Density Functionalized Drug-Surfactant Interaction of Aqueous SDS-Tartrazine

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ARTICLE INFORMATION

ABSTRACT

Study of molecular density theory is considered nowadays as a powerful tool to speculate various physical and chemical properties of materials. Herein, we report the theoretical inference of associated changes in chemical properties of sodium dodecyl sulphate and tartrazine when allowed to go through pre- and post-micellization phenomena. Because of the involvement of the two compounds in manifold industrial applications, the study reflects some important conclusions of drug-surfactant chemistry. The computational work involves the use of Polarizible Continum Model (PCM), water as solvent and 631g(d,p) basis set with B3LYP as functional. Each molecule was run individually first to arrive at an optimized structure followed by a final optimization of assumed network (mesh of proposed binary mixture) to visualize the changes that occur on combination. Each set of energy minimal calculation was then run for frequency calculation, electronic spectral evaluation and molecular natural population analysis. Molecular electrostatic potential surfaces were discussed in linking the appropriate hydrophobic and hydrophilic interaction.

1. Introduction

Dye-surfactant chemistry represents a vast field of immense industrial and medicinal application. Surfactants are candidates of valuable interest in dyeing processed by incorporating the principle of absorption (Ghoreishi *et al.*, 2007). Investigations of molecular interaction existing between cation surfactant and anion azo-dyes has brought keen interests among scientists (Gracia *et al.*,1986; Shaikh *et al.*, 2007; Ali *et al.*, 2009). Investigations relevant to micellization interaction are of great value in designing desirable properties among coloring substances (Ray *et al.*, 2009; Abu-Hamdiyyah *et al.*, 1979). Tartrazine is an effective anionic food additive known to show significance in amyloid fibril formation (Al-Shabib *et al.*, 1979). The literature survey has indicated that due to tartrazine bears electrostatic potential that results in the formation of induced amorphous aggregations (Yamamoto *et al.*, 2004; Al-Shabib *et al.*, 2017). On the other hand, sodium dodecyl sulphate (SDS) is also an important compound in respect to colloidal and surface chemistry (Al-Shabib *et al.*, 2017; Saeed *et al.*, 2017). Hence, a special attention is being given to these molecules to depict their significance in dye-surfactant chemistry.

Density functional theory (DFT) is an effective tool to explore science of theoretical insights. Computational approach can be used to arrive at the basic structural parameters of the involved dye-surfactant interaction. This technique helps to save time and labour to infer desired properties of materials under question. It is evident from the literature survey that there are very less number of reports over DFT based dye-surfactant chemistry. Herein, a binary mixture of SDS and tartrazine has been theoretically evaluated to verify the chemical aspects for the respective suggested pre- and post-micellization of its form. Both the selected molecules *viz,* tartrazine and SDS were separately optimized to arrive at stable (energy minimal) geometric state. After optimization, successive infra red and electronic simulations were run. Each calculation was run using water as solvent. The respective optimized forms were finally mingled to find the magnitude of difference in various involved parameters to establish the link between pre- and post-micellization.

2. Experimental and Methods

Gaussian09 software package was used to carry out the required calculation. GaussView 5.0 which is an animation programme associated with the software was employed to visualize the data. 631g(d,p) basis set and B3LYP functional was the combinatory level of theory applied throughout

the work. In the present work, in addition to molecular specification solvent system (Wwater)was schematically used to get the optimized frame-work as reported elsewhere in the similar type of theoretical work (Mir and Itoo 2017).

3. Results and discussion

In order to arrive at a molecular aggregation of ground state stable energy, the geometry optimal state showed total energy continuum of −1333.36 a.u. and −2782.75 a.u., for SDS and tartrazine, respectively. The tendency of anionic behaviour is thus shown by the ligands for micellization. Moreover, from the molecular structure appearance tartrazine shows an automatic alignment to get oriented in a tripodal system. Two arms stretched on one side and one as tail. Hence, two regions get assigned as a tail and as a head. The respective 3D optimal structures are shown in figure 1. From the fig. it is obvious that the variation in the nature of chemical attachments near the hydrophobic and hydrophilic zones is depicted via bond length and orientation changes brought about by the interactions. The target molecular pair shows persistence of suitable molecular orbital band gaps as shown in figure 2. This observed molecular orbital difference can serve as a source to relate it with global chemical parameters that intervene during molecular interactions.
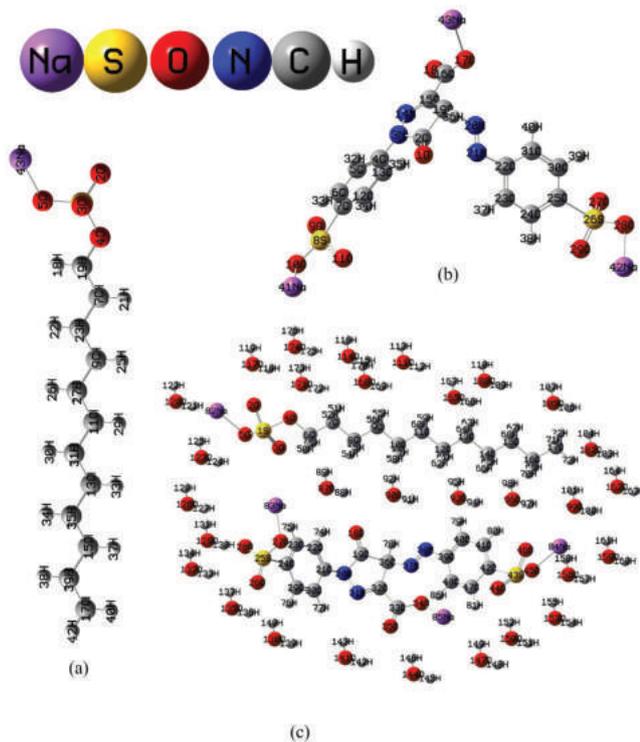

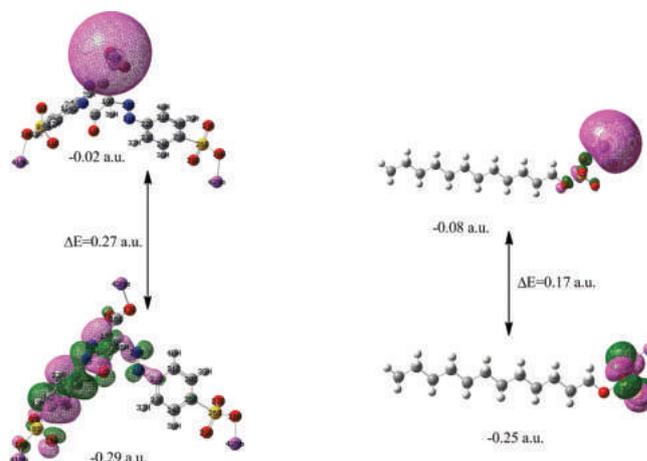**Figure 1.** Optimized 3D structures (a) SDS (b) tartrazine (c) 1:1 mesh of SDS:tartrazine.

Figure 2. Frontier orbital diagrams of the target molecules

The band gap in tartrazine is greater than SDS by 0.1 a.u. From charge density plots it is apparent that LUMO is oriented towards middle part of sodium locus in tartrazine, while as the same speculation is clear in SDS. In SDS HOMO is also mainly confined to the same spot. The valleys generated because of intermolecular communication may be stabilizing spot for incoming solutes. This has also an effect over resultant dielectric constant depending on nature of solvent. This relevance can be thought of better understanding in referring the electron dense regions. Taking the fixed concentration of tartrazine when subjected to serial diluted solutions of SDS can thus favour the chances of successful interaction in micellization by looking at the comparable band gaps as found theoretically.

TD-DFT calculations have shown that for the evaluation of three excited states of tartrazine 2.87 eV (λ = 319.66 nm), 4.48 eV (λ= 276.75 nm) and 4.5335 eV (λ = 273.48 nm) are favourable. Whereas, the similar observation for tartrazine comes out to be 3.0801 eV (λ = 402.54) nm, 4.6552 eV (λ = 266.34 nm) and 5.0057 eV (λ = 247.69 nm), respectively. On comparing the two excitation data it seems reliable to assign the respective loci of electronic shift at comparable cost of energy. Since this formalism provides instant information regarding the electronic transition, the behaviour can serve as a nice probe to formulate the energy barrier overview of a molecular system. The respective TD-DFT diagrams are given in figure 3 and 4.

Similar behaviour can be understood by looking at the electrostatic potential surfaces of the two molecules (figure 5). These theoretical potential surfaces are explained on the color code system available within GaussView animation programme (Paul *et al.*, 1998; Frisch *et al.*, 2010; GaussView 5.0). Three distinctive

regions *viz,* electronegative, electropositive and neutral loci are designated by red, blue and green color, respectively. From the fig it is apparent that middle sodium region in tartrazine and terminal sodium in SDS bear similar behaviour of electron density and hence would shows similarity in reactive behaviour at this spot.

The remaining regions of the two molecules are neutral and will behave in similar fashion. Hence, two regions are mainly predicted, which are called as hydrophobic and hydrophilic regions or head and tail for the investigated micellization (Mir *et al.*, 2017).
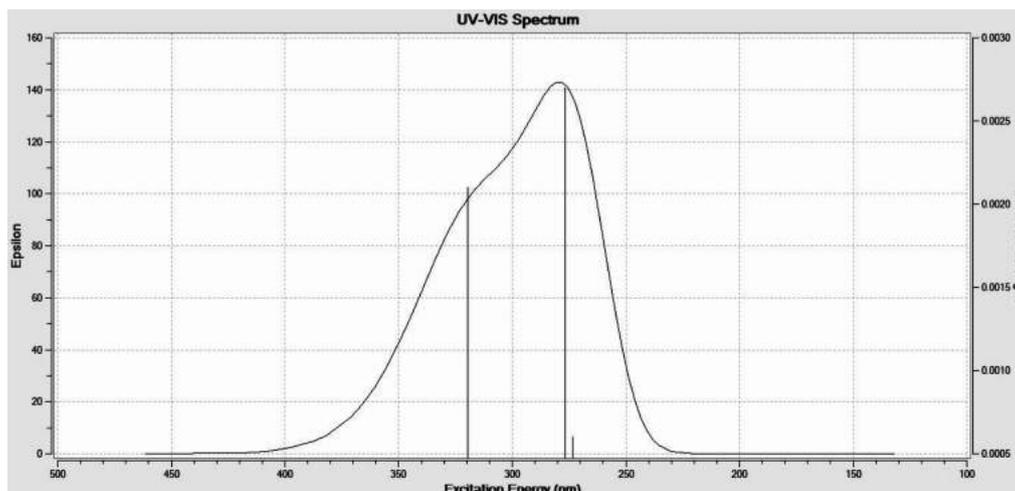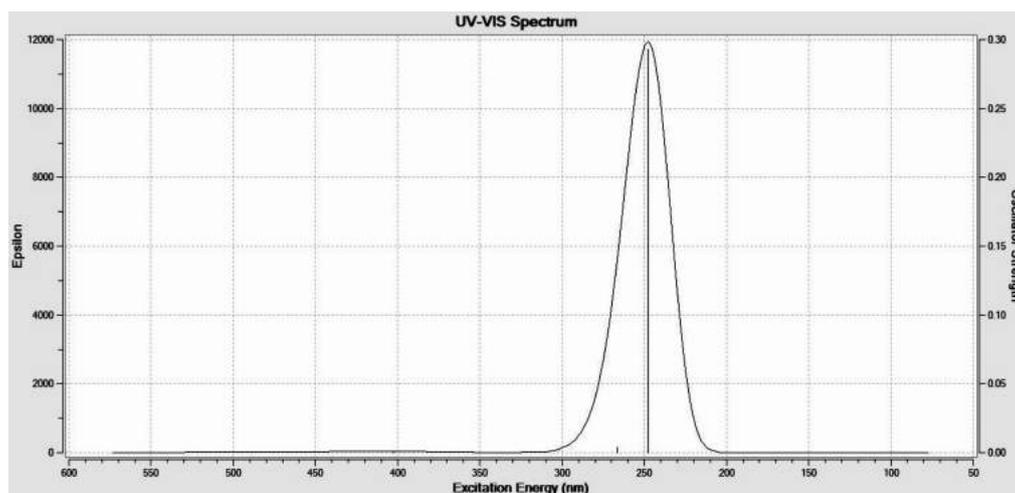

Figure 3. TD-DFT UV-Vis. Spectrum of SDS

Figure 4. TD-DFT UV-Vis. Spectrum of Tartrazine

In order to go through the thermodynamic status of the targeted molecular mesh, the FT−IR calculation was done following the same formalism scheme as applied in the respective optimization. Theoretical IR spectra of the molecules under study are given in figure 6. Theoretically evolved thermodynamics of the model systems at room temperature and pressure of 1.00 atm shows that the zero-point content energy is −0.59, thermal −0.57,

thermal enthalpy −0.56, thermal free energy −0.65 (a.u.) for tartrazine and for SDS respectively are −0.12, −0.11, −0.11, −0.16. From the thermodynamic analysis it again follows that both the target compounds differ slightly in their stability. The differences between thermodynamic parameters are the real driving forces that result in their mutual interaction to favour micellization (Mir *et al.*, 2017).
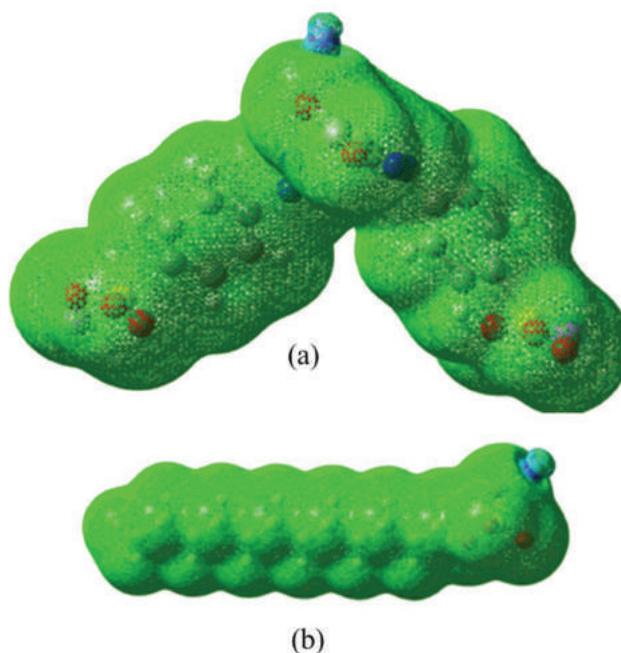
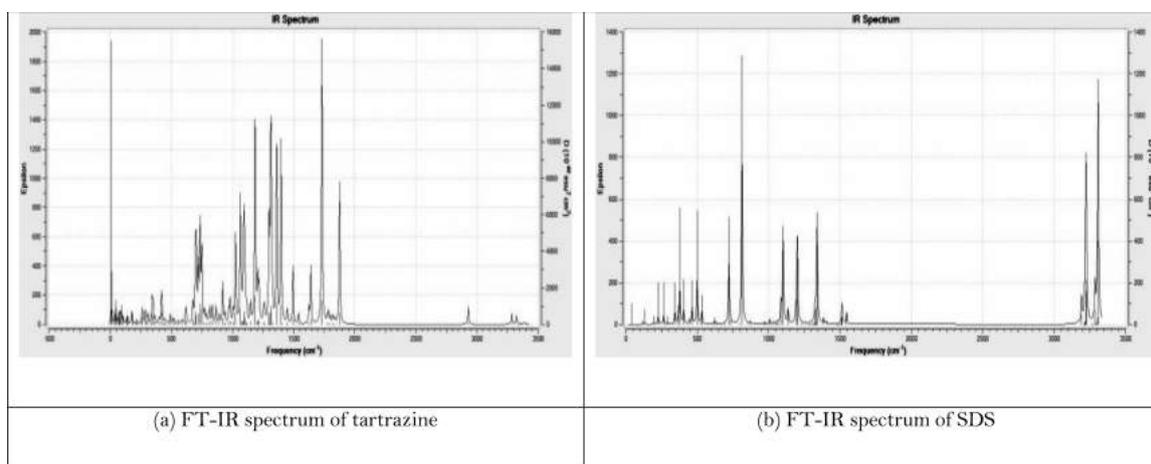**Figure 5.** Charge topography of (a) Tartrazine (b) SDS

Figure 6. FT-IR spectra of the target compounds

Conclusions

From the overall study it can be remarked that the micellization is favourable under theoretical discussion evident from the DFT analyzed components. The theoretical results can be made comparable to experimentally known observations. From the results involving molecular charge analysis, thermodynamic study and TD-DFT the favorability of the binary mixture interaction is quite supported. These energy parameters are assumed as the real factors behind the physiochemical factors discussed so far. Theoretical speculation regarding identification and visualization of binding/interaction spots can thus be easily labeled. The study can further be explored in respect of other dyes to infer desirable chemical and physical processes of industrial relevance. The area of this study may open interesting aspects of in context to other solvents for a fathomable investigation of solution chemistry.

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