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Ultrafast Vibrational Dynamics induced by the Photodetachment of Aqueous Phenylalanine Anion

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Abstract

The interaction of biomolecules with ionising radiation in an aqueous environment is a fundamental process that is not well researched [1]. Understanding the photoionization or photodetachment of amino acids can help us better understand and solve problems related to radical chemistry and radioactive processes in natural systems [2]. In this study, we use femtosecond optical pump-probe spectroscopy to explore the photodetachment of the phenylalanine anion, an aromatic amino acid. Photodetachment of phenylalanine anion in aqueous alkaline solution triggers vibrational wave packet dynamics as well as a rapid, picosecond decay of the phenylalanine radical population (Fig. 1. (a)). Both existing literature [3–5] and our ab initio calculations suggest that the photodissociation of phenylalanine radical into carbon dioxide and benzeneethanamine radical is a dominant process. While we have yet to uncover experimental evidence of this phenomenon on the sub-picosecond to picosecond timescale, we identified several key vibrational modes belonging to phenylalanine radical by comparing experimental and ab initio results (Fig 1. (b)). Overall, studying the vibrational wave packet dynamics of phenylalanine induced by photodetachment can provide a more nuanced understanding of the effects of ionising radiation on aromatic amino acids.

Fig. 1: (a) Time-resolved differential absorption spectrum of phenylalanine showing time traces at different probe wavelengths (Wavelengths in legend are in nm). Solid lines represent fitted function. (b) Normalised fast Fourier transform (FFT) amplitude spectrum of first moment time trace from 320 to 340 nm.

Keywords: Phenylalanine, femtosecond laser spectroscopy, radical, photodetachment

References:

- [1] T. Debnath, M. S. Bin Mohd Yusof, P. J. Low, and Z. H. Loh, "Ultrafast structural rearrangement dynamics induced by the photodetachment of phenoxide in aqueous solution," *Nat. Commun.*, vol. 10, no. 1, pp. 1–8, 2019.
- [2] Z. H. Loh *et al.*, "Observation of the fastest chemical processes in the radiolysis of water," *Science* (80-), vol. 367, no. 6474, pp. 179–182, 2020.
- [3] L. J. Mittal, J. P. Mittal, and E. Hayon, "Primary Processes in the Photochemistry of Phenylalanine and Derivatives in Aqueous Solution. Biphotonic Photoionization and Photodissociation Reactions," *J. Am. Chem. Soc.*, vol. 95, no. 19, pp. 6203–6210, 1973.
- [4] D. Wang, H. P. Schuchmann, and C. Sonntag von, "Phenylalanine: Its $\cdot\text{OH}$ and $\text{SO}_4^{\cdot-}$ -Induced Oxidation and Decarboxylation. A Pulse Radiolysis and Product Analysis Study," *Zeitschrift fur Naturforsch. - Sect. B J. Chem. Sci.*, vol. 48, no. 6, pp. 761–770, 1993.
- [5] N. Ludwig *et al.*, "Radiolysis of phenylalanine in solution with Bragg-Peak energy protons," *Radiat. Meas.*, vol. 116, no. March, pp. 55–59, 2018.