



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.

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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, visco-

metric, 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).

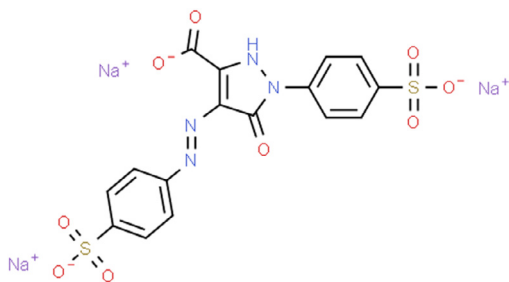
Tartrazine represents one of the effective anionic species that has been found relevant as drug-additive in proposing treatment to neural defects (Al-Shabib et al., 2018). Studies have revealed efficient electrostatic interactions exhibited by tartrazine which is important factor in induced amorphous 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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Scheme 1. Chemical structure of tartrazine.

and surface chemistry (Saeed et al., 2017; Enache and Toader, 2018). Therefore a combined experimental-theoretical study of these compounds represents a significant contribution towards dye-surfactant chemistry. Density functional theory (DFT) is considered as a modern powerful tool to validate the experimentally observed properties almost in all fields of science. The molecular interactions can be examined under both solvent-free and solvated fashion to unveil the hidden information of applied interests.

In the conspicuous fascination as aforementioned, this study involves physico-chemically evaluated thermodynamics of tartrazine and SDS mixture in combination with density functional aspects. The primary data in the form of specific conductance and surface tension of 0.002, 0.004, 0.006, 0.008, 0.010, 0.015, 0.020, and 0.025 M sodium dodecyl sulphate in 0.001 M aqueous tartrazine at 298.15, 303.15, and 313.15 K is investigated. The experimental values of conductivity and surface tension have been used to estimate various thermodynamic parameters like standard free energy, ΔG_{mic}° , enthalpy, ΔH_{mic}° , and entropy, ΔS_{mic}° , of micellization; standard free energy, ΔG_{ad}° , enthalpy, ΔH_{ad}° , and entropy, ΔS_{ad}° of adsorption, maximum (or simply) surface concentration values at the air-liquid interface, Γ_{max} at cmc, minimum area per molecule, A_{min} (nm^2) at the liquid- air- interface, and the surface pressure at the cmc, π_{cmc} . DFT based calculations were used to arrive at the basic structural parameters of the involved dye-surfactant interactions involving electron-density plots and various other descriptors to speculate the pre- and post-micellization phenomena.

2. Experimental, chemicals and methods

Double distilled water was used for making the respective solutions. Ostwald's viscometer was adjusted vertically in water bath (thermostated retained for half an hour to record thermal fluctuations if any during the experiment) to find the viscosity. Systronics conductometer and pH meter were other instruments used to record thermodynamic primary data. The pH of the studied system was not maintained to particular pH for specific group interactions but the overall effect of the tartrazine in aqueous medium at neutral pH was investigated. All the required experiments were carried out after calibration of each involved instrument. Analytical grade Sodium dodecyl sulphate (SDS), an anionic surfactant were purchased from sigma Aldrich

3. Results and discussion

3.1. Experimental discussion

The values of specific conductance, κ , surface tension, γ , and molar conductance, Λ , for sodium dodecyl sulphate in 0.001 M aqueous tartrazine are given in Table 1 as a dependent moiety of surfactant concentration at 298.15, 303.15, and 313.15 K. The specific conductance values are plotted against surfactant concentration and are shown in Fig. 1 at three different temperatures. The

Table 1

Values of surface tension, γ , molar conductance, Λ , and specific conductance, κ , of solutions of SDS in aq. Tartrazine (0.001 M) at different temperatures.

M (mol. dm ⁻³)	T (K)		
	298.15	303.15	313.15
γ (dyne / cm)			
SDS + (0.001 M) aq. Tartrazine			
0.00	61.1	56.6	52.0
0.002	33.1	34.9	35.9
0.004	31.0	32.6	33.8
0.006	29.6	31.0	32.7
0.008	28.5	29.2	30.8
0.010	28.3	29.0	30.7
0.015	28.4	29.1	30.8
0.020	28.3	29.0	30.6
0.025	28.3	29.0	30.6
Λ (mS cm ² mol ⁻¹)			
SDS + (0.001 M) aq. Tartrazine			
0.002	0.3850	0.4300	0.4750
0.004	0.2225	0.2475	0.2725
0.006	0.1750	0.1900	0.8023
0.008	0.1475	0.1550	0.1713
0.010	0.1230	0.1350	0.1470
0.015	0.0913	0.0980	0.1047
0.020	0.0740	0.0795	0.0850
0.025	0.0644	0.0692	0.0756
κ (mS cm ⁻¹)			
SDS + (0.001 M) aq. Tartrazine			
0.002	0.81158	0.90644	1.0013
0.004	0.93806	1.04346	1.14886
0.006	1.0670	1.20156	1.3175
0.008	1.24372	1.30696	1.44398
0.010	1.29642	1.4229	1.54938
0.015	1.44398	1.54938	1.65478
0.020	1.55992	1.67586	1.7918
0.025	1.69694	1.82342	1.99206

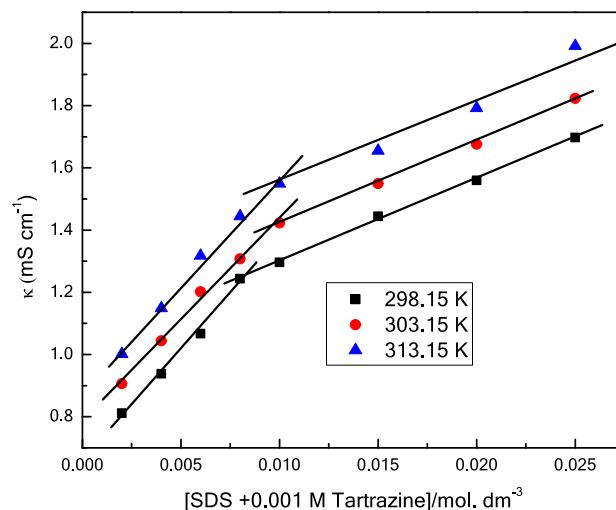


Fig. 1. Graphical presentation of specific conductance [κ (mS cm⁻¹)] vs. molarity (mol. d m⁻³) at varying temperatures for SDS in aq. Tartrazine solution.

effect of various serially dilution solutions of SDS upon Tartrazine (0.001 M aq.) at different temperatures can be thought of the prominent way to build a relation for post-micellization and pre-micellization processes.

The slope ratio method was used to determine the fraction of counter ions bound to micelles conductometrically. In this method, the ratio of the pre- and post- miceller slopes S_1 and S_2 , respectively, of the specific conductance versus concentration plots are considered. The ratio of S_2 / S_1 ($=\beta$) is taken as the fraction of the counter ion dissociated from the micelle so that the fraction bound

is given as $\alpha = (1 - S_2 / S_1)$. β and α represent the surfactant counterion dissociation and association constants, respectively. The values of β , α , and Λ^0 are given in Table 2 together with the cmc values determined by conductivity method.

The values of molar conductance at infinite dilution, in the pre-micellar region, are obtained by using Onsager equation (Paul et al., 1998) by a graphical method

$$\Lambda = \Lambda^0 - (A\Lambda^0 + B) c^{1/2} \quad (1)$$

where Λ , is the molar conductance, c is the concentration in mol. dm^{-3} of surfactant and A and B are the constants having their usual significance. The observed decrease in α , and the observed increase in Λ^0 with the increase in temperature suggests that counterion dissociation increases with the micelle formation in the presence of tartrazine. This may be due to the fact that the tartrazine dye in aqueous solution behaves as an anionic dye. As is well known that the SDS is itself an anionic surfactant, thus there are obvious anionic-anionic repulsions causing the cmc to increase and also affecting the values of α and β but increasing temperature owing to the thermal fluctuations causes slight increase in degree of dissociation (Malik, 2016). The cmc of SDS in aqueous medium in absence of tartrazine is found to be 0.8 mM in aqueous medium. As tartrazine is having three $-\text{COO}^-$ groups, when it is dissolved in water it bears three negative charge centres and SDS is itself an anionic surfactant. Thus, the repulsive interactions between the micelles of SDS and tartrazine have a profound effect on the CMC increase when TAR is added. It is also generally observed that the magnitude of β is strongly influenced by the attractive Coloumbic force operating between the counterions and the head groups of the surfactants, as well as by the increased thermal energy; the former force tends to bind the counterions to the polar head groups, whereas the latter enhances the dissociation of the counterions from the polar head groups. The increase in β suggests the dominance of the thermal force over the Coloumbic force, inducing dissociation of the counterions from the surfactants with rise in temperature. A similar increase in β with temperature has been reported for alkyltrimethylammonium bromides in aqueous solutions (Zana, 1980; Markina et al., 1997).

In other words, the value of counterion dissociation, β , increases with temperature. This is in close agreement with the variation of β and α with temperature also reported elsewhere (Paul et al., 1998). Table 1 shows that the molar conductivity, Λ , decreases with increase in concentration of surfactant, while it shows reverse trend with temperature. The Λ^0 values can be used to estimate the limiting molar ionic conductivity for sodium dodecyl sulphate, DS^- (λ_{DS}^0) ions by subtracting the value of λ_{Na}^0 in water ($=50.1 \text{ S cm}^2 \text{ mol}^{-1}$). The values of λ_{DS}^0 thus obtained at 298.15, 303.15 and 313.15 K is $276.8 \text{ S cm}^2 \text{ mol}^{-1}$.

Surface tension values have been shown as a function of $\log [\text{SDS}]$, are plotted in Fig. 2. It is observed from the surface tension plot that a steep, almost linear, decline occurs and after adding

Table 2

Values of molar equivalent conductance at infinite dilution (Λ^0), the counterion association (α), counterion dissociation (β), minimum area per molecule (A_{min}), surface pressure at cmc (Π_{cmc}), surface excess concentration (Γ_{cmc}), values of cmc for SDS in aqueous tartrazine solution (0.001 M) at different temperatures. a; by conductivity measurements. b; by surface tension measurements.

	298.15 K	303.15 K	313.15 K
Λ^0 ($\text{mS cm}^2 \text{ mol}^{-1}$)	0.327	0.360	0.396
α	0.7123	0.6500	0.3648
β	0.2878	0.3500	0.351
A_{min} (nm^2)	0.0189	0.0194	0.0211
Π_{cmc} (dyne cm^{-1})	32.5	27.4	12.2
Γ_{max} (mol cm^{-2})	8.76×10^{-5}	8.56×10^{-5}	7.87×10^{-5}
cmc^a (mol dm^{-3})	8.12×10^{-3}	8.51×10^{-3}	9.10×10^{-3}
cmc^b (mol dm^{-3})	8.14×10^{-3}	8.49×10^{-3}	8.89×10^{-3}

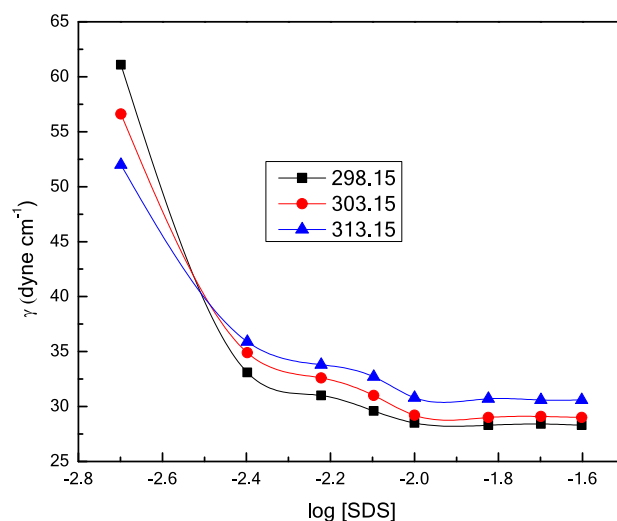


Fig. 2. surface tension (γ) as a function of $\log [\text{SDS}]$ for aq. Tartrazine + SDS at Different temperatures.

more concentration of surfactant an abrupt leveling at the critical micelle concentration (cmc) is observed. The air/water interface is assumed to be saturated with surfactant monomers from the steep descent (Voorst and Vader, 1960; Perez et al., 1998). There are clear breaks in γ vs $\log[\text{SDS}]$ plots (Fig. 2), which correspond to the cmc of the surfactant in presence of tartrazine dye. From Table 2, the cmc values of SDS in presence of tartrazine are observed to increase with temperature and in the presence of dye. This increase in cmc in the presence of tartrazine may be attributed to the anionic-anionic repulsions, as the tartrazine in aqueous solution is itself negatively charged and surfactant SDS is also anionic. Here we can conclude that the tartrazine acts as a structure breaker in the aqueous solution with SDS. On comparing the cmc values obtained by the surface tension method and conductivity method, it is observed that the cmc values from surface tension method are lower. It is already reported that cmc determination is about 7–20% lower from surface tension method (Bazito and El Seoud, 2002; Ray et al. 2009). The cmc values calculated by the surface tension as well as conductance measurements are given and compared in Table 2. It may be mentioned here that using Gibbs adsorption equation maximum surface excess concentrations, Γ_{max} values can be calculated at the air-liquid interface. This helps to assign the excess of solute per unit area of the surface over what would be presented if the bulk concentration prevailed all the way to the surface. It has a unit of mol. cm^{-2} .

$$\Gamma_{\text{max}} = 1/RT(d\gamma_{\text{cmc}}/d\ln c)_{T,P} \quad (2)$$

where γ_{cmc} is the surface tension at cmc and c is the molarity in terms of mol dm^{-3} ($d\gamma_{\text{cmc}}/d\ln c$)_T represents the slop of the surface tension, γ versus $\log c$ plot below the cmc at constant temperature. The surface tension values are dependent upon the nature of solutes differing in their structure, when surfactants are solutes the surface tension decreases and once, a minimum is reached, no more change in surface tension occurs, showing constant value in Table 1. Above the cmc, surface tension shows no change with the concentration, hence, surface tension values at the cmc have been used to calculate effectiveness as surface pressure at cmc which is an index of reduction in surface tension as given below:

$$\pi_{\text{cmc}} = \gamma_0 - \gamma_{\text{cmc}} \quad (3)$$

where γ_0 is the surface tension measured for solvent at different temperatures and γ_{cmc} is the surface tension at cmc and are included in Table 2. The effectiveness of a surface active molecule

Table 3

Thermodynamic parameters of the micellization and adsorption of SDS in aqueous tartrazine solution (0.001 M).

Temperature (K)	298.15	303.15	313.15
ΔG_{mic}^0 (10^2 KJ / mol)	-2.71	-1.98	-1.55
ΔG_{ad}^0 (10^5 KJ / mol)	-3.71	-3.20	-1.55
ΔH_{mic}^0 (10^2 KJ / mol)	-2.10	-1.90	-1.46
ΔC_{pmic}^0 (10^4 KJ / mol K)	4.29		
ΔH_{ad}^0 (10^5 KJ / mol)	-3.71	-3.20	-1.55
ΔS_{mic}^0 (10^{-2} JK ⁻¹ mol ⁻¹)	2.33	2.49	2.81
ΔS_{ad}^0 (10^{-3} JK / mol ⁻¹)	8.47	7.46	5.47

in reducing the surface tension at the cmc measured as surface pressure (π_{cmc}). It is evident from the Table 2 that π_{cmc} shows a

decreases with the increase in temperature. This trend is also followed by the α with respect to the temperature. On the other hand decrease in π_{cmc} with respect to temperature can also be ascribed to the micelle formation. So, leads to a shift of surfactant molecules from the air-liquid interface to the bulk, thereby, resulting in lower π_{cmc} values with increase in temperature. The Γ_{max} values for the present system at 298.15, 303.15 and 313.15 K are given in Table 2. The Table 2 reveals that the Γ_{max} values decreases with an increase of temperature. This is attributed to the existence of the increase of temperature making the surfactant more favourable for the solvent mixture, thereby creating a shift of surfactant agents from the air-liquid interface toward the bulk or may be enunciated for the reason to enhance molecular thermal collision at higher degree of temperature.

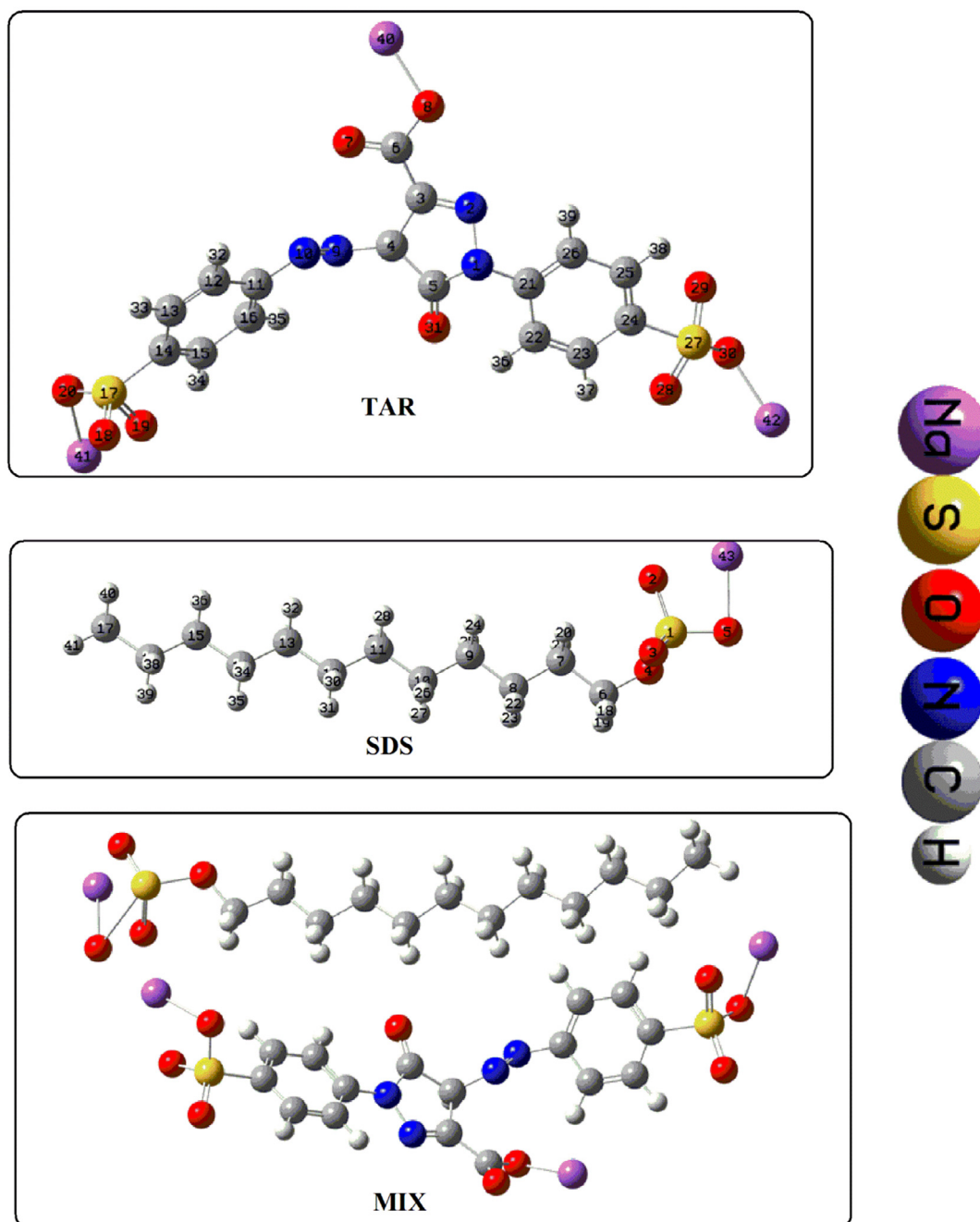


Fig. 3. Optimized 3D structures of SDS, tartrazine and SDS-tartrazine binary mixture.

The other important parameter called as minimum area per molecule A_{min} (nm^2) at the liquid – air interface has been calculated using the relationship:

$$A_{min} = 10^{18} / NT_{max} \quad (4)$$

where, N represents the Avogadro's number. The increase in the minimum area per molecule, A_{min} , on elevation of temperature may be again due to the increased thermal agitation at higher temperature. Further, Γ_{max} and A_{min} values are found to be inversely dependent, as expected. This is in good agreement with the reported variations of Γ_{max} and A_{min} with temperature for sodium *N*-dodecyl sarcosinate, an amino acid surfactant, in aqueous medium.

The standard Gibbs free energies of micellization ΔG_{mic}° were calculated using the relationship, 5:

$$\Delta G_{mic}^{\circ} = (2 - \beta)RT \ln X_{cmc} \quad (5)$$

where, X_{cmc} is the cmc value expressed in mole fraction.

The entropy (ΔS_{mic}°) and enthalpy (ΔH_{mic}°) of micellization were calculated from the equations:

$$\Delta S_{mic}^{\circ} = -d(\Delta G_{mic}^{\circ})/dT \quad (6)$$

$$\Delta H_{mic}^{\circ} = \Delta G_{mic}^{\circ} + T\Delta S_{mic}^{\circ} \quad (7)$$

The main thermodynamic characters calculated from the given data including of ΔG_{mic}° , ΔS_{mic}° , and ΔH_{mic}° are given in Table 3. As it is known that the sign of the numerical values of these parameters matters to define the feasibility of a physical or chemical process. Herein, the negative value of ΔG_{mic}° is an indicative of the fact that micellization is a thermodynamically favoured process. The escalation in temperature in the presence of co-solvent (tartrazine) for the target solution has shown direct impact on the micellization in a direct proportional way. The solvation of the surfactant hydrophilic molecular site at increased temperature can be related with the increase in the free energy of micellization, ΔG_{mic}° , on increasing the temperature. From the data it is clear that the ΔG_{mic}° becomes less negative or micellization becomes less feasible. The ΔH_m° vs. T plot gives a slope ($\partial \Delta H_m^{\circ} / \partial T$)_p called heat capacity at constant pressure of the surfactant upon micellization ($\Delta C_{p,mic}^{\circ}$). The calculated value of $\Delta C_{p,mic}^{\circ}$ in this study is $4.29 \times 10^{-4} \text{ kJ mol}^{-1} \text{ K}^{-1}$. A negative value of $\Delta C_{p,mic}^{\circ}$ indicates release of water molecules from the hydrophobic tails of surfactant molecules as micelles are formed. The system under investigation shows positive value of $\Delta C_{p,mic}^{\circ}$, which can be attributed to the structure breaking property. Moreover, due to the fact that the tartrazine acts as a structure

Table 4

Some selected bond lengths of TAR, SDS and MIX.

Bond	TAR (Å)	MIX (Å)	Bond	SDS (Å)	MIX (Å)
O(8)-Na(41)	2.22	2.27	O(5)-Na(43)	2.27	2.22
O(31)=C(5)	1.23	1.24	O(5)-S(1)	1.62	2.78
S(27)=O(28)	1.63	1.60	S(1)=O(2)	1.63	1.61
C(21)-N(1)	1.42	1.42	O(4)-S(1)	1.76	1.77
N(9)=N(10)	1.28	1.27	C(6)-O(4)	1.47	1.48
N(1)-N(2)	1.39	1.42	C(7)-C(8)	1.54	1.54
C-H (Phenyl)	1.08	1.08	C(10)-H(26)	1.10	1.10

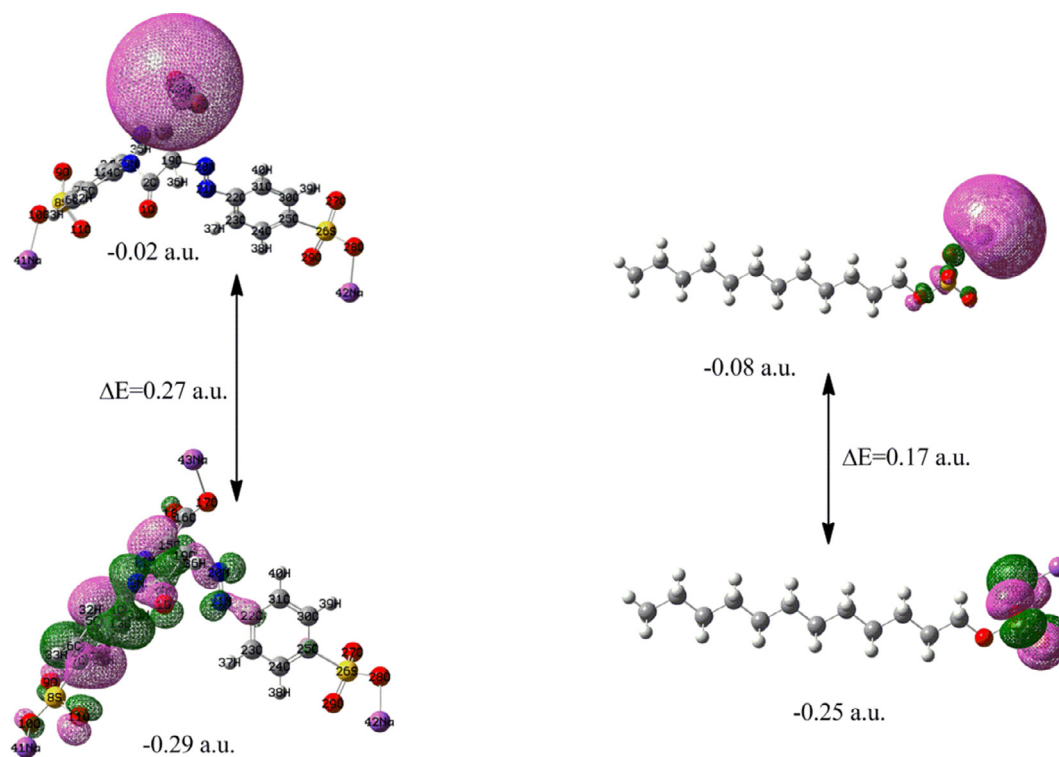


Fig. 4. Frontier orbital diagrams of TAR and SDS.

breaker, that is, destruction of the hydrophobic chain structure of the water molecular system occurs. Also owing to thermal agitation the cmc increases thereby rendering ΔG_{mic}^0 less negative. The higher positive values of change in entropy of micellization ΔS_{mic}^0 for the model system prevail over the low negative numerical values of ΔH_{mic}^0 , that can be the fact behind the micellization process predominantly controlled by the entropy again rather by any other effect. Hence, entropy is the main driving force to achieve this process.

From Table 2, it is observed that the cmc values follow a direct relation with temperature. This can be explained on the basis of the assumption that the temperature elevation can result in destruction of the hydrophobic chain structure of the water molecular system. The standard free energy values of adsorption, ΔG_{ad}^0 , at the air – liquid interface were calculated using equation:

$$\Delta G_{ad}^0 = \Delta G_{mic}^0 - \pi_{cmc}/\Gamma_{cmc} \quad (8)$$

where π_{cmc} is in dyne / cm. values of ΔS_{ad}^0 and ΔH_{ad}^0 were obtained by using the corresponding Eqs. (6) and (7). The values of ΔG_{ad}^0 , ΔS_{ad}^0 and ΔH_{ad}^0 are given in Table 3. It is evident that ΔG_{ad}^0 values are lower than ΔG_{mic}^0 values for the system studied. This is obvious, since in the micelle formation process, the system has to perform work in transforming the monomeric surfactant molecules from the air–liquid interface to the aqueous bulk med-

ium. The ΔH_{ad}^0 and ΔS_{ad}^0 values suggest that the adsorption process is also controlled by the entropy change rather than an enthalpy change.

3.2. DFT based pre-micellization and post-micellization study

In order to present a comparative description of several properties of free compounds (dye and surfactant) and finally the mixture of the two compounds selected for the study, SDS and TAR were separately optimized followed by the optimization of the mixture (MIX). The three sets of calculations were carried out in water as solvent system. The true minimal energy surface was confirmed by vibrational analyses which showed the absence of imaginary frequency. The respective 3D optimal structures are shown in Fig. 3. Out of different optimization parameters some selected bond lengths have been given in Table 4. The variation in bond-lengths depicts the impact of change in chemical environment. The data indicates the fact that head regions show more variation as compared to the tail regions. Similar explanation can be obtained in case of bond angles and dihedral angles showing the modifications in orientation of different atoms in the mixture. The total energies of the interacting species can be used to find the binding energy (B.E.) of the mixture. B.E is equal to the total energy of MIX subtracted by total energy of SDS and TAR. The calculations have shown the value 0.1 a.u. The distinctive stability of

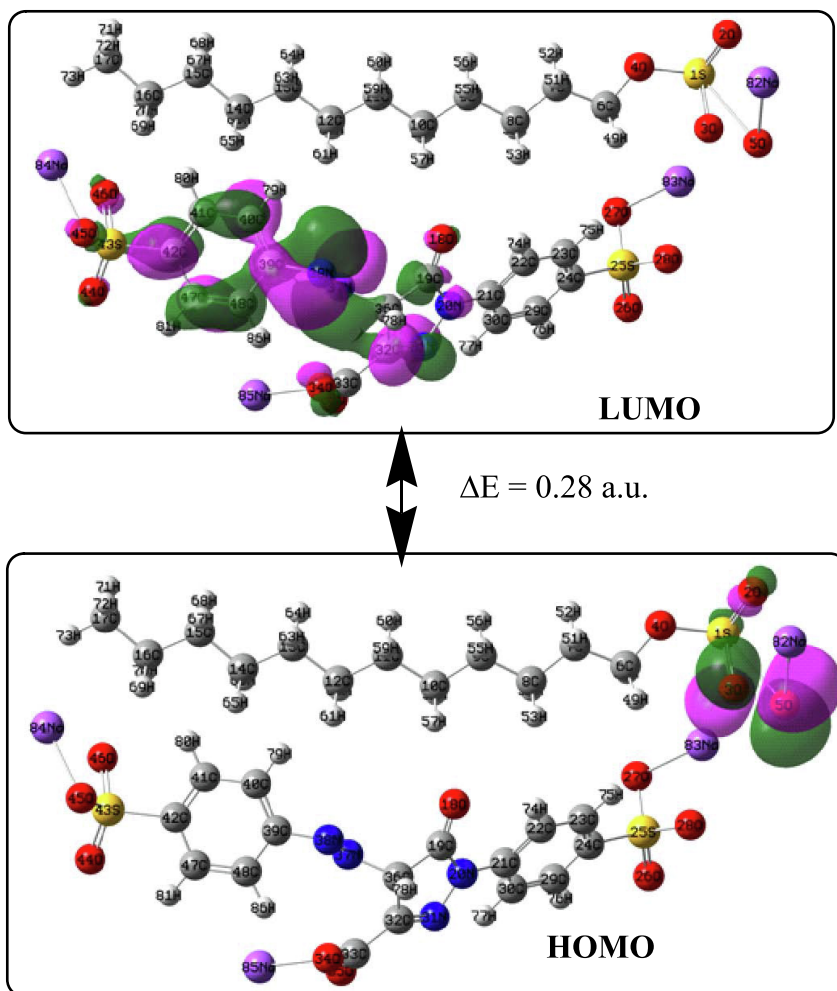


Fig. 5. Frontier orbital diagrammatic representation of MIX.

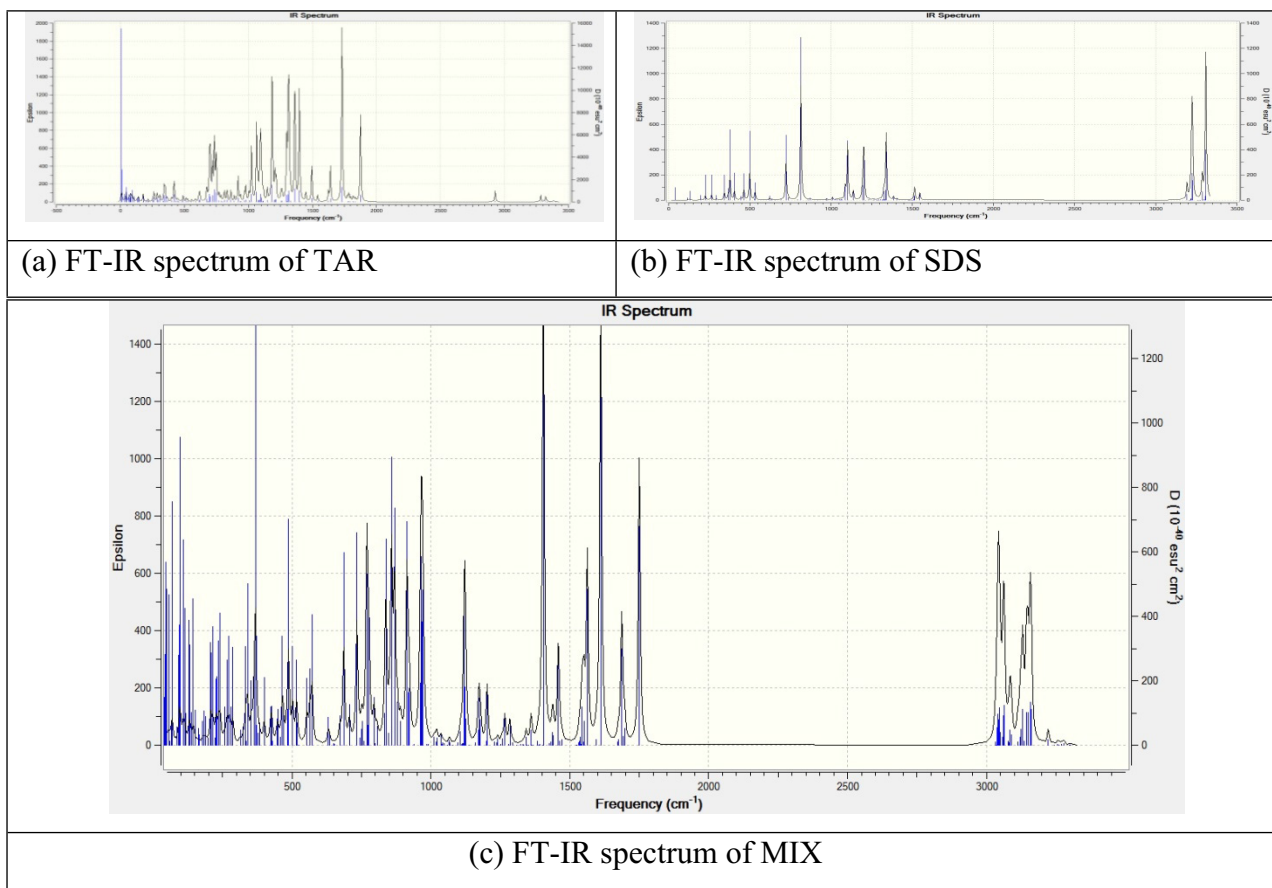


Fig. 6. Theoretical FT-IR spectra of the free compounds and the resulting mixture.

the resultant mixture can also be determined by zero point energy calculation. In the case of TAR, SDS and MIX the calculated zero-point (Z.P.) energies (Kcal/mol) were found as 158.07, 233.99 and 392.52, respectively. This indicates the resultant Z.P.E. of mixture is the summed up values of individual compounds leading to a difference of 0.46.

In addition to conformational analysis, molecular orbital evaluation can also serve as a speculative tool to find the extent of the existence of molecular interaction of target compounds in their free form as well as mixture by looking at the respective highest occupied molecular orbital (HOMO)-lowest unoccupied molecular orbital (LUMO) gaps shown in Figs. 4 and 5. The HOMO-LUMO gap of mixture corresponds to the gap of TAR. The SDS showing minimum gap out of the three sets of orbitals (Malik and Mir, 2018). This exhibits the impact of dye-surfactant interface to modify this gap to 0.28 a.u. and thus pronouncing more stability in the MIX. The observed energy gaps can be found in good relevance with other chemical reactive parameters that come into play to discuss solute-solute interactions. From the respective charge density plots it is clear that HOMO 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 projection of HOMO is thus towards SDS in MIX and LUMO is towards TAR part of the mix. This behaviour can also be implicated by the nature of solvent.

In order to find the DFT based thermodynamic parameters of the targeted molecular species, Frisch et al. (2010), GaussView 5.0, 0000, Mir and Itoo (2017), Mir and Maurya (2018), Mir et al. (2017), the vibrational spectral analysis was carried out and the respective spectra are shown in Fig. 6. The entire sets of FT-IR cal-

culations were carried out at room temperature. The magnitude of energy has been expressed as Hartree per particle. The results show enthalpy (H) and free energy (G) of TAR to be -0.570 and -0.658 , respectively. In the similar order, the properties (H and G) of SDS come out to be -0.115 and -0.167 . The summation effect of both the free compounds is clear by the resultant data of H and G in MIX as -0.804 and -0.958 , respectively. These significant characters can be used to find the difference among their values in pre- and post-micellization. The calculations over the furnished data shows ΔG to be -0.183 and ΔH as -0.119 . By applying the relation of these two factors with ΔS and taking room temperature in consideration the change in entropy can also be calculated by using $\Delta G = \Delta H - T\Delta S$.

Despite, the fact that the DFT based thermodynamic parameters are not so closely in agreement with the experimental results, the change in the respective thermodynamic parameters are significant in elaborating the interaction. On one hand the computed data is restricted to some default commands and the values are mainly confined to room temperature and on the other hand the several ion-ion interactions are ignored in theoretical results Ali et al. (2014), Azum et al. (2018), Waren (2000). The factors like hydration of sodium ions, geometry deformation and dipole-dipole interaction can be suggested as the factors that might be responsible for the disagreement between experimental and theoretical data of thermodynamics.

4. Conclusions

From the convergent theoretical and experimental results it may be remarked that the micellization is favourable under the

suggested conditions. Theoretical speculation regarding identification and visualization of binding/interaction spots can thus be easily labeled. The results have shown molecular charge analysis as the real factor behind the presented physicochemical parameters. The study can further be explored in respect of other dyes to infer desirable chemical and physical processes of industrial relevance. The well pronounced agreement between the suggested interactions and the collaborative theoretical approach thus fits to considerable level with the solution behaviour aimed in the subject matter. The area of this study may open interesting aspects of in context to other solvents for a fathomable investigation of solution chemistry.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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