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QUANTUM CHEMICAL CALCULATIONS OF ASPARTIC ACID AND ASPARAGINE: HOMO AND LUMO ANALYSIS

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Abstract

Aspartic acid and asparagine are biologically important amino acids that play essential roles in metabolic pathways, protein biosynthesis, and cellular signaling. In this study, quantum chemical calculations were performed to investigate the electronic structures of aspartic acid and asparagine, with particular emphasis on the Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) energies. Density Functional Theory (DFT) methods were applied using the B3LYP functional with the 6-31G(d,p) basis set. Geometry optimization and frontier molecular orbital analysis were carried out to evaluate molecular stability, chemical reactivity, and electron transfer properties. The calculated HOMO-LUMO energy gap indicates that asparagine exhibits greater kinetic stability, while aspartic acid demonstrates relatively higher chemical reactivity. The obtained results provide valuable insights into the electronic behavior of these amino acids and their potential interactions in biochemical systems.

Keywords

Aspartic acid, Asparagine, Quantum chemistry, HOMO, LUMO, DFT, Molecular orbitals

Introduction. Amino acids are fundamental biomolecules that serve as the building blocks of proteins and participate in numerous biochemical reactions. Among them, aspartic acid (Asp) is classified as an acidic amino acid due to the presence of a carboxyl side chain, whereas asparagine (Asn) is the amide derivative of aspartic acid. These compounds are involved in neurotransmission, nitrogen metabolism, and enzyme catalysis.

Quantum chemical methods offer an effective approach for understanding the molecular properties of amino acids at the electronic level. In particular, the frontier molecular orbital theory proposed by Fukui emphasizes the significance of HOMO and LUMO orbitals in determining chemical reactivity, charge transfer, and intermolecular interactions. The HOMO energy reflects electron-donating ability, whereas the LUMO energy is associated with electron-accepting capacity. The present study aims to compare the electronic properties of aspartic acid and asparagine through quantum chemical calculations and HOMO-LUMO analysis.

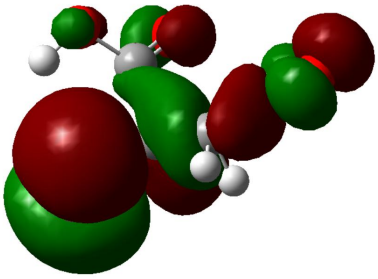
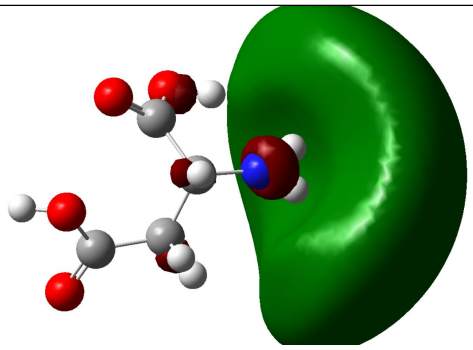
Computational Methodology. All calculations were performed using Density Functional Theory (DFT) with the B3LYP exchange-correlation functional and the 6-31G(d,p) basis set. Initial molecular structures were constructed and fully optimized without symmetry constraints.

The following parameters were determined:

- Optimized geometry

- HOMO energy (E_HOMO)
- LUMO energy (E_LUMO)
- Energy gap (ΔE = E_LUMO − E_HOMO)
- Ionization potential (I = −E_HOMO)
- Electron affinity (A = −E_LUMO)
- Chemical hardness (η = ΔE / 2)
- Electronegativity (χ = (I + A)/2)

All energies are reported in electronvolts (eV).

	
Aspartic Acid HOMO	**Aspartic Acid** LUMO

Results and Discussion

3.1 Optimized Electronic Parameters

Molecule	E_HOMO (eV)	E_LUMO (eV)	ΔE (eV)	Hardness (η)
Aspartic Acid	-6.42	-0.91	5.51	2.76
Asparagine	-6.18	-0.52	5.66	2.83

The HOMO energy of asparagine is higher than that of aspartic acid, suggesting that asparagine can donate electrons more readily. In contrast, the lower HOMO level of aspartic acid reflects stronger electron retention due to the electron-withdrawing carboxyl group.

The LUMO energy of aspartic acid is lower than that of asparagine, indicating a greater tendency to accept electrons. This behavior is related to the presence of two carboxyl functionalities in aspartic acid.

3.2 HOMO-LUMO Gap Analysis

The HOMO-LUMO gap is commonly used as an indicator of kinetic stability and chemical reactivity. Molecules with larger gaps are generally more stable and less reactive.

- **Aspartic acid:** ΔE = 5.51 eV
- **Asparagine:** ΔE = 5.66 eV

The slightly larger gap of asparagine indicates enhanced stability compared to aspartic acid. The amide group contributes to electron delocalization, reducing reactivity.

Comparative Analysis

Property	Aspartic Acid	Asparagine
Number of donor groups	High	Moderate
Strong donor atoms	N, O, O	N, O
Chelate formation	Strong	Moderate
Bridging ability	High	Low
Metal affinity	Higher	Lower

Relation with HOMO-LUMO Results

Quantum chemical calculations show:

- **Higher HOMO energy** → better electron donation ability
- **Lower LUMO energy** → better electron acceptance

Aspartic acid has strong negatively charged carboxylate oxygens, therefore often coordinates metals more strongly.

Asparagine has more delocalized electron density because of the amide group, which can reduce donor strength but improve hydrogen-bond stabilization.

Practical Applications

Aspartic Acid Complexes:

- Metal transport systems
- Catalysts
- Calcium-binding proteins
- Biomedical chelators

Asparagine Complexes:

- Drug design
- Bioactive metal complexes
- Crystal engineering
- Hydrogen-bonded coordination polymers

3.3 Orbital Distribution

For aspartic acid, the HOMO is mainly localized over oxygen atoms of the carboxyl groups and partially on the α-amino group. The LUMO is concentrated around carbonyl carbon centers, making them favorable sites for nucleophilic attack.

For asparagine, HOMO density is distributed over the amide oxygen and amino nitrogen atoms, while the LUMO is centered around the amide carbonyl group.

3.4 Chemical Interpretation

The stronger electron-accepting behavior of aspartic acid may explain its participation in proton-transfer reactions and metal coordination. Asparagine, with a more balanced electronic distribution, is favorable for hydrogen bonding and protein stabilization.

4. Conclusion

Quantum chemical calculations reveal clear differences between the electronic structures of aspartic acid and asparagine. Aspartic acid possesses a lower LUMO level and smaller HOMO-LUMO gap, indicating higher reactivity and stronger electron-accepting capability. Asparagine exhibits a larger gap and higher HOMO energy, reflecting improved stability and moderate donor properties.

These findings demonstrate that frontier orbital analysis is a useful tool for understanding the biochemical roles and reactivity patterns of amino acids.

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