QUANTUM-CHEMICAL STUDY OF A NOVEL BIS-THIOUREA DERIVATIVE

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ABSTRACT

The present work focuses on the quantum-chemical characterization of a newly synthesized N2,N3-hexamethylene-bis-[(p-nitroaniline) N2,N3-(phenylthiourea)-urea] derivative. Density Functional Theory (DFT) calculations were carried out at the B3LYP/6-31G(d) level to investigate its molecular geometry, electronic properties, charge distribution, molecular electrostatic potential, and frontier molecular orbitals. The optimized structure demonstrated high thermodynamic stability. Mulliken population analysis revealed significant charge accumulation around heteroatoms, particularly oxygen and sulfur atoms. Electrostatic potential mapping identified the most probable reactive regions responsible for intermolecular interactions. Frontier orbital analysis showed effective electron-donating and electron-accepting capabilities, suggesting favorable adsorption behavior and potential application of the compound as a corrosion inhibitor.

Introduction. Organic compounds containing sulfur, nitrogen, and oxygen atoms have attracted considerable scientific interest due to their ability to interact strongly with metallic surfaces. Such interactions are primarily governed by the electronic structure of the molecule and the availability of electron-rich adsorption centers. Thiourea-based derivatives are among the most promising classes of compounds because their heteroatoms and conjugated systems facilitate electron transfer processes[1-3].

Advances in computational chemistry have made it possible to predict molecular reactivity and adsorption characteristics through theoretical calculations. In this context, Density Functional Theory (DFT) has become a powerful tool for understanding the relationship between molecular structure and physicochemical properties. Therefore, the present study aims to investigate the electronic characteristics of a newly synthesized bis-thiourea derivative using quantum-chemical methods[4-6].

Computational Method. All calculations were performed within the framework of Density Functional Theory using the B3LYP exchange-correlation functional and the 6-31G(d) basis set. Geometry optimization was carried out without imposing any symmetry restrictions. Following optimization, Mulliken atomic charges, molecular electrostatic potential (MEP), and frontier molecular orbitals were analyzed to evaluate the electronic behavior of the molecule[6-9].

Results and Discussion. The optimized molecular structure exhibits a stable conformation characterized by two aromatic nitro-substituted fragments connected through a hexamethylene bridge and thiourea functional groups. The absence of imaginary frequencies confirms that the optimized geometry corresponds to a true energy minimum on the potential energy surface.

The calculated thermodynamic parameters indicate that the molecule possesses substantial energetic stability. Furthermore, the dipole moment value suggests the presence of significant molecular polarity, which may enhance intermolecular interactions and surface adsorption processes.

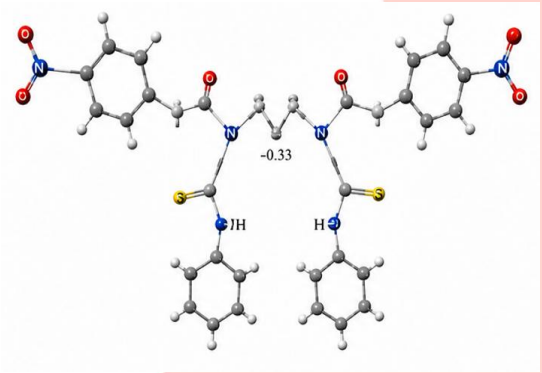

Figure 1. Optimized molecular geometry calculated at the DFT/B3LYP/6-31G(d) level.

Analysis of the Mulliken atomic charges demonstrated a non-uniform distribution of electron density throughout the molecule. The oxygen atoms of the nitro and carbonyl groups, together with sulfur atoms of the thiocarbonyl fragments, carry the highest negative charge density. These centers are expected to participate actively in coordination and adsorption phenomena.

Conversely, hydrogen atoms attached to nitrogen atoms exhibit positive charge values, creating potential sites for hydrogen-bond formation. The observed charge separation contributes to the overall electronic polarization of the molecule.

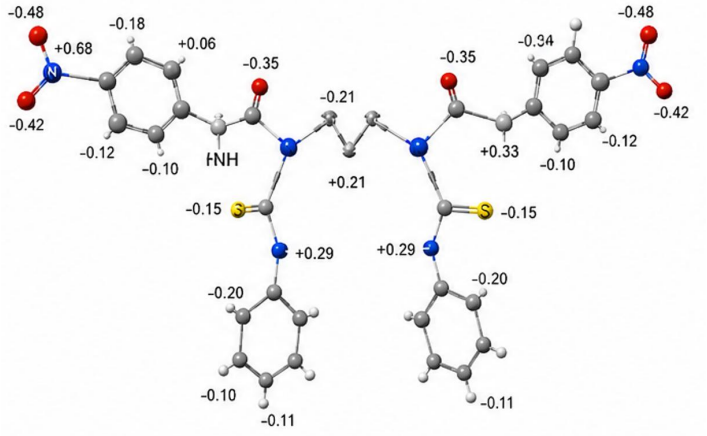

Figure 2. Mulliken atomic charge distribution.

The molecular electrostatic potential surface provides a visual representation of electron density distribution. Regions with negative electrostatic potential are concentrated around oxygen and sulfur atoms, indicating preferred sites for electrophilic attack. Positive potential zones are mainly localized near NH groups.

The presence of both electron-rich and electron-deficient regions within the same molecular framework suggests enhanced reactivity and the ability to interact with different chemical environments.

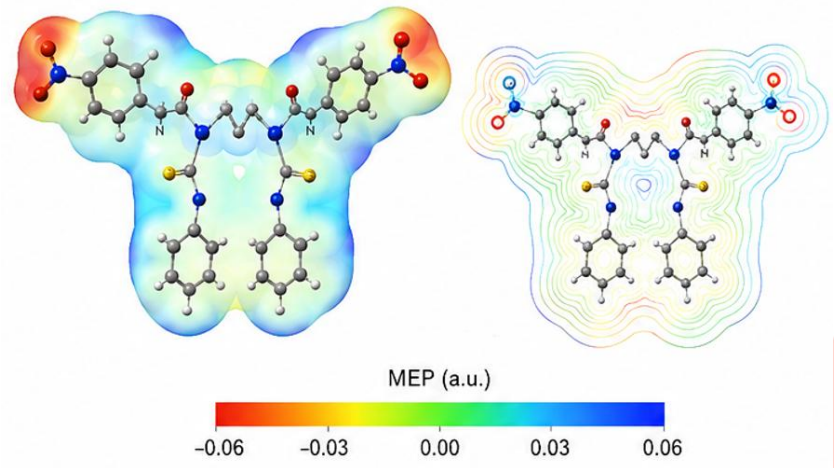

Figure 3. Molecular electrostatic potential (MEP) map and contour plot.

The frontier molecular orbital analysis revealed that the HOMO is primarily localized over sulfur-containing thiourea fragments and aromatic rings, indicating their role in electron donation. In contrast, the LUMO is concentrated mainly around nitro-substituted aromatic fragments and carbonyl groups, which function as electron acceptors.

The calculated HOMO–LUMO energy separation of approximately 3.55 eV indicates moderate chemical hardness and relatively high electronic mobility. Such characteristics are generally associated with efficient charge-transfer processes and strong adsorption tendencies on metal surfaces.

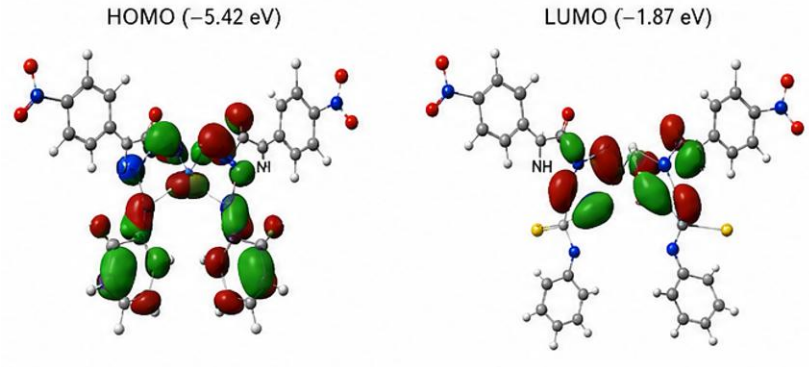

Figure 4. Frontier molecular orbitals (HOMO and LUMO).

Conclusion. Quantum-chemical calculations have demonstrated that N^2,N^3-hexamethylene-bis-[(p-nitroaniline) N^2,N^3-(phenylthiourea)-urea] possesses a favorable electronic structure characterized by distinct donor and acceptor regions. Mulliken charge analysis and molecular electrostatic potential mapping identified oxygen and sulfur atoms as the principal reactive centers. The HOMO–LUMO distribution further confirmed the molecule's capability for effective electron exchange. These findings suggest that the investigated compound may

exhibit promising adsorption behavior and could serve as a potential corrosion-inhibiting material.

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