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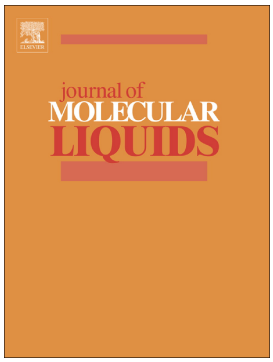

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ACCEPTED MANUSCRIPT

All-trans-β-Carotene Absorption Shift and Electron-phonon Coupling Modulated by Solvent Polarizability

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Abstract: Absorption, resonance Raman spectra are reported on *all-trans*-β-carotene dissolved in different polarizability solvents. The absorption spectra of *all-trans*-β-carotene are analyzed by Franck-Condon principle and the Huang-Rhys factors are calculated. With the increasing solvent polarizability, the Huang-Rhys factor and the electron-phonon coupling constant decrease, while the Raman scattering cross section increases. The red-shift of absorption would leads to an increasing spectral overlap with the laser excitation leading to an enhanced resonance effect. Through electron-phonon coupling, the ground state structure of *all-trans*-β-carotene will be modulated by the electronic transition and is assumed to lead to a modulation of energy flow. Results present insights on the solvent's polarizability dependence on electron-phonon coupling of carotenoid. This work is expected to be helpful for exploring the surrounding medium effects on the electronic transition and carbon-carbon vibrations.

Keywords: *all-trans*-β-carotene; polarizability; electron-phonon coupling

1. Introduction

Carotenoids play an important part in a lot of physiological processes and show critical importance for life. In a majority of natural processes, they are assumed to be the carriers of electrons and energies[1-5].Carotenoids have the function of collecting light and play roles in regulating light harvesting and photosynthetic efficiency[6,7]. The *all-trans*-β-carotene (*β*-Car), with 11 conjugated double bond, has unique biochemical and optical properties and is considered to be a model in studying conjugated molecules. Carotenoids have a photoprotection role in photosynthetic membranes by preventing photooxidation damage through quenching of chlorophyll singlet and triplets. It is also suggested that the nearby *β*-Car participates the ^{3}Chl* quenching and prevents the production of harmful singlet oxygen, which indicates the key role of the carotenoids in organic life process [7,8]. Carotenoids present such a key role through their electronic properties because they possess the linear conjugated chain and their lowest excited state have large contributions. Extensive studies on predicting the electronic state of *β*-Car showed difficulties in picturing the full electronic structure [9].

Linear polyenes and polymers have been synthesized extensively in order to modulate the energy gap [10]. Doped *β*-Car has been studied by optical absorption, Raman, and infrared spectra [11]. Many spectroscopic observations on relatively short polyenes combining with theoretical considerations suggested that the increase of the conjugation length would strongly change the

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