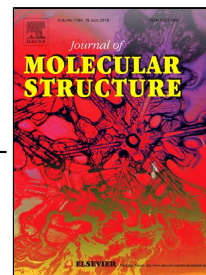


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Theoretical Investigation on Excited State Intramolecular Proton Transfer of 1-Aryl-2-(furan-2-yl) butane-1, 3-diones Substitutions

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The effect of different substituents on the excited state intramolecular proton transfer (ESIPT) of 1-aryl-2-(furan-2-yl)butane-1,3-diones (AYFBD), namely OFBD, TFBD, MFBD and FFBD are studied by employing the density functional theory (DFT) and time-dependent density functional theory (TDDFT) methods. By comparing the geometric configurations and infrared vibrational spectra of the first excited state (S_1) with those of the ground state (S_0), it can be concluded that the intramolecular hydrogen bonds are strengthened in S_1 state. The calculated peaks of absorption and fluorescence spectra of AYFBD derivatives in keto form are consistent with experimental results reported previously (*Journal of Organic Chemistry*, 2017, **82**, 12097). We can also confirm that the intensities of the intramolecular hydrogen bonds in the S_1 state are enhanced by analyzing the frontier molecular orbitals and the infrared spectra. To further investigate the ESIPT mechanism of AYFBD derivatives, the potential energy curves (PECs) of S_0 and S_1 states are scanned by varying O_1 - H_2 distance, which demonstrates that ESIPT occurs in the S_1 state of all the AYFBD derivatives and follows the order: FFBD > MFBD > TFBD > OFBD.

1. Introduction

The investigations of excited-state hydrogen bond dynamics are essential for exploring the process of photophysics, photochemistry, and photobiology.¹⁻¹¹ Since the phenomenon of excited state intramolecular proton transfer (ESIPT) was first observed in salicylic acid by Weller *et al.* in 1965,¹² a wide range of experimental and theoretical studies have been carried out on picosecond kinetics, thermodynamics, proton transfer dynamics and so on.¹³⁻²¹ Especially for the hydrogen bond kinetics research, comparing with the ground state, the study of the excited state is more complex but has more significance. Garza *et al.* studied the hydrogen bonds in methane-water clusters.²² Moreover, García-Hernández and Garza investigated the reactivity sites in dopamine depend on its intramolecular hydrogen bond.²³ Upon the photoexcitation, the hydrogen-bonded molecules will transfer protons or hydrogen atoms to achieve rearrangement during intermolecular or intramolecular excited state proton transfer. Recently, a series of new mechanisms to explain the excited hydrogen bonding dynamics, such as photoelectron transfer (PET), fluorescence resonance energy transfer (FRET), intermolecular charge transfer (ICT) and so forth, have been proposed by Han and co-workers.²⁴⁻²⁸ In addition, Zhao *et al.* have also investigated the excited state proton transfer mechanism.²⁹⁻³¹ With the development of hydrogen bond dynamics, the substituent effects on ESIPT have been studied in previous literatures.³²⁻³⁶ Pearson *et al.* studied the substituent effects in the

keto-enol tautomerism of fused 1,4-naphthalenediols experimentally.³⁷ Moreover, Ma *et al.* investigated the different substituent effects on ESIPT of 1-(amido)-anthraquinone molecule.³⁸ Manojai *et al.* explored heteroatom effect on photophysical properties of 2-(2'-Hydroxyphenyl) benzimidazole with its derivatives.³⁹

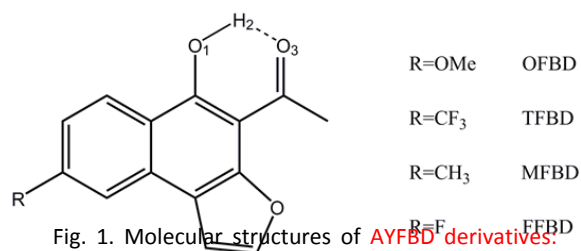


Fig. 1. Molecular structures of AYFBD derivatives: OFBD, TFBD, MFBD and FFBD.

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