Title

Role of Triplet States in the Photolysis of Proteogenic Amino Acids

Abstract

This investigation delves into the UV photodissociation of pivotal amino acids (Alanine, Glycine, Leucine, Proline, and Serine) at 213 nm, providing insights into triplet-state deactivation pathways. Utilizing a comprehensive approach involving time-dependent density functional calculations (TD-DFT), multi-configurational methods, and ab-initio molecular dynamics (AIMD) simulations, we scrutinize the excited electronic states (T1, T2, and S1) subsequent to 213 nm excitation. Our findings demonstrate that α-carbonyl C−C bond-breaking in triplet states exhibits markedly lower barriers than in singlet states (below 5.0 kcal mol−1). AIMD simulations corroborate the potential involvement of triplet states in amino acid fragmentation, underscoring the significance of accounting for these states in photochemistry. Chemical bonding analyses unveil distinctive patterns for S1 and T1 states, with the asymmetric redistribution of electron density characterizing the C−C breaking in triplet states, in contrast to the symmetric breaking observed in singlet states. This research complements recent experimental discoveries, enhancing our comprehension of amino acid reactions in the interstellar medium.

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Author(s) ID

57222029039; 57195727205; 6507908577

Year

2024

Source title

ChemPhysChem

Volume

25.0

Issue

3

Art. No.

e202300655

DOI

10.1002/cphc.202300655

Link

https://www.scopus.com/inward/record.uri?eid=2-s2.0-85178889110&doi=10.1002%2fcphc.202300655&partnerID=40&md5=1d0318e59b2974c4edec0f45644b9920

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Author Keywords

amino acids; C−C breaking; photodissociation; photolysis; triplet-state

Index Keywords

Amino acids; Chemical bonds; Molecular dynamics; Photodissociation; Reaction kinetics; alanine; amino acid; carbonyl derivative; glycylleucine; proline; serine; Ab initio molecular dynamics simulation; Amino acid alanines; Amino-acids; Breakings; C−C breaking; Deactivation pathways; Singlet state; Time-dependent density functional calculations; Triplet state; UV photodissociation; ab initio calculation; article; chemical binding; density functional theory; drug development; human; molecular dynamics; photochemistry; photolysis; triplets; ultraviolet radiation; Photolysis

Chemicals/CAS

alanine, 56-41-7, 6898-94-8; amino acid, 65072-01-7; glycylleucine, 869-19-2; proline, 147-85-3, 7005-20-1; serine, 56-45-1, 6898-95-9

Funding Details

Andrés Bello University, (DI-05-23/REG)

Funding Texts

The authors thank the Center for Theoretical and Computational Chemistry (CQTC) at Andrés Bello University. Y. A. R. N acknowledges to project UNAB N° DI-05-23/REG.

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Publisher

John Wiley and Sons Inc

ISSN

14394235

CODEN

CPCHF

PubMed ID

38057134.0

Language of Original Document

English

Abbreviated Source Title

ChemPhysChem

Document Type

Article

Publication Stage

Final

Source

Scopus

EID

2-s2.0-85178889110