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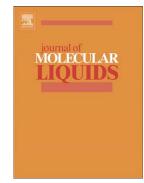
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## ACCEPTED MANUSCRIPT

#### Solvatochromism of Fluorescein in Aqueous Aprotic Solvents

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#### ABSTRACT

Fluorescein solvatochromism was studied in pure aprotic solvents dimethylsulfoxide, N,N-dimethylformamide, acetonitrile and acetone, and their aqueous mixtures. The type and extent of solvent effects were identified and interpreted based on the electronic structure of fluorescein and the nature of the solvent. The main effect of hydrogen bonding interaction was observed on solvatochromism. A modified preferential solvation model was used to gain a reliable insight into the contribution of solvent-solvent interactions to solvatochromism as well as the local and bulk mole fraction distribution of solvation species. Results indicate that the solvation shell of the solute is mainly affected by the solvent-solvent interaction.

*Keywords:* Fluorescein; solvatochromism; nonideality; preferential solvation; local composition

#### 1. Introduction

The solvent effect is a fascinating subject of research in solution chemistry because the environment has an essential role on the solute behavior, and therefore on the thermodynamics and kinetics of reactions in solution. In this direction, solvatochromism, defined as the spectral changes of solute induced by the solvent, opens a convenient way to achieve a molecular understanding of the solvent effects [1, 2]. The electronic transition energy,  $E_{\rm T}$ , of the solute in its absorption spectra depends on the energy level of the ground and excited state of the solute; by change in the surrounding media, the ground and excited state enjoy different stabilization due to its different electronic structure and consequently, solvatochromism occurs as a function of the magnitude of the solvent effect. Such behavior makes experimental

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