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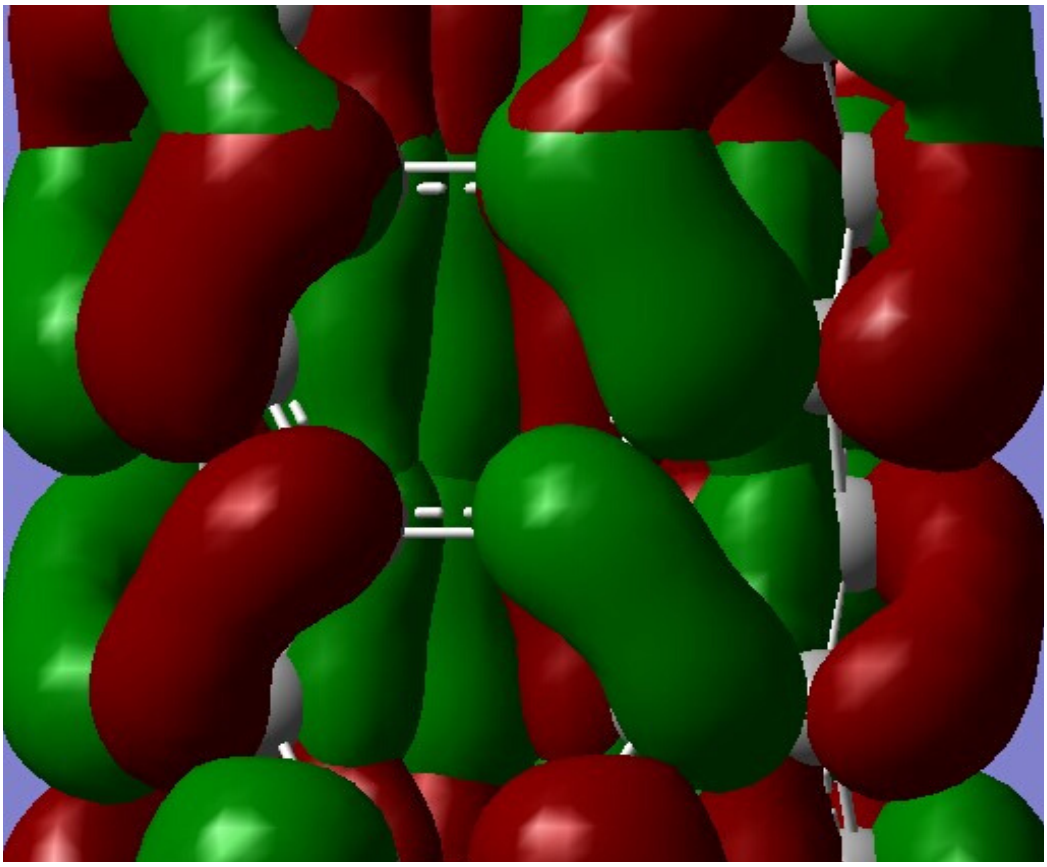

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Muonium behavior in amino acids (tyrosine, tryptophan and phenylalanine)

Research Article

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Abstract: To interpret the muon spin rotation and relaxation (μSR) data on cytochrome c protein, the stopping site and charge states of muon and muonium in constituents (amino acids) of the protein have been studied through the first-principles approach. The stopping site of muonium in amino acids containing aromatic side rings –tyrosine, tryptophan and phenylalanine with extended main chain structure (like a peptide chain in real protein) have been estimated in aromatic side chain. It indicates that existence of those amino acids may contribute for intra-molecular electron transfer in the protein.

Keywords: Muon stopping site • Muonium • Electron transfer • Muon spin rotation

1. Introduction

Since muon acts as promising tool for the study of life and materials, its application to study life phenomena remains limited owing to complex bio-samples and functional dynamics, and energy of conventional muon beams (∼MeV). Kanetada Nagamine et al initiated the study of electron transfer in cytochrome protein [1], DNA [2] and aqueous biological solutions [3]. But the stopping of site of muon and electron dynamics are not completely understood yet. To estimate the stopping site of muon and its charge state in the system, in addition to muon spin rotation and relaxation (μSR) study [4], the first-principles calculation is necessary.

Positive muon μ^+ is a spin half elementary particle lies in second generation leptons in standard model of particles. It is like a light proton (mass $m_\mu \approx 1/9\ m_p$; magnetic moment $\mu_\mu = 3.18\ \mu_p$) which acts as sensitive probe in materials. It is available in cosmic rays and accelerator facilities. The muon can be produced by decay of pion. In accelerator, muon can be generated by bombarding a muon production target (graphite etc.) by proton beam. The muon decays (2.2 μs) to positron and neutrinos. The positive muon probes the local electronic and spin states of surrounding atoms and molecules at the stopping site. Its bound state with electron is known as

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muonium (Mu) which behaves as light isotope of hydrogen (H) in materials. The wide time window ($\sim ps$ to few μs), measurement without perturbations (at any temperature, without external field) and characteristics of muon (100% spin polarized and asymmetric decay to positron in weak interaction) are advantages of this methods over other spectroscopic/resonance methods. Details of (μSR) technique can be available elsewhere [5, 6].

To interpret the (μSR) experiment and estimate the muon stopping site in cytochrome c protein, it is expected that the systematic study starting from its constituents amino acids will helpful to understand electron transfer mechanism and function of the protein system. The (μSR) experiments in amino acids are in progress and the theoretical study has also been performing. Collaborating with K. Nagamine, T. P. Das group reported the stopping site of muon in amino acids using cluster Hartree-Fock method is around unsaturated O carboxyl group of the amino acids [7, 8]. In real biological system there is peptide bond in the main chain [9] so we made three model structures for calculation in which the main chain of amino acids was terminated by different groups [10]. In glycine, the stopping site was estimated around O of carboxyl group that shows agreement with previous result by Das group but when the calculation is performed in triglycine the stopping site was around O of central glycine moiety [11]. In the histidine which has aromatic ring in side chain, stopping site of muon is estimated around N of side aromatic ring [12]. Then it is interesting to check the stopping site of muon in other amino acids (with extended main chain structure) having aromatic side ring - tyrosine, tryptophan and phenylalanine. In this paper, the stopping site of muon in those three amino acids - tyrosine, tryptophan and phenylalanine is discussed.

2. Methodology

Theoretical calculations were performed using hybrid density function B3LYP with basis sets 6-31G(d) in Gaussian 16 package [13]. In the B3LYP level of calculation, both gradient and exchange correlations are included. The basis set 6-31G(d) describes well the orbitals of first and second rows elements. The optimization of structures with different sets were confirmed as mentioned in previous work [12]. The initial charge state of muon is taken as Mu as mentioned in the muon labelled electron method [5]. The Mu is formed in the biomolecules stops somewhere in the reactive site. The stopping site is estimated based on the minimum potential energy (PE) for H or Mu (hereafter H(Mu)) in the system. The potential energy in term of optimized energies (Es) for H was calculated as,

$$PE = E(aminoacid + H) – [E(aminoacid) + E(H)]$$

3. Results and Discussion

Fig. 1(a) shows the optimized structure for H(Mu) in tyrosine amino acid with extended main chain. The potential energy for H(Mu) at different positions is presented in Fig. 1(b). Mu near C10 shows deep potential. Another optimized structure is also estimated when H16 of OH shows stable structure when it lies to the left

side. In this case, stopping of H(Mu) is estimated around C11. Based on potential energies, it is found that the stopping site of H(Mu) is in aromatic side chain rather than main chain.

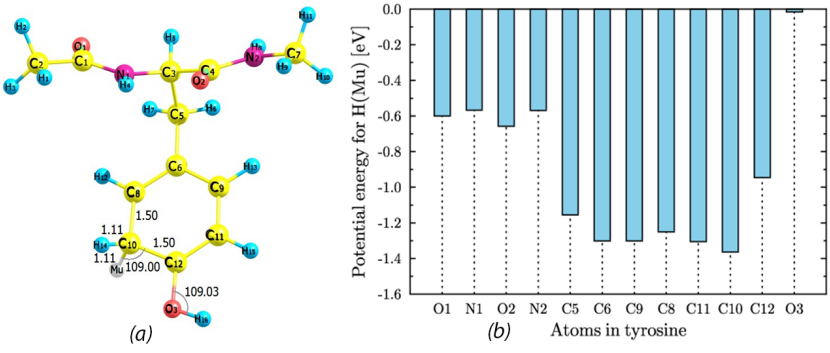

Figure 1. (a) Optimized structure of H(Mu) in tyrosine, (b) Potential energy for hydrogen at different sites. Aromatic side ring is possible site for muonium. Bond length presented in A and angle in degree.

Optimized structure for H(Mu) in tryptophan is shown in Fig. 2(a) and potential energy in Fig. 2(b). In this system the stopping site for Mu is the vicinity of C8 and N3. Similarly, the optimized structure and potential energy for H(Mu) in the phenylalanine is presented in Fig. 3(a) and 3(b), respectively. Muonium stopping site is estimated around side ring.

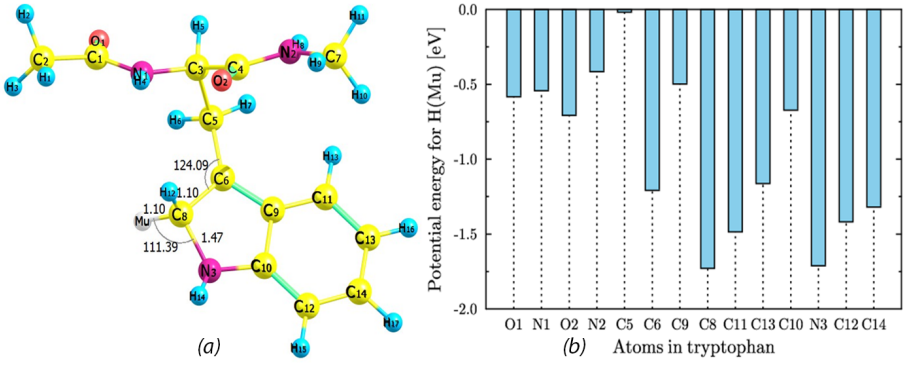

Figure 2. (a) Optimized structure of H(Mu) in tryptophan, (b) Potential energy for hydrogen at different sites. Region around C8 and N3 are possible stopping site for muonium. Bond length presented in A and angle in degree

The stopping sites for Mu in gas phase amino acids containing aromatic side chain are estimated in the aromatic side ring. It is possible that those amino acids in the protein may contribute for intra-molecular electron transfer process. Further calculation for hyperfine coupling constant and electric field gradient, and high transverse field (μSR) measurement will help to understand the stopping sites of muon and electron dynamics in the system.

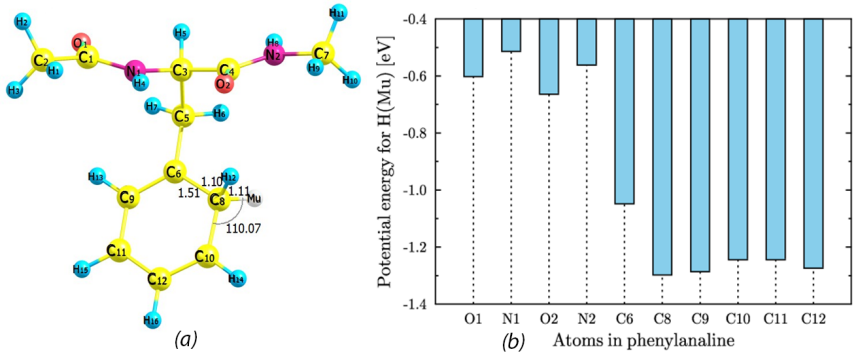

Figure 3. (a) Optimized structure of H(Mu) in phenylalanine, (b) Potential energy for hydrogen at different sites. Aromatic side ring is possible site for muonium. Bond length presented in A and angle in degree.

4. Conclusions

The first-principles calculations to estimate the stopping site of muonium in amino acids containing aromatic side ring shows the stopping site of the muonium is in aromatic side ring using the extended main chain structure model. It indicates that these amino acids may contribute for intra-molecular electron transfer in the protein in muon spin rotation and relaxation measurement.

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