Electron-hole analysis of Phe electron excitation characteristics under implicit H_2O solvent

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ABSTRACT

Implicit expression H_2O solvent S-Phe molecular system(S-Phe-1) electron-hole diagram analysis is not reported, for this reason, the excited state wave function of S-Phe- electronic structure characteristics of S-Phe-1. Based on the PBE0 method, TDDFT electronic excitation calculations were performed using two different basis sets (6-311G(d) and defTZVP), and electron-hole analyses were conducted for the S0 to S7 excited states of the S-Phe-1 system. It is show that: through electron and hole diagrams, the electron excitation characteristics of the S-Phe-1 molecular system are demonstrated, and the two base groups can see that the analysis of S1, S2, S3, S4, S5, S6 excitation electron excitation characteristics is qualitatively consistent, and the results of the analysis are basically the same; S7 excitation state is different, with polarization function of the 6-311G (d) base group and defTZVP base group is different, the former refers to the benzene-based to the niobium-based pi→pi* charge transfer excitation, the latter is the amino-to-pyridine n→pi* field excitation.

Keywords: Phenylalanine, electron-hole, electronic stimulation, implicit H_2O solvents

1. INTRODUCTION

Phenylalanine(Phe) is one of the important components of proteins such as organisms, and the molecular characteristics of Phe molecular system are widely concerned. Reference [1] drew a complete reaction potential energy surface for chiral transition path of Phe molecule by finding structures of the extreme value points including the transition states and intermediates. Reference [2] study reports a theoretical study of the mechanism of Phe molecular chiral transition under the action of a single water molecule. Reference [3] drew a reaction potential energy surface for chiral transition path by finding the structures of extreme value points including the transition states and intermediates, and analyzed the geometric and electronic structure properties of extreme value points for Phe. Implicit expression H_2O solvent S-Phe molecular system(S-Phe-1) electron-hole diagram analysis is not reported, for this reason, the excited state wave function of S-Phe-1 and the electron-hole diagram analysis of three different group levels, so as to reveal the electronic structure characteristics of S-Phe-1.

2. THEORY AND COMPUTATIONAL METHODS

The electron excitation process is usually accompanied by the transfer of the electron distribution range, and the electron transition process of a certain system is quantitatively described by theoretical calculations. The electron-hole module of the Multiwfn [4] is super powerful, not only can give electron and hole distribution, but also can do a lot of analysis to help judge the degree of CT, such as the distance between electron and hole centroid, electron and hole overlap integral, draw density difference (namely electron distribution minus hole distribution), the electron and hole into easier to investigate smooth distribution form, track or fragment contribution to electron and hole, etc.

This work used the density functional(DFT) B3LYP method to optimize the S-Phe-1 geometry at the 6-31G(d) base group level; using PBE0 [5] method based on the TDDFT electron excitation calculation of 6-311G(d) and defTZVP with gradually enhanced polarization function, the excited state wave function of the S-Phe-1 is calculated, and is studied by graphically identifying the electron transition region Electron-excitation properties of the S-Phe-1. Calculated in Gaussian 16 [6], all graphics processing, wave function analysis by program Multiwfn_3.7(dev) [4,7-11] accomplish.

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3. RESULTS AND DISCUSSION

3.1 Ground state configuration of S-Phe-1

S-Phe-1[1] as shown in figure 1, based on the implicit for the electron-hole analysis the properties of the excited states of the S-Phe-1 are analyzed theoretically.

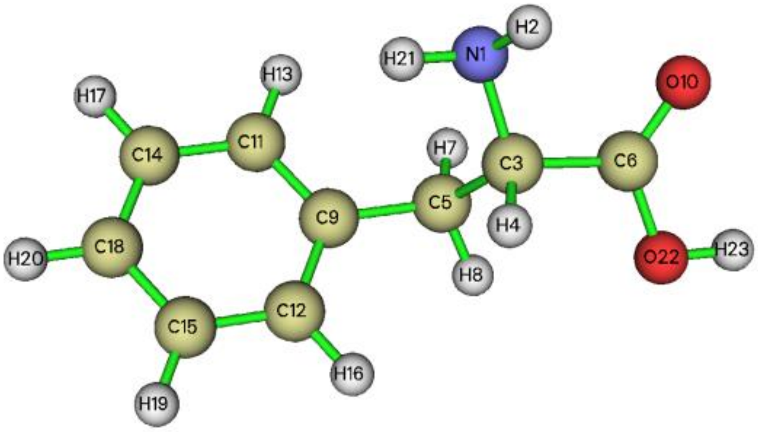


Figure 1. S-Phe geometric configuration in an implicit solvent environment.

3.2 Electron-hole diagram analysis of the electron excitation properties of the S-Phe-1

Based on PBE0 method, 6-311G(d) and defTZVP with polarization function, electron-hole analysis of each excited electron excitation of ground states S0 to S1-S7 in the S-Phe-1. Based on the electron-hole analysis of Multiwfn program, the corresponding distribution map of electron and hole is presented, and is studied by graphically identifying the electron transition region electron-excitation properties of the S-Phe-1.

3.2.1. Graphram analysis of electron excitation properties of S-Phe-1 at PBE0/6-311G(d) level.

Assist in determining the degree of charge transfer (CT) based on electron and hole analysis. The level of PBE0/6-311g(d) is shown by the electron and mole diagram electron-excitation properties of the S-Phe-1.

Discuss the excited state of S1, visualize the simultaneous distribution of hole, electron, electron and hold respectively. Investigate the simultaneous distribution of electron and hole, and use green and blue isosurfaces respectively (ρ=0.003a.u.) representation, as shown in figures 2,3,4.

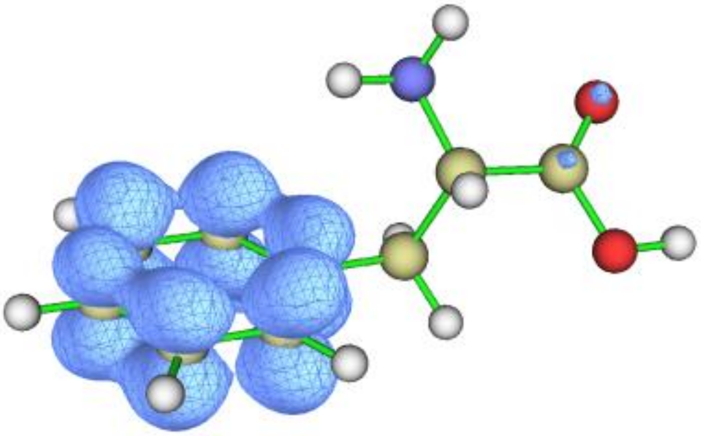


Figure 2. Distribution map of holes in the S1 excitation state of S-Phe-1, highlighting the regions with the highest hole density.

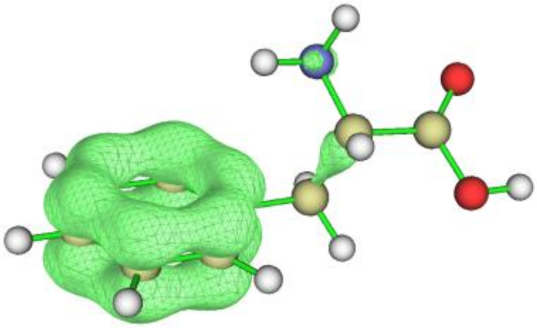


Figure 3. Distribution map of electrons in the S1 excitation state of S-Phe-1, highlighting the regions with the highest electron density.

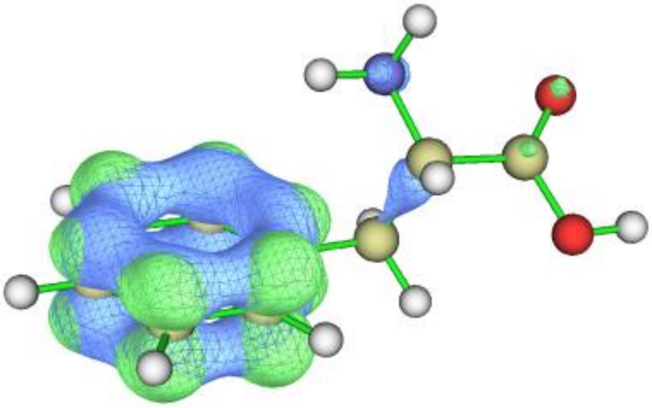
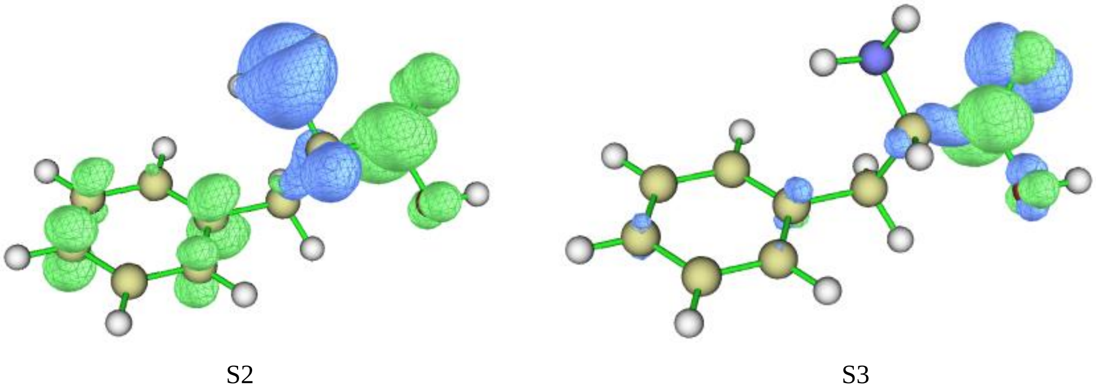


Figure 4. Distribution map of electron-holes in the S1 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.

The hole is mostly in the phenyl region, very few in the carboxyl region, while electron is mostly in the phenyl region, and a few on the amino, chiral C3 atoms. It can be known that after the electron transition, there will be a little electron flow from the phenyl and carboxyl region to amino and chiral C3 atoms, with a little CT feature, but the LE feature is more important, so it is suitable to belong to LE excitation, that is, local excitation from phenyl to phenyl pi→pi*.

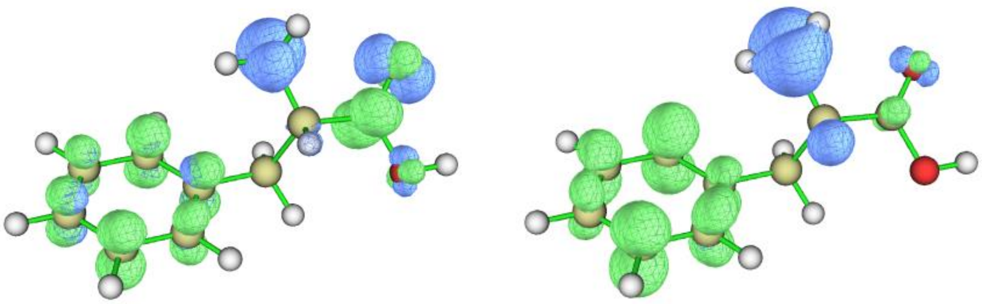
To explore the specific excitation mode of each excited state of S2-S7, the following is the isosurface diagram of the simultaneous distribution of electron and hole of each excited state, as shown in figures 5,6,7.



S2

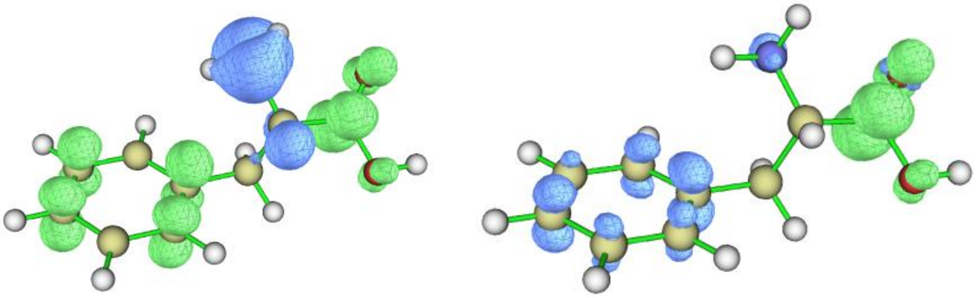
S3

Figure 5. Distribution map of electron-holes in the S2、S3 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.



S4 S5

Figure 6. Distribution map of electron-holes in the S4、S5 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.



S6 S7

Figure 7. Distribution map of electron-holes in the S6、S7 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.

In the same way, S2 excited from charge transfer from amino to phenyl and phenyl carboxy n→pi*, S3 excited from carboxy to carboxy n→pi*, S4 excited from amino, carboxyl to phenyl and carboxy n→pi*, S5 excited from charge transfer from amino to phenyl n→pi*, S6 excited from amino to phenyl and carboxy n→pi*, and S7 excited from charge transfer from phenyl to carboxy pi→pi*.

3.2.2. At the PBE0/defTZVP level Graphram analysis of the electron excitation properties of S-Phe-1.

Plot shown by electron and hole analysis at the PBE0/defTZVP level electron-excitation properties of the S-Phe-1.

Discuss the S4 excited state situation (ρ=0.009a.u.), as shown in figures 8,9,10.

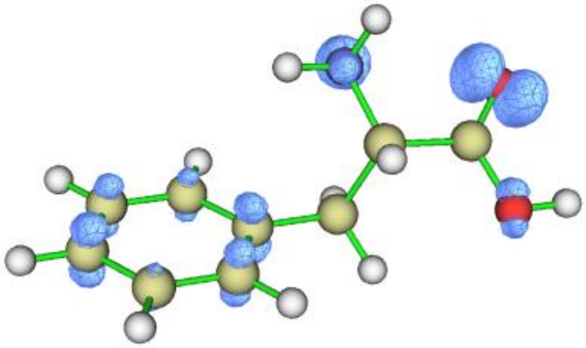


Figure 8. Distribution map of holes in the S4 excitation state of S-Phe-1, highlighting the regions with the highest hole density.

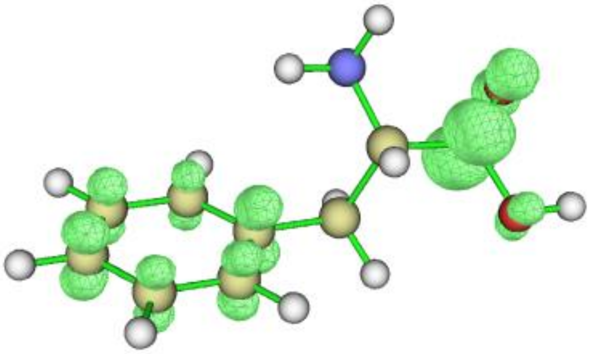


Figure 9. Distribution map of electrons in the S4 excitation state of S-Phe-1, highlighting the regions with the highest electron density.

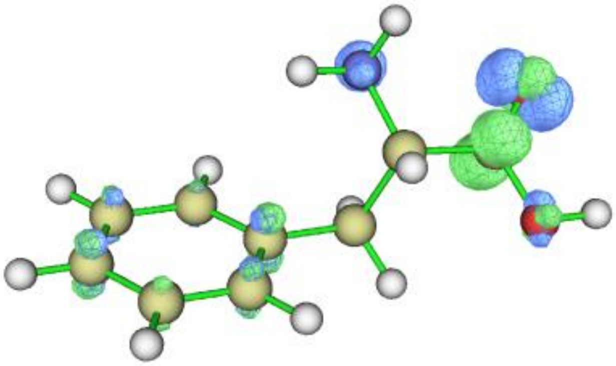
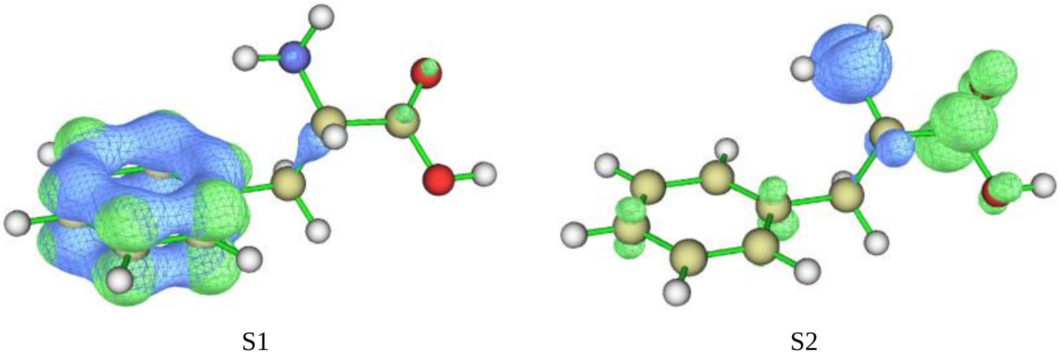


Figure 10. Distribution map of electron-holes in the S4 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.

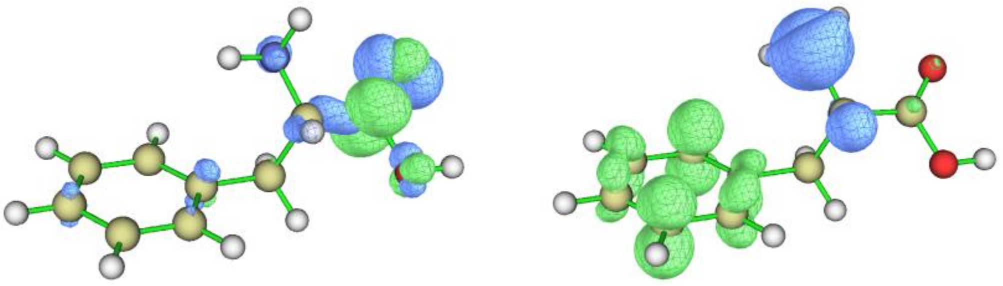
According to the figure, hold appears mostly in the amino and carboxyl regions, and very few in the phenyl region, while electron appears mostly in the carboxyl region and a small part in the phenyl region. It can be known that after the electron transition, some electron will flow from amino and carboxyl region to phenyl, with a little CT feature, but the LE feature is more important, so it is suitable to belong to LE excitation, that is, local excitation from amino, carboxy to carboxy n→pi*.

To explore the specific excitation mode of each excited state of S1-3 and S5-7, the following is the isosurface diagram of electron and hole simultaneous distribution of each excited state, as shown in figures 11,12,13.



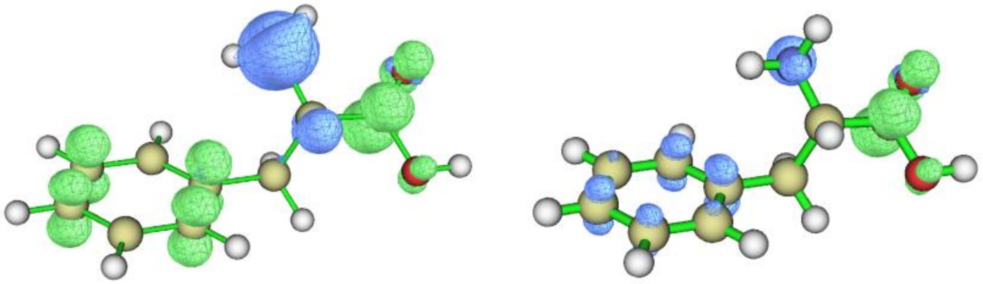
S1 S2

Figure 11. Distribution map of electron-holes in the S1、S2 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.



S3 S5

Figure 12. Distribution map of electron-holes in the S3、S5 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.



S6 S7

Figure 13. Distribution map of electron-holes in the S6, S7 excitation state of S-Phe-1, highlighting the regions with the highest electron-hole density.

In the same way, S1 excited from localized excitation from phenyl to phenyl pi→pi*; S2 excited from amino to carboxy n→pi*, S3 excited from carboxy to carboxy n→pi*, S5 excited from amino to phenyl n→pi*, S6 excited from amino to phenyl and carboxy n→pi*, and S7 excited from amino to carboxy n→pi*.

4. CONCLUSION

By examining the excited state characteristics of S-Phe-1 of 6-311G(d) and defTZVP with polarization function, judging the excited state electron excitation characteristics of S1-S7 by using electron-hole diagram analysis method, summarizing: it is displayed in S-hole figure by electron and Phe-H_2O molecular system, the two groups show that the excited state of S1-S6, the analysis results are basically the same; S7, the 6-311G(d) group with polarization function is different from defTZVP groups, the former refers to the charge transfer excitation from phenyl to carboxy pi→pi*; the latter is the local excitation from amino to carboxy n→pi*.

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