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# Theoretical Study of Hydrogen Bonding Excited States of Fluorenone with Formaldehyde

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**Abstract:** Time-dependent density functional method was performed to investigate the intermolecular hydrogen bond between fluorenone and formaldehyde in the electronically excited states. The geometric structures of the hydrogen bonding complex in the ground state and the first singlet and triplet excited states  $S_1$  and  $T_1$  are optimized respectively by the DFT and TD DFT methods, the vibrational spectra, electronic absorption spectra and fluorescence spectra are calculated. The two intermolecular hydrogen bonds  $C=O\cdots H-C$  formed between fluorenone and  $CH_2O$  in the complex are strengthened in the  $S_1$  and  $T_1$  states relative to the ground state. The excited states  $S_1$  and  $T_1$  are locally excited, where fluorenone is excited but  $CH_2O$  remains in the ground state. The hydrogen bonds cause a frequency blue shift of the involved CH bond in formaldehyde in the ground state, the electron excitations  $S_0 \rightarrow S_1$  and  $S_0 \rightarrow T_1$  mainly lead to large frequency red shift of the C=O bond in fluorenone.

**Keywords:** Time-dependent density functional method(TD DFT), excited states, vibrational spectra, electronic spectra, blue shifted hydrogen bonds

## 1. Introduction

In recent years noncovalent interactions are interesting and valuable topics attracting theoretical and experimental chemists. Hydrogen bonding as the most important noncovalent interaction [1-3] is critical to understand microscopic structures, properties and functions of many molecular and supermolecular systems, proteins and DNA [4-10]. The nature of hydrogen bonds in the ground state has been explored by various theoretical methods and experimental techniques. The investigation of hydrogen bonding in electronically excited states expands the contemporary hydrogen bond research interests [4-13].

Upon photoexcited to electronically excited states, the hydrogen bonding complex is significantly changed with charge density redistributing and the hydrogen donor and acceptor reorganizing. This process is called electronic excited-state hydrogen bonding dynamics (ESHBD) [3,10,14,15]. There are three different ways for ESHBD, one of the hydrogen acceptor or donor is photoexcited whereas the other remains in the ground state, or both the acceptor and donor are photoexcited [5].

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