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Original article

Density functional aspects and thermodynamic evaluation of sodium dodecyl sulphate in aqueous tartrazine

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ABSTRACT

Sodium dodecyl sulphate (SDS) and tartrazine (TAR) are involved in manifold industrial and medicinal applications. Under such a fascination, this work describes the conjoint experimental-theoretical investigation of a binary mixture containing SDS in aqueous TAR (0.001 M). The study involves the evaluation of some primary thermodynamic parameters due to SDS-TAR micellization and a special focus on computational density functional theory (DFT) approach using water as solvent under 631-g(d,p) as basis set and B3LYP as the respective functional. Structures of both the SDS and TAR were separately optimized first, followed by the calculation of their mixture under the same quantum chemical theory. After confirming the absence of imaginary frequency in the frequency calculation of each set further theoretical calculations were done to get the respective molecular orbital energies and several other descriptors to reveal the difference of chemical behaviour in relation to pre- and post-micellization processes. The study shows remarkable agreement between DFT and experimental outcomes.

1. Introduction

The study of dye-surfactant interactions is one of the prominent disciplines bearing huge industrial and medicinal application. It is a known fact that surfactants are candidates of valuable interest that assist in dyeing by wetting, leveling or dispersing dyes of low solubility following the principle of absorption by fibers (Ghoreishi et al., 2007; Malik and Mir, 2018). The dye-surfactant systems and their investigation of interactions are currently used in analytical chemistry, photography, luminescence and lasers (Barni et al., 1991). The profound application of dye-surfactant systems makes these systems of interest for investigation. In this connection investigations leading to explore ionic interactions among surfactants and azo dyes have gained keen interests to design desirable agents (Garcia and Medel, 1986; Shatkh et al., 2007). These studies involve primarily the evaluation of volumetric, viscometric, spectroscopic and refractive index insights to arrive at some significant conclusions (Ali et al., 2009; Deshpande et al., 2018; Vinarov et al., 2018). Hence, knowledge of the dye-surfactant interface is indeed of great value in understanding the respective mechanism of chemical equilibrium and kinetics of surfactant- sensitized color and / or fluorescence reactions intervening in the process (Ray et al., 2009; Abu-Hamdiyyah and Al-Mansour, 1979). The investigation of tartrazine-surfactant interactions would help in understanding and development of new spectrophotometric and fluorimetric methods for the determination of micro amounts of metal ions, anions, and biological compounds. These systems are not investigated to be incorporated as food additives but to explore these systems for sensing purposes (Scheme 1).

Tartrazine represents one of the effective anionic species that has been found relevant as drug-additive in proposing treatment to neural defects (Al-Shabib et al., 2018). Studies have revealed efficient electrostatic interactions exhibited by tartrazine which is important factor in induced amorphous aggregations (Al-Shabib et al., 2017a). Similarly, the potentiality of hydrophobic interaction plays a key role in tartrazine-amyloid fibrillations (Al-Shabib et al., 2017b). These findings suggest the importance of non-covalent binding of tartrazine in applying the compound as additive in drug-surfactant interface. On the other hand, sodium dodecyl sulphate is also worthy scaffold in the respect of colloidal

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