Table for Atoms of molecule 2-amine-4,6-bis(4chlorophenylthio) pyrimidine

SN	SCALED FREQUENCY	IR FREQUENCY	VIBTRATION
1	3689.61	55.1525	υ_{as}(H9-N8-H10)
2	3558.12	122.1049	υ(H9-N8-H10)
3	3279.87	5.1647	υ(N4-H7)
4	3222.76	0.2515	υ_{as}(H19-C15,H22-C18)
5	1665.11	373.8825	α(H9-N8-H10)
6	1599.97	9.1135	α(R2)+ υ(C13-S12) +υ(C28-Cl33)
7	1599.24	27.2843	α(R3)+ υ(C23-S11) +υ(C30-Cl34)
8	1565.98	601.4917	α(H9-N8-H10)+ α(N6-C1-N2)+ α(R3)
9	1512.76	725.9574	υ_{as}(N6-C1-N2, C5-C4-C3)+α(H10-N8-C1, R2-H7, R1-H)
10	1422.74	28.2576	υ_{as}(N6-C1-N2, C5-C4-C3)+α(H9-H10-N8-C1, R2-H7, R1-H)
11	1310.36	2.5800	υ_{as}(C13-C14-C16-C20-C18-C15-C13)
12	1188.99	56.2737	υ_{as}(N6-C1-N2)+α(H7- R1)
13	1114.15	40.8807	α(R3)
14	1111.62	69.7736	α(R2)
15	1099.46	34.0733	ρ(R3)+ υ(C30-Cl34, C23-S11)
16	1099.02	16.4491	ρ(R2)+ υ(C20-Cl33, C13-S12)
17	1003.76	3.7051	β(H17-C14, H21-C16)
18	876.10	59.9413	β(R3)-H
19	867.39	43.9069	β(R2)-H
20	831.12	32.7795	υ_{as}(β(R1)-H)
21	786.59	111.1978	α(R1)+υ_{as}(C5-S12, C3-S11)+ β(R3-H27-H29)
22	616.69	0.5920	τ(R1(C5-C3), H9-N8-H10)
23	505.29	267.2749	β(H10-N8-H9)

υ-Streching, υ_{as}-Antisymmetric stretching, α- Inplane Bending, β- Out of Plane Bending, χ- Scissoring, ρ- Shrinking, τ- Twisting

VII. Conclusion

This computational study provides invaluable insights into the structural, electronic, and nonlinear optical (NLO) properties of 2-Amino-4,6-bis(4-chlorophenylthio) pyrimidine.

Density Functional Theory (DFT) calculations employing the B3LYP/6-31G(d,p) level of theory reveal that the molecule exhibits substantial NLO properties, rendering it a promising candidate for NLO applications. Furthermore, the Prediction of Activity Spectra for Substances (PASS) analysis indicates that the title molecule has potential as a therapeutic agent, particularly as an antineoplastic (0.914) and peptidyltransferase inhibitor (0.969).

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