Investigation of the Interaction of Tetradecyltrimethylammonium Bromide Drug with Cetyltrimethylammonium Bromide at Different Temperatures

ABSTRACT

At solution and within the attending of salts at the several of temperatures (25℃, 30℃, 35℃, 40℃ and 45℃), the interaction of the antibacterial between tetradecyltrimethylammonium bromide (TTAB) and cetyltrimethylammonium bromide (CTAB) has been investigated. For the pure CTAB and their mixture with the drug tetradecyltrimethylammonium bromide (TTAB), one vital particle concentration (CMC) was determined. Within the presence of salt, the CMC values for mixed systems (TTAB + CTAB) showed lower in magnitude compared to the absence of the salt within the mixture. By remarking the first micellization of the mixture of TTAB and CTAB, all the G0m values were found to be negative for all systems. The values of H^0_m and S^0_m indicated that hydrophobic and static interactions were boosted within the presence of salts than the absence of salt at the lower and therefore the higher temperatures severally. Transfer energy ($G^0_{m.tr.}$), transfer enthalpy ($H^0_{m.tr.}$) furthermore as transfer entropy ($S^0_{m.tr.}$) was called the physical science parameters were additionally determined and mentioned intimately. The intrinsic H gain compensation temperature (T_c) were also evaluated and mentioned. Molecular dynamics simulation reveals that liquid furthermore as salt setting have impact on the hydrophobic interaction between tetradecyltrimethylammonium bromides (TTAB) with cetyltrimethylammonium bromide (CTAB).

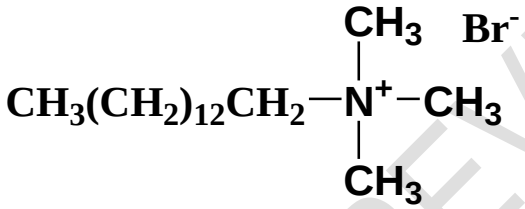
Keywords: TTAB; CTAB; CMC; Micelle.

1. INTRODUCTION

Both hydrophobic and hydrophilic components in a private chemical agent is responsible to make aggregates in aqueous/ non-aqueous resolution, termed as particles and this development takes place on the far side a precise chemical agent concentration that is acknowledged as important micelle concentration (CMC) [1–3]. The micelles of surfactants are used as a model of biological membranes. Appliances of surfactants are in the main addicted to the advanced formation behavior of surfactants with solutes like medication, dyes, organic molecules etc. [1– 7]. Micelles have massive surface area; thus, they're befittingly exploited to perform as catalysts for varied chemical reactions, able to modify the reactions pathways, rates likewise as equilibria [8-9]. Amphiphiles mixed systems are sound reportable within the previous study, being of key interest so as to advance their self-assembly and convenient applications [1,4–6,10,11]. Cetrimonium bromide ($[(C_{16}H_{33})N(CH_3)_3]Br$; cetyltrimethylammonium bromide; CTAB) may be a quaternary ammonium ion chemical

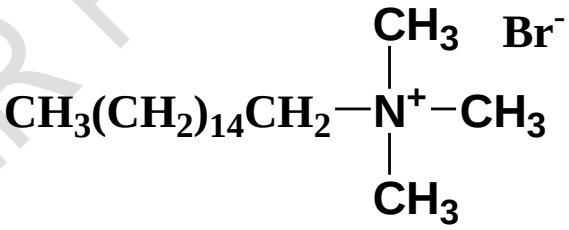
agent.

It is the foremost in all the parts of the topical antiseptic antimicrobial. The cetrimonium (hexadecyltrimethylammonium) ion is an efficient antiseptic agent against microorganism and fungi. It's conjointly one in all the most parts of some buffers for the extraction of desoxyribonucleic acid. It's been wide utilized in synthesis of gold nanoparticles (e.g., spheres, rods, bipyramids), mesoporous silicon dioxide nanoparticles and hair learning product. The closely connected compounds cetrimonium chloride and cetrimonium stearate also are used as topical antiseptics and should be found in several family product like shampoos and cosmetics. CTAB, because of its comparatively high price, is often solely utilized in choose cosmetics.



Scheme1. Molecular structure of tetradecyltrimethylammonium bromide (TTAB)

Moreover, it is typically utilized to cure respiratory illness, tract ill-ness, and abdominal infections in conjunction with those opposing to different antibiotics. On the opposite hand, among an outsized range of standard wetting agent, we have chosen the cationic wetting agent CTAB that have useful uses like removal ability of significant metal from magnetic nanoparticles [5] associated use as an adsorbent to remove of poisonous and harmful compounds like herbicides from the water.



Scheme2 Molecular structure of cetyltrimethylammonium bromide (CTAB)

Although literature surveys show the presence of an outsized range of studies on the mixed wetting agent systems, to the simplest of our information a detail study on the mixed particle formation between tetradecyltrimethylammonium bromide (TTAB) and cetyltrimethylammonium bromide (CTAB) (Schemes one and 2) has not been nonetheless studied. Considering these views during this study totally different micellar parameters like CMC, ideal price of the essential particle concentration, micellar mole fractions and their ideal values, activity coefficients (fRub1 and fRub2), degree of dissociation (g) similarly as totally different physics parameters (standard free energy change (G^{o}_{m}), standard enthalpy change (H^{0}_{m}), standard entropy change (S^{0}_{m}) of micellization as well as excess free energy of micellization (G^{Rub}_{ex})) of micellization similarly as excess

free energy of micellization are determined from conduction technique and theoretical calculations to explore the interactions between the parts gift in mixtures.

In this study, the interaction between TTAB and CTAB (cationic surfactant) within the absence and also the presence of some inorganic salts like binary compound, sodium chloride, potassium chloride, and sal ammonium chloride was investigated by the conductometric methodology. Exploitation of inorganic salts, drugs etc. could be an acquainted method to switch the micellization performance of amphiphiles. The presence of salts reduces the electricity repulsion among the charged head cluster that decreases the essential particle concentration (CMC). Additionally, sturdy electricity interactions considerably influence the sorption of amphiphile molecules at the interface of air and water [19, 20]. Hence, it will simply be assumed that the degree of sorption within the presence of salts ought to be significantly totally different as compared to the absence of the salts within the wetting agent answer. In presence of salts the varied parameters like essential particle concentration (CMC), counter particle binding (β), physics parameters (G^0_m, H^0_m, and S^0_m) connected with the TTAB and CTAB interaction in solution are calculable may be the interaction behavior between TTAB and CTAB at totally different temperatures..

2. MATERIAL AND METHODS

2.1. Preparation of solutions

At the absence or presence of a better-known concentration of common salt, potassium chloride, and ammonium chloride (NaCl, KCl, NH_4Cl) and mistreatment double deionized H_2O having the precise physical phenomenon within the vary of 1.5–2 μScm^{-1}, the stock solutions of TTAB (drug) and surface-active agent were ready. Within the gift study, all the utilized materials were used while not extra purification. Cetyltrimethylammonium bromide (CTAB) was purchased from Aldrich, USA. TTAB as USP commonplace sample common salt, potassium, and sal ammoniac (NaCl, KCl and NH_4Cl) were utilized in this study.

2.2. Conductivity technique

In the absence or the presence a celebrated concentration of common salt, potassium, and salt, A solution twenty five $mmolL^{-1}$ CTAB ready in water or (TTAB+ water) is step by step other to twenty cc of water or (TTAB + water) solution of a specific drug (TTAB) concentration at fastened temperature. After that, the particular electrical phenomenon of the ready mixtures was evaluated by means that of a physical phenomenon meter having a dip cell (glass electrode) of cell constant 0.97 cm^{-1} [5–8, 14–18, 21, 22]. This instrument was mark exploitation solutions of KCl of the acceptable vary of concentration. For electrical phenomenon measurements, An Alternative current (AC) voltage supply at a frequency of 60cycles/second was applied. The accuracy of the electrical phenomenon measurements is within the difference of ±0.5%. By current water throughout the answer having error of ± 0.2 K, the temperature of systems was controlled among the expressed vary. each the TTAB additionally as CTAB solutions area unit ready in presence of common salt, Potassium, and salt, therefore, all the solutions hold a similar concentration of salt to examine the impact of salt.

2.3. Molecular dynamics simulations

In the presence of salt and also the absence of salt, molecular dynamic (MD) simulation was performed on 2 systems containing surfactant-drug with water. For wetting agent, thirty two molecules of CTAB were thought of. The initial wetting agent molecule was optimized by Universal physical phenomenon [23] in mathematician 09 package. [24] Then every wetting agent molecular are paired up and clustered along through continuous step-down. Six medications molecular are indiscriminately placed in every system. For considering salt-containing surfactant-drug system, 10 sodium ions, and 10 chloride ions were added. All molecular dynamics simulations were conducted exploitation star physical phenomenon within the suite of YASARA Dynamic program [25]. A cut-off radius of eight.0 Å was utilized for short-range van der Waals also as Coulomb interactions. The particle-mesh Ewald methodology [26] was applied to cypher the long-range electro-static interactions. Periodic precondition (cell box of 54 Å × 68 Å × 46 Å) and temperature of 298 °C were thought of for all simulations. Time step of one fs was used and simulation snapshots were saved at the each one hundred PS 2261 water molecules were added to stay the solvent density of one g/mL for each system. A complete of 17,008 atoms was gift in those systems.

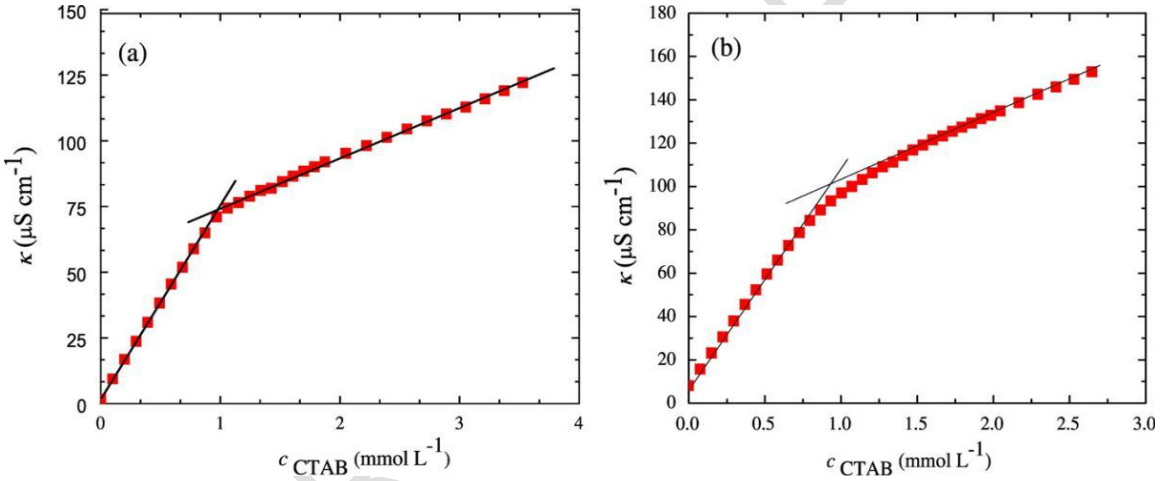


Fig.1. Specific electrical phenomenon versus concentration of CTAB for (a) pure CTAB in water and (b) (TTAB + CTAB) mixed system in water containing 0.032 mmolL^{-1} TTAB at 303 K.

The systems were reduced together with equilibrated with the default protocols of the YASARA dynamic. Lastly, three ns non-constrained molecular dynamic simulation was dead for all system.

3. RESULTS AND DISCUSSION

3.1. Critical micelle concentration (CMC) and binding counter ion (β)

In the current investigation, by perceptive modification in specific electrical phenomenon values versus the concentration of CTAB in water or TTAB and water mixture, the values of important particle concentration (CMC) square measure evaluated. In the Fig.1 the variation of specific electrical phenomenon (κ) vs. concentration of chemical agent (C_{CTAB}) of pure CTAB in solution or (TTAB + water) mixed system is incontestable at 303 K. The conduction price of answer modified linearly with the concentration of amphiphile within the pre and post micellar regions. A transparent break purpose shows within the κ versus $C_{CTAB.}$

Table 1

In solution and within the presence of various salts of various concentrations, chemistry parameters for CTAB and (TTAB + CTAB) system containing 0.032 mmolL^{-1} TTAB drug at mounted and numerous temperatures.

Systems	Medium	T (K)	C_{salts} (mmolL^{-1})	CMC (mmolL^{-1})	$X_{CMC} \times 10^5$	A	B
CTAB	H_2O	298.15	0.00	1.01	1.82	0.27	0.73
		303.15		0.99	1.78	0.28	0.72
		308.15		1.05	1.89	0.29	0.71
		313.15		1.16	2.09	0.30	0.70
		318.15		1.23	2.21	0.30	0.70
		323.15		1.33	2.39	0.31	0.69
(TTAB+ CTAB)	H_2O	298.15	0.00	0.95	1.71	0.31	0.69
		303.15	0.00	0.93	1.67	0.30	0.68
		308.15	0.00	1.00	1.80	0.34	0.66
		313.15	0.00	1.06	1.91	0.35	0.65
		318.15	0.00	1.16	2.09	0.37	0.63
(TTAB + CTAB)	H_2O	303.15	0.00	0.93	1.67	0.30	0.68
(TTAB + CTAB)	(NaCl + H_2O)	303.15	0.505	0.83	1.49	0.31	0.69
			1.067	0.70	1.35	0.29	0.71
			2.035	0.60	1.21	0.29	0.71
			3.013	0.60	1.08	0.28	0.72
(TTAB + CTAB)	(KCl + H_2O)	303.15	0.506	0.84	1.51	0.31	0.69
			1.078	0.77	1.39	0.31	0.69
			2.038	0.70	1.26	0.29	0.71
(TTAB + CTAB)	(NH_4Cl+H_2O)	303.15	0.507	0.86	1.55	0.31	0.69
			1.035	0.80	1.44	0.32	0.68
			2.009	0.74	1.33	0.27	0.73
			3.003	0.68	1.22	0.26	0.74

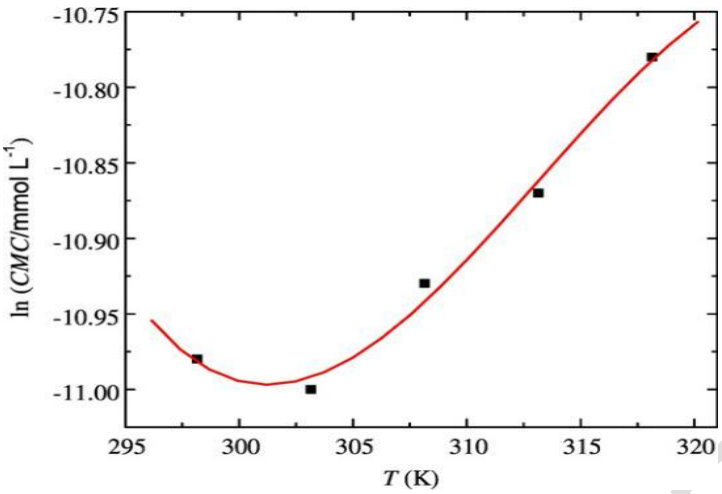


Fig.2. ln (CMC/mmolL^{-1}) versus T for (TTAB + CTAB) mixed system in water.

Plot was obtained in between pre-micellar and post-micellar region is considered the vital particle concentration (CMC) and it's such as the concentration of amphiphile comparable to the break purpose [3, 14– 18, 27, 28]. The initial rise of specific electrical phenomenon values were thanks to the involvements of the free CTA+ and Br− ions at low surface-active agent concentrations. On top of the CMC, thanks to the formation of CTAB micelles and also the condensation of the Br− ions with CTAB micelles to create physicist layer, the rise of specific electrical phenomenon values becomes smaller. By suggests that of surface charge neutralization and thence lowering unit repulsion potential, this stabilizes the self-micellized amphiphile [29]. Thus the fashioned micelles have poorer quality compare to the free ions of CTAB. The literature showed that the worth of CMC of pure CTAB in water at 303.15 K lies within the different of 0.8–1.1 mmolL−1 that is in fine agreement with our obtained values [4, 11, 8, 18].

From the quantitative relation of the slopes of the pre and post-micellar regions associated with the on top of likewise as below CMC, the degree of ionization (α) of micelles is evaluated [4, 14–18, 21, 22]. From the ratios S2/S1, the worth of α is often calculated if S1 and S2 area unit the slopes on top of and below CMC. At CMC, the fraction of counter particle binding, β is evaluated by deducting the worth of α from unity i.e. β = 1 − α.

At temperature 303 K within the group action of salts, the values of CMC or X_{CMC}, α likewise as β for (TTAB + surfactant) mixture area unit shown in Table one. The concentration of electrolytes within the body membranes could vary from time to time. The presence of varied electrolytes and its concentration could influence the interaction propensity of surface-active agent. Hence, it's essential to own awareness of aggregation phenomena for pure CTAB and TTAB + CTAB mixtures by suggests that of temperature along with attending of electrolytes. Herein, at 303.15 K within the presence of all the inorganic salt, the values of CMC of (TTAB + CTAB) mixture utilized in the current study area unit found to be lower in magnitude compared to salt-free resolution. The CMC worth of pure CTAB and their mixtures with TTAB decreases within the presence of salt (Table 1). Because the inorganic salt accessorial CMC decreases just in case of ionic surfactants, [4, 27, 28]. The values

of CMC also are reduced with the rise of the ionic strength (concentration) of salts. For micellization of our studied (TTAB + CTAB) system, higher concentration of salts provides a convenient setting. The co-ions for pure likewise as the mixed system micelles area unit Na^+, K^+,and NH_4^+. The result of salts on the decrease of CMC or XCMC values of mixed systems followed the order: $CMC_{NaCl} > CMC_{KCl} > CMC_{NH4Cl}$ (Table 1). This shows that NaCl is simpler within the reduction of CMC of the present studied system compared to KCl and NH4Cl. thanks to the tiny size together with large hydrous radius, the amendment of CMC values presumably thanks to the group action of various cations within the salts keeping identical ion (Cl−), NH_4^+ area unit the smallest amount effectual in alteration the CMC. Therefore, this salt performs as a water-structure promoter alteration the accessibility of binary compound to the micelles. Similar behavior of those cations on the CMC values of ionic surface-active agent has additionally been reportable earlier [4].

In solution or in presence of various solutes, this behavior of nonlinearity/minimum position within the CMC versus T plots is additionally found within the literature for numerous different ionic surfactants [14]. By suggests that of the mode of association getting ready to the monomers of CTAB and also the TTAB arbitrated micelles of CTAB, the result of temperature on the values of CMC are often processed. At low concentration of surface-active agent, the monomeric kind the hydrophobic likewise as the hydrophilic hydrations area unit possible, whereas solely hydrophilic association is possible for assembled CTAB. Every kind of hydrations area unit presupposed to be reduced through the increase of temperature. By suggests that of the rising of temperature barred the formation of particle, a scale back in hydrophilic association promotes the particle formation whereas a scale back of hydrophobic dehydration [4,15,15]. Therefore, the extent of each option decides whether or not the values of CMC increase or decrease at a selected vary of temperatures. Usually, the primary issue dominates at lower temperature vary Associate in Nursingd when an assured temperature, the second issue initiates governing.

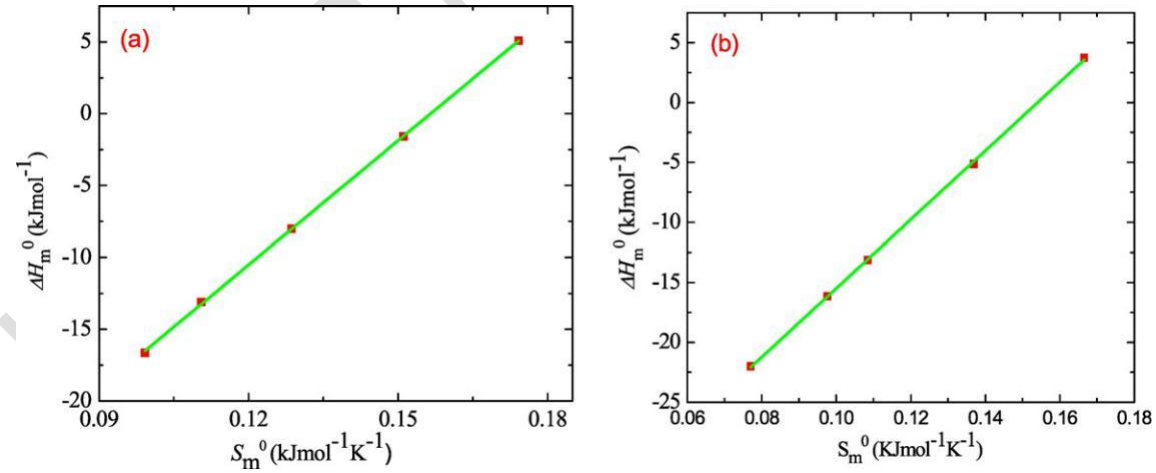


Fig.3. Enthalpy-entropy compensation plot for (a) CTAB in liquid and (b) (TTAB + CTAB) mixed system in binary compound medium

In the higher than equation, CMC values are in used in mole fraction unit. ln(CMC) versus T plot (Fig. 2) is obtained to be nonlinear. The plots are utilized to judge H^0_m and slopes are drawn at each studied temperature that's thought to be cherish to ∂ln(CMC) / ∂T [15, 25, 28].

In case of pure CTAB together with TTAB and CTAB mixtures, the G^0_m values are found to be negative. From the tables, it's obvious that the values of G^0_m for CTAB are achieved to be negative in absence yet as attending of TTAB indicating the micelles formation is spontaneous phenomena. By increasing of drug concentration within the mixtures of TTAB and CTAB, G^0_m is found to be bit by bit further negative. This signifies that within the mixed systems particle formation manifest itself simply alongside the method of micellization is a lot of spontaneous for drug-CTAB mixtures than CTAB alone. Attending of salt, the negative G0m values ar obtained to be further negative signifying favorable association phenomena, whereas in presence of NaCl/ KCl/ NH_4Cl, dynamic force for aggregation is significantly accumulated. The H^0_m values for TTAB + CTAB mixtures in solution are found to be positive at 298 K. However, in absence yet as attending of salt, at higher temperature, these values become negative and accumulated with increase in temperature. At all temperatures and their worth decreases with a rise of temperatures, the S^0_m values are found to be positive. The negative values of H^0_m and positive S^0_m values for TTAB-surfactant mixed systems signify that besides hydrophobic, static interactions conjointly participates an important role within the association of TTAB. At higher temperature, this happens by suggests that of wetter throughout formation of TTAB supported wetter micelles [34]. Within the gift study, the hydrophobic involvement reduces whereas the static interaction enhances by suggests that of the increase of temperature, keeping the negative values of G0m virtually constant at each temperature utilized. Similar behavior of H^0_m is additionally obtained for varied ionic surfactants earlier [35, 36]. Nusselder and Engberts [37] projected that it's the London-dispersion forces that ar responsible within the micellar progression for negative H values. The positive values of $H^0_{m,}$ at lower temperature are probably because of harm of structured water molecules within the region of hydrophobic parts viewing the importance of hydrophobic interactions within the development of particle formation. Within the case of each single well as mixed system, positive together with negative H values also are antecedently rumored [38–39].

Upon addition of salt within the answer at higher temperatures, the negative H^0_m values of (drug + CTAB) mixtures accumulated compared to the binary compound medium. This means that H contribution on the micellization of (drug + surfactant) mixtures is accumulated within the attending of salts as compared to in solution. At each studied in absence and incidence of salt, the worth of S^0_m for pure CTAB and TTAB + CTAB mixtures are obtained positive. The magnitude of the positive values of S^0_m for (TTAB+CTAB) mixed systems within the attending of salt is larger compared to binary compound system at the bottom temperature. By suggests that of enhance of the salts concentration, the positive values are obtained to be accumulated. The positive values of S^0_m are often explained by the rupturing of iceberg structures close the hydrophobic parts of wetter compound in the middle of the accumulated the randomness within the micelles core [40]. At higher temperature, the values of S^0_m become lower in presence of salt within the solution. At lower temperatures, the positive values of H^0_m are determined to be accumulated with the rise of the concentrations of salts. In presence of salts, the upper positive values of each S^0_m and H^0_m at lower temperatures are an honest indication of accumulated hydrophobic interactions between the hydrophobic chains of wetter and interaction

among the hydro-phobic chain of drug and CTAB. The upper negative values of H0m and comparatively lower positive S^0_m values at higher temperatures in presence of salts conjointly acknowledged those static interactions ar a lot of necessary in presence of salts compared to the salt-free answer. Besides temperatures, NaCl, KCl & NH4Cl destroy hydrophobic association of wetter monomers; so, in presence of salts abundant lower energy is required for aggregation. Within the mixed system of TTAB and CTAB in solution, the contribution of G^0_m reduces together with that of entropy enhance by suggests that of the increase of temperatures. In presence of salt within the answer follow the lot of or less similar trend with few exceptions. In presence of salt at totally different concentrations, the G^0_m.tr worth for TTAB + CTAB mixtures is obtained to be negative whereas, in solution and lower concentrations of salt, the G^0_m.tr worth is determined to be positive. The values of H^0_m.tr. and S^0_m.tr. for TTAB+CTAB mixtures in solution and attending of salts are obtained to be positive at lowest temperatures whereas the values are negative at higher temperatures. For the transport of salt and proteins from aqueous solution to a carbamide solution, the negative values of H0m.tr. also are accounted [41]. The negative worth of H0m.tr. acknowledged that the move of the hydrophilic portion of CTAB from solution to the TTAB (drug) yet as TTAB associate degreed salt mixtures is heat-releasing method whereas similar phenomena for the hydrophobic cluster is an heat-absorbing development. Both within the absence and also the attending of salts The Tc values for TTAB + CTAB mixture are obtained to be within the vary of 286–302 K. For the contribution of liquid within the supermolecule answer, the Tc values of associate degree system within the different of 270–300 K suggests that this method are often utilized as an indicative check [40]. Therefore, within the current system, the obtained values of Tc ar in fine conformity with the quality values of Tc for the biological fluid. A lot of negative values of H^0_m signify that the association of wetter, yet as drug-CTAB mixtures, are happens even at S^0_m = 0. The raise of the negative values of H^0_m discloses the upper stability of the micelles shaped within the solution. [44]

From all the system utilized in this study, we tend to acquire a linear line between the plots of H^0_m versus S^0_m with parametric statistic (R2) values within the different of 0.990–0.999 that is acquainted as entropy-enthalpy compensation. Similar behavior is additionally antecedently obtained by others researchers in solution [45]. The negative intercept is that the intrinsic H gain (H^0_m) and also the slope of the compensation plots is that the compensation temperature (Tc). The intercept H^0_m discloses the solute-solute interaction. It stands for associate degree index of the potency of the hydrophobic portion to contribute to the particle growth. The Tc values for TTAB + CTAB mixture each in absence and attending of salts are obtained to be within vary of 286–302 K. The Tc values of associate degree system within vary of 270–300 K suggests that this method is often utilized as an indicative check for the contribution of liquid within the supermolecule solution [43]. Therefore, the obtained values of Tc within the current system are in fine conformity with the quality values of Tc for the biological fluid. The negative values of H^0_m signify that the association of wetter, yet as drug-CTAB mixtures, are happens even at S^0_m = 0. The raise of the negative values of H^0_m discloses the upper stability of the micelles shaped within the solution.

4. CONCLUSION

In the absence and the group action of salts, the role of the variation of temperature and also the concentration of drug on the micellization development of cationic wetter CTAB is delineated during this study. At the various

temperature, the addition of drug decreases CMC price of pure wetter. Within the presence of salts, the decrease of the CMC of the mixture of CTAB with the drug is additionally ascertained. With gradual increase of the concentration of varied electrolytes supports the soundness of micelles, the rise of the values of counter particle binding (β). Molecular dynamics simulation disclosed the very fact that so salt setting promotes the particle formation of the surfactant-drug complicated compared to the no-salt setting. Within the totally different medium, the all values of G^0_m area unit found to be negative just in case of each studied system showing the formations of particle area unit spontaneous phenomena. At lower and better temperatures severally, the values of H0m and S^0_m values reveal that hydrophobic and static interactions area unit increased in presence of salts compared to those in absence of salts in water. The subsequent observations area unit obtained from molecular dynamics simulation: (1) salt promotes the particle formation; (2) particle adopts nearly spherical shape; (3) medication acts with the outer-sphere of the particle closed to the cationic head and (4) particle structure stays compressed over the simulation time.

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