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Investigating Aggregation and Interaction for Stearalkonium Chloride in Methanol at 301 K

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Abstract

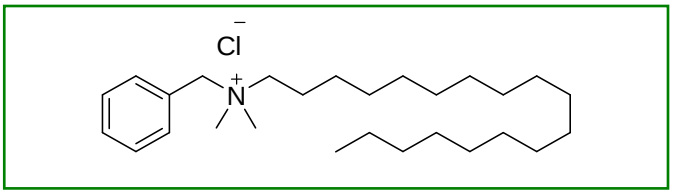
Density and viscosity measurements of Stearalkonium chloride (SAC) in methanol at different concentration show that there is marked change in aggregation at critical micellar concentration (CMC). The results obtained from density and viscosity methods have been satisfactorily explained by well-known equations with their parameters. Treatment of data obtained from density and viscosity measurement showed that there is significant interaction between SAC and methanol molecules in dilute solutions and SAC molecules do not aggregate appreciably below the CMC.

Keywords: Cationic surfactants; Ionic species; Critical micellar concentration

Abbreviations: CMC: Critical Micelle Concentration; η: Viscosity and ρ: Density; SAC: Stearalkonium Chloride; CPB: Tetra Decyltriphenyl Phosphonium Bromide; CAB: Tetra Decyltrimethyl Ammonium Bromide.

Introduction

Surfactants are main components of household detergents include laundry detergent, home cleansing supplies and personal toiletries. Physical properties of surfactants provide an introduction to the nature and emphasizing their ability to radically alter surface and interfacial properties and to self-associate and solubilize themselves in micelles. On the basis of charge of head groups, the surfactants are classified in four types - anionic, cationic, nonionic and amphoteric surfactants [1]. Cationic surfactants are dissolved in solvent with generating the surface active positive ions on hydrophilic part. These surfactants are widely used as disinfectant as preservatives, due to good bactericidal property e.g. Octadecylammoium chloride. Cationic surfactants are widely used for sterilization, corrosion inhibitors and mineral flotation [2]. Stearalkonium Chloride is classified as cationic surfactant. It is represented as:



Mehrotra et al. [3] reported the specific conductance of the dilute solutions increases with increasing concentration of CTAB, temperature and dielectric constant of the solvent. The plots of specific conductance

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v/s concentration for aqueous solutions are characterized by an intersection of two straight lines at a concentration which corresponds to the CMC. The molar conductance of aqueous and methanolic solution decreases with increasing concentration of CTAB.

Moulik et al. [4] Studied interfacial and bulk behaviors of binary and ternary combinations of tetra decyltrimethyl ammonium bromide (C_{14}TAB), tetra decyltriphenyl phosphonium bromide (C_{14}TPB), and tetra decylpyridinium bromide (C_{14}PB) by using tensiometry, conductometry, fluorimetry, and microcalorimetry and found that out of the three surfactants used in this study, C_{14}TPB alone produced two types of micelles, whereas both C_{14}TAB and C_{14}-PB produced one in aqueous solution. The mixed binary combinations C_{14}TAB-C_{14}TPB and C_{14}TPB-C_{14}PB in aqueous solution produced two kinds of micelles with two CMCs, whereas C_{14}TAB-C_{14}PB produced one type of micelle.

Many physical properties of surfactant solutions exhibit a characteristic transition over a narrow range of concentration. This transition is generally related to association of surfactant molecules arising from the intrinsic amphiphilic nature. The transition region could be used to determine the critical micellar concentration, CMC above which multi-molecular aggregates (micelles) are formed. Critical micellar concentration (CMC) is a measure of surfactants efficiency. A lower CMC indicates less surfactant is needed to saturate interfaces and form micelles. The forces which hold surfactant molecules together in micelles arise from weaker vander Waal's, hydrophobic, hydrogen-bonding and screened electrostatic interactions. Keeping in view the above points, present investigation has been taken with determination of densities and viscosities and its variation with stearalkonium chloride concentration at 301 K temperature. An attempt has been made to determination of intermolecular interactions between stearalkonium chloride & methanol; and critical micellar concentration (CMC) values from densities and viscosities data with help of some well known equations.

Materials and Methods

The cationic surfactant, Stearalkonium chloride (SAC) (CASNO- 122-19-0, Himedia Mumbai India) was used as received except dried in a vacuum desiccator. All glassware used to air sensitive experiment were oven-dried at least 1hrbefore use. Prior to use, the solutions of SAC in best solvent were prepared. Stearalkonium chloride has shown maximum solubility in methanol mixtures i.e., solution behaviour of SAC was carried out in this solvent system. The calculated amount of SAC was taken in standard flask and the solution was made up by adding the required amount of methanol. By this method, a number of solutions containing different concentration of SAC in methanol were prepared. The density and viscosity were measured to identify the solution behavior, molecular interactions at different concentrations. Ostwald's type viscometer was used for measuring the viscosity of the SAC in methanol at 301 K. The viscosities of the SAC solutions were calculated by using the equation.

$$\frac{\eta_1}{\eta_2} = \frac{\rho_1 t_1}{\rho_2 t_2} \text{ - - - - - - - - - - (1)}$$

Where η_1, η_2, ρ_1, ρ_2, t_1 and t_2 are the viscosity, density and flow time for known SAC solution and distilled water respectively. The densities were determined with the help of specific gravity bottle.

Results and Discussion

Density measurements

The densities (ρ) of Stearalkonium chloride (SAC) have been measured in methanol solvent with different concentration at temperature 301 K (Table 1). A plot between density (ρ) against SAC concentration (C) is characterized by an intersection of two straight lines at a definite SAC concentration (Figure 1). This concentration corresponds to critical micellar concentration (CMC) at which there is a sudden change in the aggregation of SAC molecules. The plot of density (ρ) against SAC concentration (C) is extrapolated to zero concentration and it was noticed that extrapolated value of density (ρ_0) is in agreement with the density of the methanol. SAC molecules do not show appreciable aggregation below the critical micellar concentration, CMC whereas at this definite concentration there is a marked change in the aggregation of SAC molecules. The density results of SAC have been explained in terms of Root's equation [5].

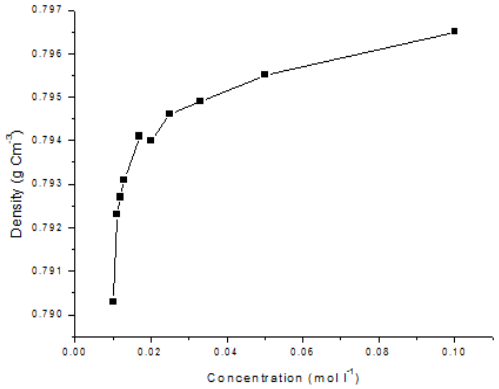

Figure 1: Density VS Concentrations.

S.N.	Concentration (mol l^{-1})	C^2 10^{-4}	$\sqrt{C}$	1/C	Density (ρ) g mol^{-1}	Viscosity (η) centipoise	$(\eta/\eta_0)^2$	$log\ (n/n_0)$	1/log (η/η_0)	$\eta_{sp}/C^{1/2}$	Specific viscosity (η_{sp})
1	0.01	1.00	0.1	100	0.7903	0.6783	1.0383	0.0081	123.4567	0.19	0.190
2	0.011	1.21	0.104	90.90	0.7923	0.6808	1.0461	0.0097	103.0927	0.2192	0.0228
3	0.012	1.44	0.109	83.33	0.7927	0.6887	1.0706	0.0148	67.5675	0.3183	0.0347
4	0.013	1.96	0.118	71.42	0.7931	0.6960	1.0932	0.0193	51.8134	0.3864	0.0456
5	0.017	2.89	0.130	58.82	0.7941	0.7042	1.1191	0.0244	40.9836	0.4453	0.0579
6	0.020	4.0	0.141	50	0.7940	0.7047	1.1208	0.0247	40.4858	0.4163	0.0587
7	0.025	6.25	0.158	40	0.7946	0.7223	1.1774	0.0354	28.2485	0.5386	0.0851
8	0.033	10.84	0.181	30.30	0.7949	0.7281	1.1966	0.0389	25.7069	0.5187	0.0939
9	0.050	25.0	0.225	20	0.7955	0.7447	1.2517	0.0487	20.5338	0.528	0.1188
10	0.10	100.0	0.318	10	0.7965	0.7812	1.3773	0.0695	14.3884	0.5493	0.1736

Table 1: Density, viscosity, specific viscosity other allied parameters of SAC in methanol at 301 K.

$$\rho = \rho_0 + AC - BC^{3/2} \quad -------- (2)$$

Where C is the concentration of the SAC solution; ρand ρ_0 are densities of the salt solutions and solvent, respectively. The constants A and B referred to SAC-solvent and SAC-SAC interactions, respectively. The values of constants A and B mention in Table 2 have been obtained from the intercept and slope of the plots of ρ-ρ_0 / C against $C^{1/2}$ below the CMC.

Viscosity measurements

The viscosities (η) of the solutions of SAC in methanol have been measured at temperature 301 K (Table 1). The viscosity (η) of the solutions of SAC increases with increasing concentration. The plot of viscosity against the SAC concentration (Figure 2) is characterized by an intersection of two straight lines corresponds to CMC of the SAC. The plots of viscosity v/s SAC concentration have been extrapolated to zero concentration. The extrapolated value of viscosity (η_0) is found to be in good agreement with the experimental value of viscosity of the methanol. The specific viscosity (η_{sp}) of SAC solutions in methanol increases with increasing the SAC concentration. The specific viscosity (η_{sp}) of SAC solution are characterized by an intersection of two straight lines at a definite SAC concentration which corresponds to the critical micellar concentration, CMC and the values so obtained is observed to be in good agreement with the value obtained from the plot of viscosity v/s SAC concentration.

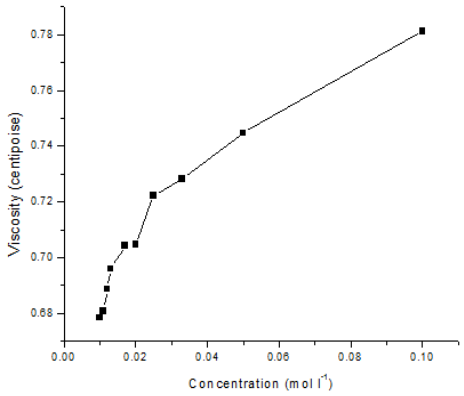

Figure 2: Viscosity VS Concentrations.

The viscosity results of SAC in methanol can be explained by the following equations.

Einstein [6], $\eta_{sp=} 2.5\overline{V}C \quad -------- (3)$

Vand [7], $\frac{1}{C} = (\frac{0.921}{\overline{V}})^{-1} \frac{1}{\log(\frac{\eta}{\eta_o})} + \emptyset\overline{V} \quad -------- (4)$

Moulik [8], $(\frac{\eta}{\eta_o})^2 = M + KC^2 \quad -------- (5)$

Jones-Dole [9], $\frac{\eta_{sp}}{C^{1/2}} = A + BC^{1/2} \quad -------- (6)$

Where $\bar{V}$, C, ϕ, η, η_0 and η_{sp} are molar volume of the SAC (liter mole^{-1}), concentration of salt (mole l^{-1}), interaction coefficient, viscosity of SAC solution, viscosity of methanol and specific viscosity, respectively. M and K' are Moulik's constants. The constant A and B of Jones Dole's equation signify the SAC-SAC and SAC-solvent interactions respectively shown in Table 2. The values of molar volume ($\bar{V}$) and interaction coefficient (ϕ) obtained from Einstein's and Vand's type plots are summarized in Table 2. The values of constant A (SAC-SAC interactions) and B (salt-solvent interactions) for SAC have been calculated from the intercept and slope of the Jones-Dole plot below the CMC are mentioned in Table 2. The result obtained from Jones dole equation indicates that the values of constant B is higher than constant A indicating the existence of strong SAC-solvent interactions.

Technique	Physical constants	Values obtained
Density	CMC (mol l^{-1}) (From the plots of ρ versus C)	0.01797
	Constant A (Root's Equation)	0.8
	Constant B (Root's Equation)	-13.33
Viscosity	CMC (mole l^{-1}) (From the plot η versis C)	0.01850
	Molar volume ($\bar{V}$) l mol^{-1} (Vand's Equation)	1.244
	Interaction coefficient (ϕ) (Vand's Equation)	7
	M (Moulik equation)	1.021
	K ′ x 10^2 (Moulik equation)	61.53
	$\bar{V}$ (Enistein equation)	2.00
	Constant A (Jones-Dole equation)	0.10
	Constant B (Jones-Dole equation)	6.72

Table 2: Various physical constants calculated from different techniques for Stearalkonium Chloride solution at 301 K.

The values of Moulik's constants, M and K' for SAC shown in Table 2 have been calculated from the intercept and slope of the plots between $(\eta/\eta_0)^2$ and C^2. The plot of $(\eta/\eta_0)^2$ vs C^2 is linear below the CMC which indicate that the Moulik's equation is applicable to the dilute solutions of SAC in methanol. It is, therefore, concluded that the equations of Einstein, Vand, Moulik and Jones-Dole have a similar probability of fitting the experimental data of SAC in methanol. The results of viscosity of SAC indicate that there is a marked change in the aggregation of the cationic species at the critical micellar concentration (CMC). The values of various constants calculated from above cited well known equations indicate that there is a significant interaction between SAC and solvent molecule. These results are in good agreement with literature [10,11].

Conclusion

A comprehensive study of cationic surfactant; Stearalkonium chloride (SAC) in organic solvent (methanol) has been carried out. The density (ρ) of SAC solutions increases with increase in concentration. The viscosity results of SAC in methanol have been satisfactorily explained in the light of Einstein, Vand, Moulik and Jones-Dole equations. It is concluded from results obtained that the equations of Einstein, Vand, Moulik and Jones-Dole have a similar probability of fitting the experimental data of SAC in methanol solutions at different concentration. The results of viscosity indicate that there is a marked change in the aggregation of the cationic species at the CMC. The values of various constants calculated from above cited well known equations indicate that there is a significant interaction between SAC and solvent molecules. The results of density, viscosity, measurements indicate that there is a marked change in aggregation of the ionic species at the critical micelle concentration (CMC). The value of CMC obtained is found to be very close to each other. The values of various constants obtained from some well-known equations indicate that there is a significant interaction between SAC and solvent molecules.

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References

1. Holmberg K, Joensson B, Kronberg B, Lindman B (2002) Surfactants solution and polymers in aqueous solution. (2nd edn), John Wiley & Sons Ltd 22: 194-214.

2. Yuan CL, Xu ZZ, Fan MX, Liu HY, Xie YH, et al. (2014) Study on characteristics and harm of surfactants. J. chem. Pharm Res 6(7): 2233-2237.

3. Mehrotra KN, Upadhyaya SK, Gahlaut AS, Sharma M (1989) Conductometric Studies on Cetyl-trimethyl-ammoniumbromide. J Electrochem Soc India 23(38): 195-197.

4. Moulik S, Ray G, Chakraborty I, Ghosh S (2007) Studies on Binary and Ternary Amphiphile Combinations of Tetradecyltrimethylammonium Bromide (C_{14}TAB), Tetradecyl triphenyl phosphonium Bromide (C_{14}TPB) and Tetradecylpyridinium Bromide (C_{14}PB). A Critical

Analysis of their Interfacial and Bulk Behaviors. J Phys Chem B 111(3): 9828-9837.

5. Roots WC (1933) An Equation Relating Density and Concentration. J Am Chem Soc 55(2): 850-851.

6. Einstein A (1906) Eineneue Bestimmung der Molekül dimensionen. Ann Phys 19: 289-306.

7. Vand V (1948) Viscosity of solutions and suspensions. I Theory. J Phys Chem 52(2): 277-299.

8. Moulik S P (1968) Proposed viscosity-concentration equation beyond Einsteins region. J Phys Chem 72(13): 4682-4684.

9. Jones G, Dole M (1929) The viscosity of aqueous solutions of strong electrolytes with special reference to barium chloride. J Am Chem Soc 51(10): 2950-2964.

10. Upadhyaya SK, AnuShri Gupta, Kishore K (2013) Acoustical behavior of Cerium & Thorium palmitate in non-aqueous binary mixture. Asian J of Adv Basic Sci 1(1): 19-25.

11. Singh C, Upadhyaya SK, Kishore K (2018) Conductometric and viscometric studies on magnesium caprylate and laurate. Asian J of Adv Basic Sci 6(1): 54- 57.