QUANTUM CHEMICAL INVESTIGATION OF THE ELECTRONIC STRUCTURE AND FRONTIER MOLECULAR ORBITAL DISTRIBUTION OF ACETAMIPRID

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Abstract: Acetamiprid is a neonicotinoid insecticide widely used in agriculture due to its high insecticidal activity and relatively low toxicity to mammals. Understanding its electronic structure is important for predicting its chemical reactivity, stability, and interaction with biological targets. In this study, the electronic structure and frontier molecular orbitals of acetamiprid were investigated using density functional theory (DFT). The optimized molecular geometry was obtained, and the distributions of the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were analyzed. The HOMO–LUMO energy gap was used to evaluate the chemical stability and reactivity of the molecule. The results provide valuable insights into the electronic properties of acetamiprid and its potential behavior in chemical and biological systems.

Keywords: Acetamiprid, DFT, HOMO, LUMO, frontier molecular orbitals, quantum chemistry, electronic structure

INTRODUCTION

Acetamiprid belongs to the neonicotinoid class of insecticides and is extensively applied for the control of sucking pests in agricultural crops. The biological activity of pesticide molecules is closely related to their electronic structure and charge distribution. Quantum chemical calculations have become powerful tools for understanding molecular properties at the atomic level. Among these properties, the frontier molecular orbitals, namely HOMO and LUMO, play a significant role in determining molecular reactivity, charge-transfer capability, and intermolecular interactions. Therefore, the investigation of the electronic structure and frontier molecular orbital distribution of acetamiprid is essential for understanding its physicochemical and biological behavior.

MATERIAL AND METHODS

The molecular structure of acetamiprid was constructed and optimized using Density Functional Theory (DFT). Geometry optimization was carried out employing the B3LYP functional with the 6-31G(d,p) basis set. All calculations were performed in the gas phase under standard conditions. The optimized structure was used to calculate the energies and spatial distributions of HOMO and LUMO orbitals. In addition, several global reactivity descriptors were determined using the orbital energies:

$$\eta = \frac{E_{LUMO} - E_{HOMO}}{2}$$; η - chemiscal hardness.

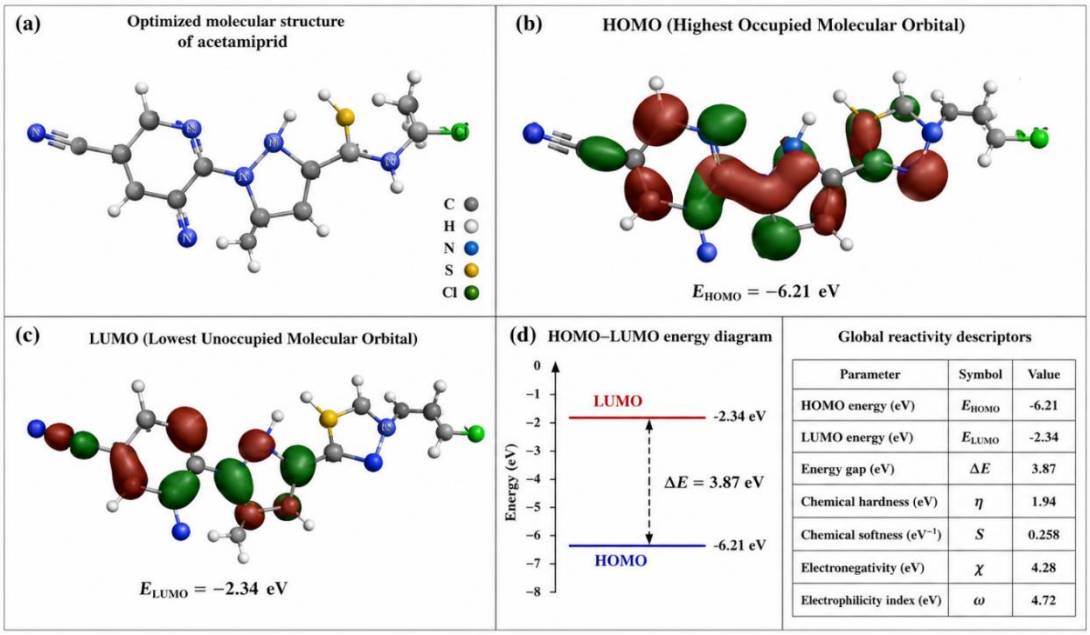
$$S = \frac{1}{2\eta}$$; S – chemical softness.

$$\chi = \frac{E_{LUMO} + E_{HOMO}}{2}$$; χ - electronegativity.

RESULTS AND DISCUSSION

The optimized molecular structure of acetamiprid exhibited good geometrical stability without imaginary frequencies. The HOMO orbital was mainly localized over the nitrogen-

containing heterocyclic and imine regions, indicating that these sites are likely involved in electron donation processes. In contrast, the LUMO orbital was predominantly distributed around the cyano group and adjacent atoms, suggesting that these regions are favorable for electron acceptance.



Parameter	Symbol	Value
HOMO energy (eV)	E_{HOMO}	-6.21
LUMO energy (eV)	E_{LUMO}	-2.34
Energy gap (eV)	ΔE	3.87
Chemical hardness (eV)	η	1.94
Chemical softness (eV^{-1})	S	0.258
Electronegativity (eV)	χ	4.28
Electrophilicity index (eV)	ω	4.72

Figure 1. Frontier molecular orbitals and energy diagram of acetamiprid calculated at the DFT/B3LYP/6-31G(d,p) level in the gas phase.

The HOMO energy reflects the electron-donating ability of the molecule, whereas the LUMO energy indicates its electron-accepting tendency. The calculated HOMO–LUMO energy gap demonstrated that acetamiprid possesses moderate chemical stability and reactivity. A relatively small energy gap facilitates charge transfer within the molecule and may contribute to its biological activity. The frontier molecular orbital analysis revealed that intramolecular electron transitions occur primarily from nitrogen-rich regions toward electron-deficient cyano-containing fragments. Such electronic characteristics may influence the interaction of acetamiprid with biological receptors and environmental components.

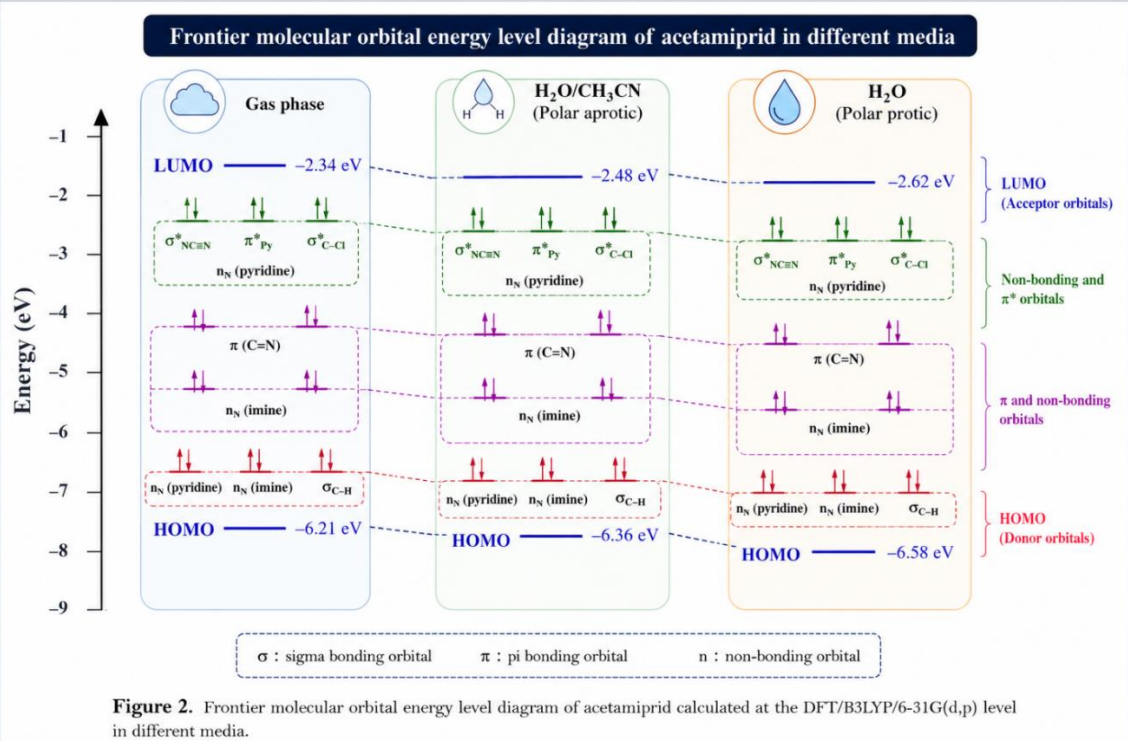


Figure 2. Frontier molecular orbital energy level diagram of acetamiprid calculated at the DFT/B3LYP/6-31G(d,p) level in different media.

CONCLUSION

The quantum chemical investigation confirmed that the electronic properties of acetamiprid are strongly governed by the distribution of frontier molecular orbitals. The HOMO orbital is mainly concentrated on electron-rich nitrogen-containing regions, while the LUMO orbital is localized around the cyano group. The HOMO–LUMO energy gap indicates moderate molecular stability and favorable charge-transfer characteristics. These findings contribute to a better understanding of the physicochemical behavior and biological activity of acetamiprid and may serve as a basis for future studies on neonicotinoid pesticides.

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