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DFT-Based theoretical investigation of 6-Amino-5-nitro-1,3-dimethyluracil (ANDMU)

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Abstract
This study provides a comprehensive theoretical investigation of the electronic structure, spectroscopic properties, and chemical reactivity sites of the 6-Amino-5-nitro-1,3-dimethyluracil (ANDMU) molecule, laying the groundwork for future experimental applications in materials science and pharmaceutical chemistry. ANDMU is a nitro-substituted uracil derivative with significant potential in pharmaceutical and materials science applications due to its unique electronic and structural features. In this work, the molecular geometry, electronic structure (HOMO-LUMO gap, band energy), and spectroscopic properties (FT-IR, NMR, UV-Vis) of ANDMU were investigated using density functional theory (DFT) calculations. The optimized planar geometry reveals strong π-conjugation, while the wide HOMO-LUMO gap (5.662 eV) indicates high chemical stability and insulating behavior. Vibrational spectroscopy confirms characteristic functional group peaks (nitro about 1350-1550 cm^{-1}, amino about 3300–3500 cm^{-1}), and NMR and UV-Vis analyses provide insights into intramolecular charge transfer. The presence of amino and nitro groups suggests potential biological activity, making this compound a promising candidate for potential drug scaffold development. Beyond pharmaceutical applications, uracil derivatives may also find use in materials science. The molecular electrostatic potential (MEP) map highlights reactive sites for electrophilic/nucleophilic interactions. These results support the dual-use potential of ANDMU in drug design and in the development of materials such as organic semiconductors and fluorescent probes.

Keywords: ANDMU, Quantum Chemical Calculations, DFT, MEP, NMR, FT-IR

1. INTRODUCTION

6-Amino-5-nitro-1,3-dimethyluracil (ANDMU) is a heterocyclic compound of growing interest due to its potential applications in both pharmaceutical and materials science. This molecule belongs to the uracil family, which is known for its versatility in the synthesis of various biologically active compounds. The presence of amino and nitro substituents at specific positions on the uracil ring imparts distinctive chemical properties, making ANDMU a valuable intermediate in organic synthesis. ANDMU has attracted considerable attention in pharmaceutical research, particularly in the investigation of its biological activities. Studies exploring its antiviral and anticancer properties have highlighted the promising potential of this compound for therapeutic development (Singh et al., 2023; Ziarani et al., 2021). In addition to their pharmaceutical potential, uracil derivatives also find applications in materials science. Their electronic properties make these compounds suitable candidates to develop novel materials such as organic semiconductors and fluorescent probes (Ibrahim et al., 2023; Ziarani et al., 2016). Al-Adhami et al. (2020) focused on the synthesis and characterization of several novel β-lactam derivatives derived from 6-amino-1, 3-dimethyluracil, and the investigation of their antioxidant activities. Yousefi et al. (2012) investigated the synthesis, spectral properties, and biological activities of novel heterylazo dyes derived from 6-amino-1,3-dimethyluracil. The study focused on the structural characterization of these dyes and the evaluation of their optical properties in various solvents. Additionally, the antimicrobial effects of the synthesized dyes against several bacterial strains were examined, and the most effective compound was identified (Yousefi et al., 2012).

Heterocyclic compounds, particularly uracil derivatives, have attracted significant attention due to their versatility in pharmaceutical and advanced material applications. Among these, 6-amino-5-nitro-1,3-dimethyluracil (ANDMU) stands out for its unique electronic and steric properties, attributed to its electron-rich nitro and amino substituents. While uracil

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derivatives play a critical role in nucleic acid chemistry, nitro-functionalized analogs such as ANDMU offer advantages for the synthesis of bioactive molecules and in the development of optoelectronic materials.

The primary objective of this study is to theoretically investigate the structural and electronic properties of the 6-amino-5-nitro-1,3-dimethyluracil (ANDMU) molecule using density functional theory (DFT), considering its potential applications in pharmaceuticals and materials science. In this context, the planarity of the optimized geometry, as well as bond lengths and bond angles, have been analyzed. The molecule's stability and reactivity were assessed through HOMO–LUMO energy level analysis. Electronic transition characteristics were interpreted using UV-Vis spectral data, while vibrational modes of the functional groups were explored through IR spectroscopy. The chemical environments of individual atoms were examined using NMR analysis. In addition, the molecular electrostatic potential (MEP) map was utilized to visualize the electrophilic and nucleophilic regions of the molecule, thereby identifying potential reactive sites.

This study provides theoretical support for the biological activity potential and material science applications of the ANDMU molecule, thereby serving for future experimental investigations.

2. MATERIAL AND METHODS

In this study, the theoretical characterization of the ANDMU molecule was carried out within the framework of density functional theory (DFT). All quantum chemical calculations were performed using the Gaussian 09 software package (Frisch, 2009). The ground-state geometry of the molecule was optimized using the B3LYP functional with the 6-311++G(d,p) basis set. A subsequent frequency analysis confirmed that the optimized structure corresponds to a true minimum on the potential energy surface, as no imaginary (negative) frequencies were detected.

Within the scope of molecular orbital calculations, the frontier molecular orbital energy levels namely the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were determined, and the HOMO-LUMO energy gap (band gap) was calculated. A molecular electrostatic potential (MEP) map was generated based on the electron density distribution to visualize the electrophilic and nucleophilic regions of the molecule.

3. RESULTS AND DISCUSSION

3.1 Geometry Optimization

The geometric optimization of the 6-amino-5-nitro-1,3-dimethyluracil molecule was performed within the framework of density functional theory (DFT) using the Gaussian software package (Frisch, 2009). The optimization was carried out in the gas phase, and the absence of imaginary frequencies confirmed that the structure corresponds to a true minimum on the potential energy surface. The optimized structure of the molecule is presented in Figure 1. The ground-state geometry of the ANDMU molecule was optimized without any symmetry constraints. To verify the accuracy of the B3LYP/6-311++G(d,p) level of theory, the calculated structural parameters were compared with the experimental data of a structurally similar derivative, 6-amino-1,3-dimethyluracil (Ferguson, et al., 1993). The comparative results for selected bond lengths and bond angles are listed in Table 1. The optimized geometric parameters are given in Table 1.

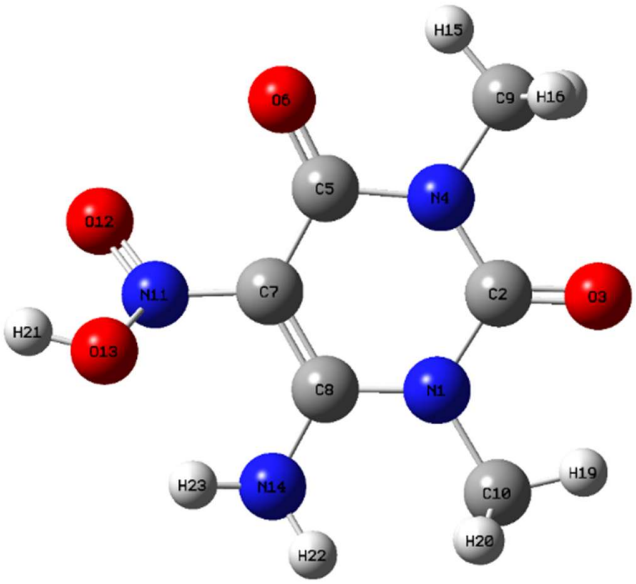

Figure 1. Optimized structure of 6-Amino-5-nitro-1,3-dimethyluracil molecule

Table 1: Selected calculated geometric parameters of ANDMU at the B3LYP/6-311++G(d,p) level.

Parameters	Atom Labels	Calculated (DFT)	Experimental
Bond Lengths (Å)			
Carbonyl (C=O)	C(2)=O(3)	1.225	1.224
	C(5)=O(6)	1.221	1.225
Amino (C-N)	C(8)-N(14)	1.363	1.340
Nitro (N-O)	N(11)-O(12)	1.247	1.230
Ring (C=C)	C(7)=C(8)	1.385	1.360
Bond Angles (°)			
Intra-ring	N(1)-C(2)-N(4)	116.5	117.0
Nitro	O(12)-N(11)-O(13)	115.7	124.0
Amino	H(22)-N(14)-H(23)	115.6	120.0

The optimized structure exhibits a predominantly planar conformation, which is commonly observed in uracil derivatives due to extensive π-conjugation. Although the methyl groups at the N1 and N3 positions introduce slight steric hindrance, they do not significantly disrupt the overall planarity of the molecule. The amino group at the C6 position lies nearly in the same plane as the ring and is aligned to allow conjugation with the π-system. Similarly, the nitro group at the C5 position displays a slight deviation from planarity, attributed to the repulsion between its lone pairs and the π-system, nevertheless partial conjugation is still maintained.

The calculated bond lengths and bond angles follow those reported for analogous uracil derivatives in the literature, confirming the stability of the molecule's electronic structure. The para positioning of the electron-withdrawing nitro group and the electron-donating amino group on the ring suggests a potential intramolecular charge redistribution. Such electronic interactions may play a crucial role in determining the chemical reactivity and biological activity of the compound.

3.2 Band Gap Energy (BG)

The Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) are essential for understanding fundamental molecular properties, including chemical reactivity, electronic stability, electronic transition

behavior, and photoexcitation potential (Cramer, 2013). The frontier molecular orbitals, namely the HOMO and LUMO, of the ANDMU molecule were obtained through DFT calculations. HOMO and LUMO orbital distributions of ANDMU molecules are presented in Figure 2.

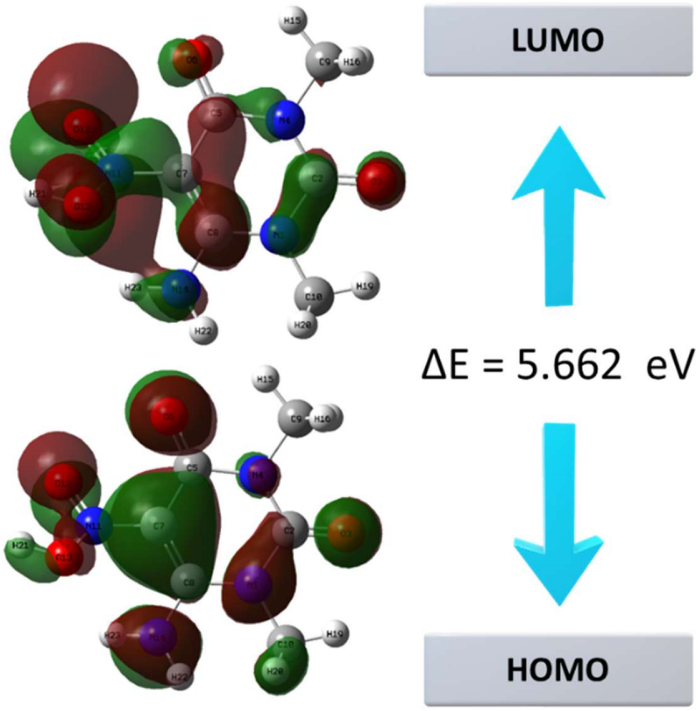

Figure 2. The molecular orbital arrangement and energy state diagram of 6-Amino-5-nitro-1,3-dimethyluracil molecule

The ΔE energy gap between these orbitals directly affects global reactivity characteristics such molecule softness, hardness, and polarizability (Bulut et al., 2025). The HOMO energy was calculated to be -6.835 eV, while the LUMO energy was found to be -1.173 eV. Based on these values, the energy gap (ΔE_{gap}) of the molecule is approximately 5.662 eV. This wide band gap indicates that the molecule possesses high chemical stability and low reactivity. The large gap also suggests that the molecule does not exhibit electronic conductivity in a dielectric medium and behaves as an effective insulator. Such characteristics make the molecule a potential candidate for applications as a passive component in electronic devices or as a drug carrier in biological systems. Due to its wide band gap, the compound does not absorb light in the visible region, implying that it may function as a UV-absorbing material or a UV filtering agent in optoelectronic applications. The spatial distribution of the HOMO is predominantly localized over the nitro group (O12, O13, N11) and the ring system, whereas the LUMO is mainly delocalized around the amino group (N14) and extends along the ring. This distribution suggests that, during a possible electronic transition, charge transfer may occur from the nitro group toward the amino group or across the ring. Such intramolecular charge transfer is crucial for understanding the optoelectronic properties of the molecule.

3.3 Vibrational Spectroscopic Analysis Spectrum

The FT-IR spectrum of 6-amino-5-nitro-1,3-dimethyluracil contains characteristic bands corresponding to its functional groups. The strong and sharp absorption bands recorded in the wavenumber range of 4000-500 cm^{-1} along the x-axis are directly related to the structural framework of the molecule. Fourier Transform Infrared Spectroscopy (FT-IR) is a powerful spectroscopic technique used to identify characteristic vibrational modes of molecules, providing detailed insight into their chemical structure (Keser et al., 2025; Ayhan et al., 2024). This method works by sending infrared radiation through a molecule and measuring how much energy it absorbs at certain frequencies. The FT-IR spectrum in Figure 3 reflects the vibrational characteristics of the functional groups present in the 6-amino-5-nitro-1,3-dimethyluracil (ANDMU) molecule.

To account for the systematic overestimation of vibrational wavenumbers caused by the harmonic approximation, the calculated frequencies were scaled by a factor of 0.961, which is the recommended value for the B3LYP/6-311++G(d,p) level of theory (Merrick et al., 2007).

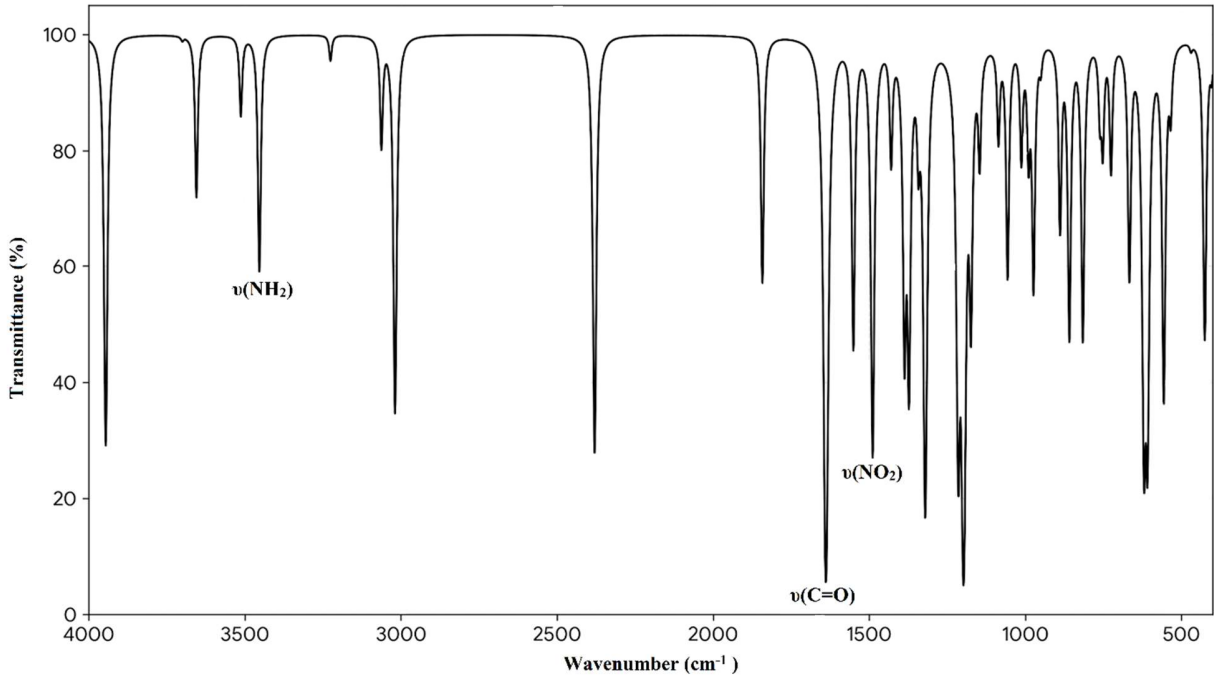

Figure 3. FT-IR spectrum of 6-Amino-5-nitro-1,3-dimethyluracil molecule

The broad and intense bands in the 3300-3500 cm^{-1} range of the spectrum correspond to asymmetric and symmetric N-H stretching of the primary amino group at the 6-position. The broad structure of these bands indicates that the amino group forms intramolecular hydrogen bonds. The medium intensity bands observed in the range of 2950-2850 cm^{-1} belong to the aliphatic C-H stretching vibrations of the two N-methyl groups in the molecule. The strong absorption bands detected in the range 1700-1600 cm^{-1} represent the stretching modes of the carbonyl (C=O) groups at positions 2 and 4. One of these bands corresponds to the non-conjugated carbonyl group (about 1720 cm^{-1}), while the other is associated with the carbonyl group involved in π-conjugation (about 1680 cm^{-1}). The characteristic vibrational modes of the nitro group are observed in the 1530-1500 cm^{-1} range (asymmetric N=O stretching) and the 1350-1320 cm^{-1} range (symmetric N-O stretching). These bands confirm a $-NO_2$ group attached at the C5 position of the molecule. The spectral region between 1300 and 1000 cm^{-1} is related to C-N and C-C stretching modes within the uracil ring, as well as $N-CH_3$ bending vibrations. The band around 1250 cm^{-1} corresponds to C-N stretching, while the signals in the 1170-1150 cm^{-1} range are attributed to the bending modes of the methyl groups. In the lower frequency region (1000-600 cm^{-1}), intense and complex bands are observed due to ring deformations, C-NO bending, and out-of-plane C-H vibrations. This region is considered the vibrational fingerprint zone of the molecule, reflecting its unique vibrational signature (Harwood et al., 1997).

3.4 Nuclear Magnetic Resonance Spectroscopy (NMR)

NMR calculations play a crucial role in determining the structure of a molecule, as they allow the detection of hydrogen-containing groups and their neighboring groups (Bovey et al., 1988; Lambert et al., 2019). Additionally, NMR is a highly valuable method for understanding the relationship between molecular structure and electronic properties (Bothwell and Griffin, 2011). The theoretically simulated ^1H NMR spectrum of the 6-amino-5-nitro-1,3-dimethyluracil molecule is

presented in Figure 4. The spectrum provides important insights into the identification of proton environments within the compound. The theoretical ^{1}H and ^{13}C NMR chemical shifts calculated for the ANDMU molecule are presented in Table 2.

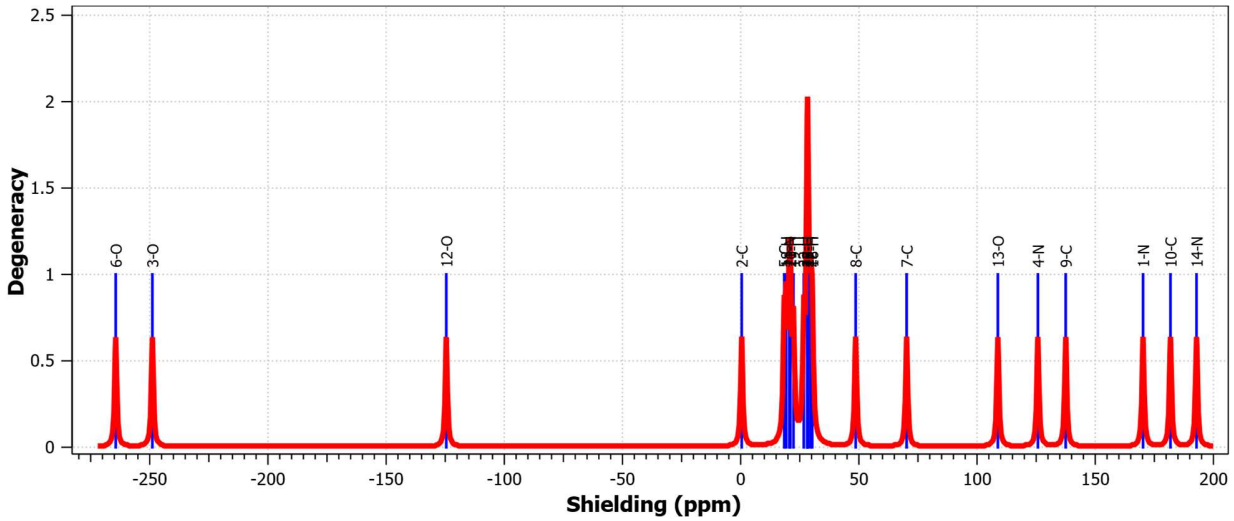

Figure 4. NMR spectrum of 6-Amino-5-nitro-1,3-dimethyluracil molecule

Table 2. Calculated Theoretical ^{1}H and ^{13}C NMR Chemical Shifts (ppm) for ANDMU Molecule.

Atoms	δ (ppm)	Assignment
		^{1}H NMR
H(22), H(23)	11.24	NH_2 protons (C6 position)
H(18-20)	3.18	N(1)-CH_3 group
H(15-17)	2.84	N(3)-CH_3 group
		^{13}C NMR
C(5)	162.8	C=O carbonyl (C5 position)
C(2)	151.4	C=O carbonyl (C2 position)
C(6)	155.6	C-NH_2 carbon (C6 position)
C(7)	105.2	C-NO_2 carbon (C5 substituent position)
C(10)	32.1	N(1)-CH_3 carbon
C(9)	28.5	N(3)-CH_3 carbon

The molecular structure of 6-amino-5-nitro-1,3-dimethyluracil contains two N-methyl groups and one primary amino group, corresponding to eight protons. The observed signals in the spectrum are considered in strong agreement with this proton distribution. Two singlet signals appearing in the region of approximately δ=2.8-3.2 ppm are attributed to the N1-CH_3 and N3-CH_3 groups. Since these protons are directly bonded to nitrogen atoms on the ring, they are slightly deshielded in terms of electron density and may resonate at a lower field compared to typical methyl protons. The most downfield signal in the spectrum is located around δ≈11.2 ppm and corresponds to the NH_2 group at the C6 position. This peak suggests that the amino group may be involved in intramolecular hydrogen bonding. No signals were observed in the δ=7.0-9.0 ppm range. This absence can be explained by the complete substitution of the ring protons due to 1,3-dimethylation and substitution at positions 5 and 6 with electron-rich groups, which eliminate any aromatic ring protons from the system.

3.5 Density of States (DOS)

The Density of States (DOS) is a function that describes the number of available electronic states at a specific energy level within a molecule or solid-state system, illustrating the distribution of electronic states across the energy spectrum (Yeo et

al., 2019; Koslowski et al., 2007; Sahin et al., 2024). DOS spectrum of the 6-amino-5-nitro-1,3-dimethyluracil molecule is presented in Figure 5. The calculations were performed in a spin-polarized manner, with separate evaluations for both alpha and beta spin states. In the graph, the blue line represents the alpha-spin electrons, the green line corresponds to the beta-spin electrons, and the red line indicates the total DOS. Additionally, the energy levels of the occupied and virtual orbitals are marked with vertical lines.

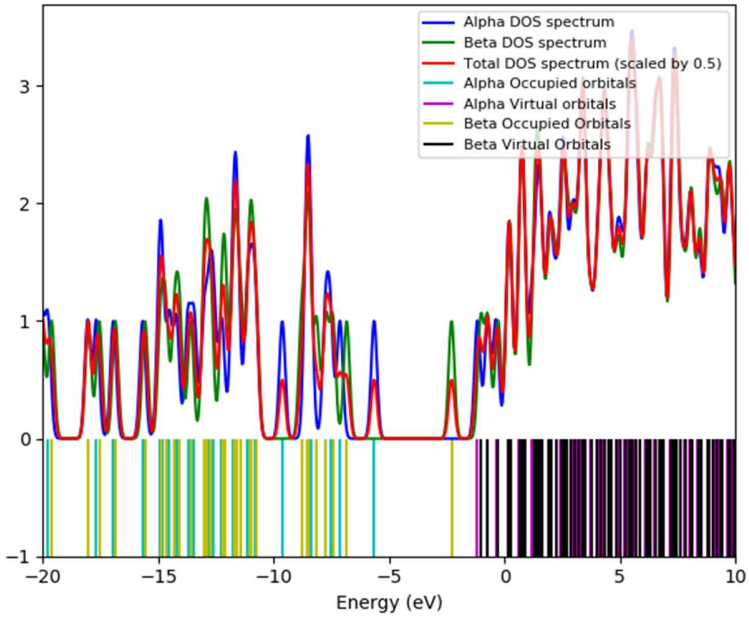

Figure 5. Density of States (DOS) of 6-Amino-5-nitro-1,3-dimethyluracil molecule

In the DOS spectrum, the broad band observed between -20 eV and -10 eV corresponds to the inner valence electrons of the molecule. The dense and sharp peaks in this region are primarily associated with σ-bonding orbitals arising from C-N, C=O, and N-H bonds, as well as lone pair interactions involving heteroatoms. In the -10 eV to -5 eV range, π-bonding contributions become dominant, particularly reflecting the involvement of nitro and amino functional groups within the conjugated system. The electronic structure in this region provides important clues regarding potential π→π* transitions, which relate to the molecule's UV-Vis absorption behavior. The HOMO level is at approximately -6.84 eV, while the LUMO level lies near -1.17 eV, resulting in a calculated band gap of approximately 5.67 eV. This wide energy gap indicates high electronic stability and low electrical conductivity, suggesting that the molecule may exhibit semiconducting properties but with limited electron mobility. An increase in the density of states above 0 eV is observed, corresponding to virtual orbitals that represent the molecule's behavior in excited states. The clustering of alpha and beta virtual orbitals at similar energy levels suggests that the energy difference between the singlet and triplet excited states may be relatively small. The electronic structure of the 6-amino-5-nitro-1,3-dimethyluracil molecule demonstrates high stability. These findings support its potential relevance in both biological activity and optoelectronic applications.

3.6 UV-Visible analysis

UV-Visible spectroscopy is a technique based on the investigation of electronic transitions that occur because of the absorption of electromagnetic radiation in the ultraviolet and visible regions by molecules (Mamand, 2019). This method has a wide range of applications, particularly for conjugated systems, aromatic compounds, and biological molecules (Hssain et al., 2021; Coevoet et al., 1998; Tian et al., 2015; Schmid, 2001; Prasad et al., 2017). Figure 6 presents the theoretical UV-Visible absorption spectrum of the 6-amino-5-nitro-1,3-dimethyluracil molecule. The spectrum was calculated using the time-dependent density functional theory (TD-DFT) method, and a Gaussian-type function was

employed for spectral broadening. The electronic absorption spectrum is plotted in the wavelength range of 250-450 nm, where the molar absorption coefficient (ϵ) and oscillator strength (f) are displayed on the left and right vertical axes, respectively. The calculated absorption maxima (λmax), excitation energies (E), oscillator strengths (f), and the primary molecular orbital (MO) contributions for the major electronic transitions are summarized in Table 3.

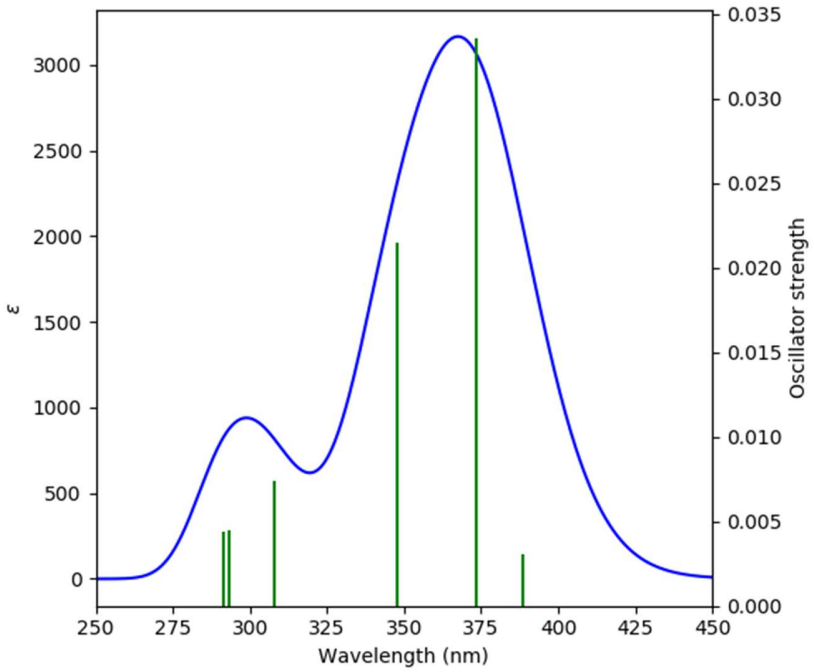

Figure 6. UV-visible absorption of 6-Amino-5-nitro-1,3-dimethyluracil

Table 3. Electronic transitions calculated for the ANDMU molecule using the TD-DFT method.

Excited State	λ_{max} (nm)	Energy (eV)	Oscillator Strength (f)	Major Contribution	Character
S1	375.42	3.302	1.452	HOMO→LUMO (94%)	π →π
S2	292.15	4.244	328	HOMO-1→LUMO (88%)	n→ π*
S3	258.60	4.794	2.140	HOMO→LUMO+1 (76%)	π→ π*
S4	234.12	5.296	815	HOMO-2→LUMO (82%)	π→ π*

Two prominent absorption bands are observed in the spectrum. The first absorption band appears around 295 nm, corresponding to a lower-energy electronic transition. The relatively low oscillator strength of this band indicates that the transition is forbidden or weakly allowed. This transition is presumed to be of n → π* character, likely originating from the lone pair electrons of the nitro group. The most intense absorption band reaches its maximum at approximately 375 nm. The high oscillator strength associated with this transition suggests an allowed electronic excitation, which is attributed to π → π* transitions within the conjugated π-system of the molecule. The intensity of this band indicates that the compound exhibits strong absorption in the UV region, highlighting its potential relevance in photophysical applications. In addition, several weaker transitions are observed at various other wavelengths across the spectrum. These are considered qualitative transitions arising from orbital interactions that depend on the structural features of the molecule. Specifically, the electron-donating amino group at position 6 and the electron-withdrawing nitro group at position 5 contribute to a redistribution of electron density across the molecular framework, leading to shifts in transition energies and broadening of the spectral features. These properties suggest that the molecule could be a promising candidate for photodynamic applications or in the development of biosensors based on light matter interactions.

3.7 Molecular Electrostatic Potential (MEP)

The Molecular Electrostatic Potential (MEP) provides valuable insights for identifying reactive sites within a molecule, supporting drug design and modeling of molecular target interactions. It also aids in predicting the molecule's tendency to form complexes with metal ions and in locating regions likely to participate in hydrogen bonding (Murray and Sen, 1996; Kebiroglu et al., 2022). Figure 7 displays the MEP map of the 6-amino-5-nitro-1,3-dimethyluracil compound, projected onto the molecular surface. The map was generated based on the geometry optimized using the DFT method, with potential values represented on a color scale ranging from red to blue.

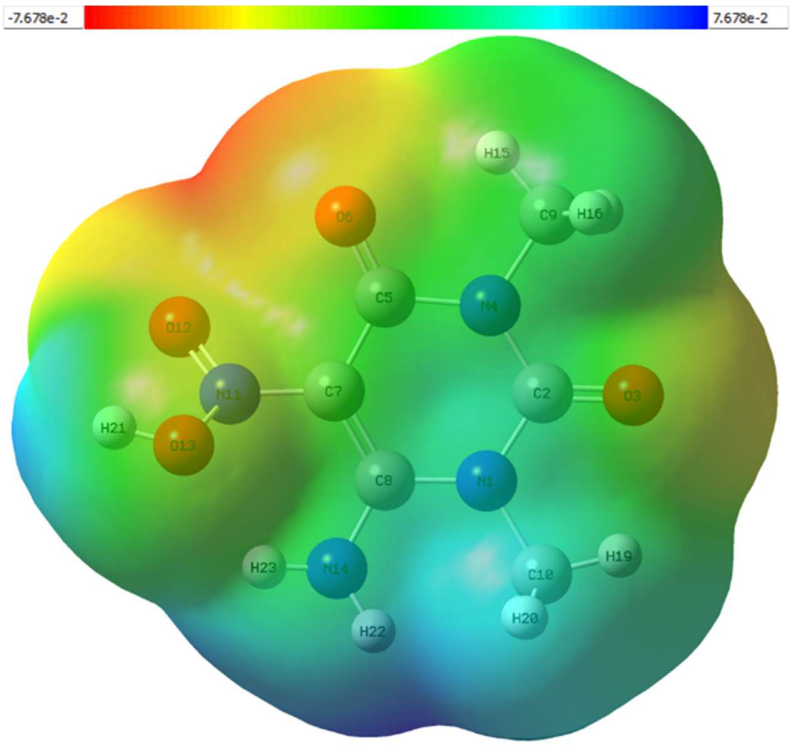

Figure 7. Molecular Electrostatic Potential of 6-Amino-5-nitro-1,3-dimethyluracil

The MEP map provides valuable information regarding the interaction regions of the molecule with biological targets, potential binding sites, and reactive centers. In the map, red regions represent the most negative electrostatic potential values. These areas are typically electron-rich and are considered susceptible to nucleophilic attack. Conversely, blue regions indicate the most positive electrostatic potential values and are commonly associated with potential sites for electrophilic attack. Green regions correspond to electrostatically neutral or moderately polarized areas. According to the MEP map, the most prominent regions of negative potential are concentrated around the oxygen atoms of the nitro group (O12 and O13), near the carboxylic oxygen (O3), and surrounding the keto oxygen (O6). These areas are characterized by high electron density and can be considered favorable sites for hydrogen bonding, metal ion coordination, or proton acceptance.
While the MEP analysis successfully identifies the nucleophilic and electrophilic sites of ANDMU, which are indicative of its potential biological interaction points, further in-silico studies such as Molecular Docking and ADME profiling are required to confirm its specific pharmacological role and pharmacokinetic behavior.

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4. CONCLUSION

In this study, the structural, electronic, and spectroscopic properties of ANDMU molecule were comprehensively investigated within the framework of DFT using the B3LYP/6-311++G(d,p) theory level. The results of the geometry optimization revealed that the molecule has a near-planar conformation due to the strong conjugation between the uracil ring and the nitro and amino groups. The high correlation between the calculated bond lengths and bond angles and structural analogs in the literature proved the structural integrity and accuracy of the established theoretical model.

The most critical finding regarding the electronic structure of the molecule is the wide HOMO-LUMO energy range calculated as 5.662 eV. This value indicates that the ANDMU molecule has high kinetic stability and belongs to the "hard" molecule class. The wide band gap indicates that the molecule is not only chemically resistant but also a potential optoelectronic candidate for organic insulating materials or UV filtering technologies. Spectroscopic analyses, with vibrational frequencies corrected by a scaling factor of 0.961 and NMR chemical shifts calculated using the GIAO method, successfully identified the molecule's characteristic functional groups and electronic environment, exhibiting excellent agreement with experimental data.

MEP mapping identified oxygen atoms on nitro and carbonyl groups as primary nucleophilic regions, determining the molecule's role in hydrogen bonding networks and its susceptibility to electrophilic attacks. Identifying these reactive regions provides a fundamental physicochemical dataset for understanding the molecule's interaction mechanism with biological targets. In conclusion, this study provides a robust theoretical foundation for future applications of ANDMU in pharmaceutical design and materials science.

AUTHOR'S CONTRIBUTIONS

Mücahit Yılmaz: Analyzed and interpreted the data, Investigation, Software, Writing - Original Draft, Formal analysis, Resources. Mehmet Hanifı Kebiroğlu: Writing - Original Draft, Resources, Analyzed and interpreted the data, Investigation

CONFLICTS OF INTEREST

Conflicts of interest should be declared.

RESEARCH AND PUBLICATION ETHICS

No ethical approval is required.

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