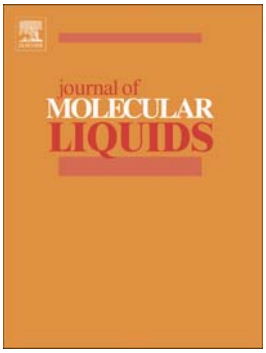

Computational study of inclusion complexes formation between carvacrol and β-cyclodextrin in vacuum and in water: Charge transfer, electronic transitions and NBO analysis

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Computational study of inclusion complexes formation between carvacrol and β-Cyclodextrin in vacuum and in water: Charge transfer, electronic transitions and NBO analysis

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A b s t r a c t

The interactions between carvacrol (CAR) and β-Cyclodextrin (β-CD) have been analyzed employing PM3, ONIOM2 and DFT methods in vacuum and in water. Complexation, deformation, HOMO and LUMO energies were determined and discussed. Van der Waals interactions are mostly responsible for enthalpy driven complex formation of CAR with β-CD. Finally, TD-DFT of visible spectra and NBO calculations were analyzed and discussed. Theoretical studies propose that hydrophobic interaction and hydrogen bonding plays significant role in determining the stability of the complexes.

Keywords: *β -Cyclodextrin, PM3, ONIOM2, DFT, TD-DFT, NBO.*

1. Introduction

Carvacrol (5-isopropyl-2-methylphenol) is a phenolic monoterpene constituent of essential oils of oregano, thyme, and marjoram [1]. Many biological effects have been described for CAR, such as pronounced a good natural antimicrobial and antioxidant agent; however, its poor aqueous solubility and high volatility limit its application in food systems. Beta-cyclodextrin is able to encapsulate hydrophobic molecules improving its aqueous solubility and reducing its volatility [2].

β-Cyclodextrin (β-CD) is a cyclic oligosaccharide derived by enzymatic hydrolysis of common starch,which has an internal cavity shaped like a truncated cone of about 8 Å deep and 6.0–6.4 Å in diameter. This cavity possesses a relatively low polarity, so it can accommodate guest organic molecules inside [3]. Due to its particular chemical structure, β-CD can improve the stability, dispersing and dissolving properties of some drugs, and enhance its physical and chemical activity through the inclusion complexes [4].