Cavity and Hydrogen Bonding Effects of β-Cyclodextrin on the Structures and Photophysics of Amino Acid Derivatives

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β-cyclodextrin (β-CyD) and its derivatives with particular structures have manifested efficient catalytic abilities in many organic reactions, which have been extensively studied in the past decades, both experimentally and theoretically. Herein, a theoretical study of structural and photophysics properties of three amino acid derivatives of β-CyD, named 6-phe-β-CyD, 6-tyr-β-CyD and 6-trp-β-CyD is presented using the density functional theory (DFT) method. We have obtained both self-inclusion and non-inclusion structures for each derivative. It is found that the amino acid moieties tend to be placed out of cavity of β-CyD in the non-polar solvents. But in the polar solvents, especially in water, the amino acid moieties have included within the cavity. This is affected by the intermolecular hydrogen bond and hydrophobic interactions. Furthermore, our calculated circular dichroism (CD) spectra are in good agreement with previous experimental data. This confirms that our theoretical results are credible. These results can be provided for the prediction of catalytic reaction and explained the experimental facts theoretically. The cavity and hydrogen bonding effects of β-CyD on the structure and photophysics of amino acid derivatives may play important role in photocatalysis.

References: