

Electronic supplementary information for Soft Matter manuscript

Tetraalkylammonium ion induced micelle-to-vesicle transition in aqueous sodium dioctylsulfosuccinate solution

U. Thapa[†] J. Dey,[†] Sugam Kumar,[‡] P. A. Hassan,[§] V. K. Aswal,[‡] and K. Ismail^{*†}

[†] Department of Chemistry, North-Eastern Hill University, Shillong – 793022, India

[§] Chemistry Division, Bhabha Atomic Research Center, Trombay, Mumbai – 400085, India

[‡] Solid State Physics Division, Bhabha Atomic Research Center, Trombay, Mumbai – 400085, India

Address for Manuscript Correspondence: Prof. K. Ismail, Department of Chemistry, North-Eastern Hill University, NEHU Campus, Shillong - 793022, India. E-mail: kismail@nehu.ac.in; kinehu@hotmail.com, Telephone: 91-364 – 2722610, Fax: 91-364 – 2550486

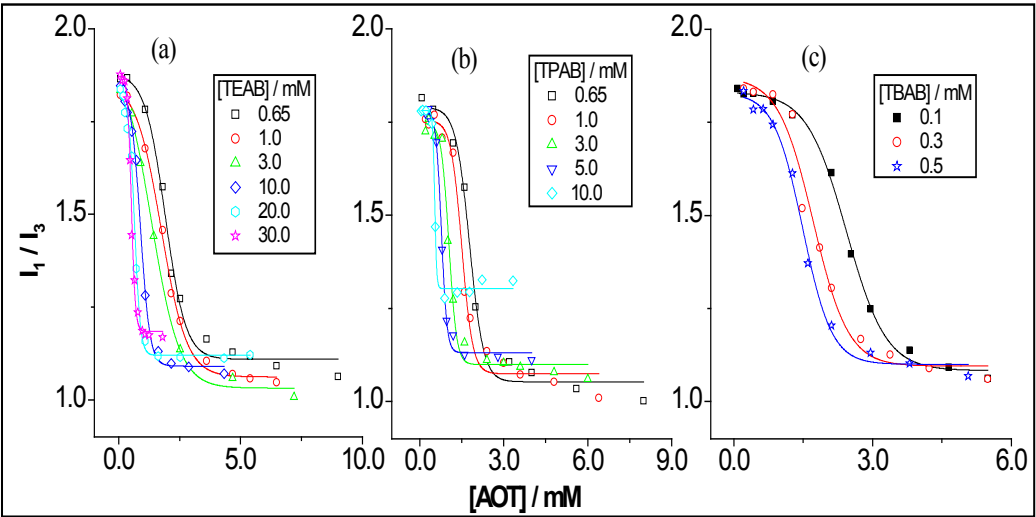


Fig. S1. Variation of I_1/I_3 of pyrene with AOT concentration in aqueous medium in the presence of TAAB. (a) TEAB, (b) TPAB, (c) TBAB.

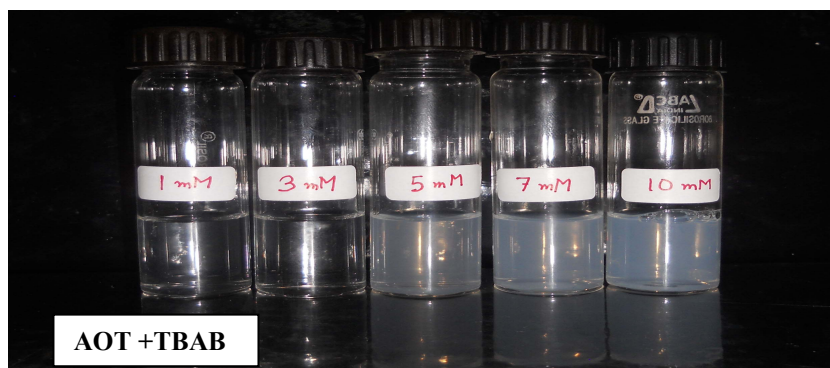
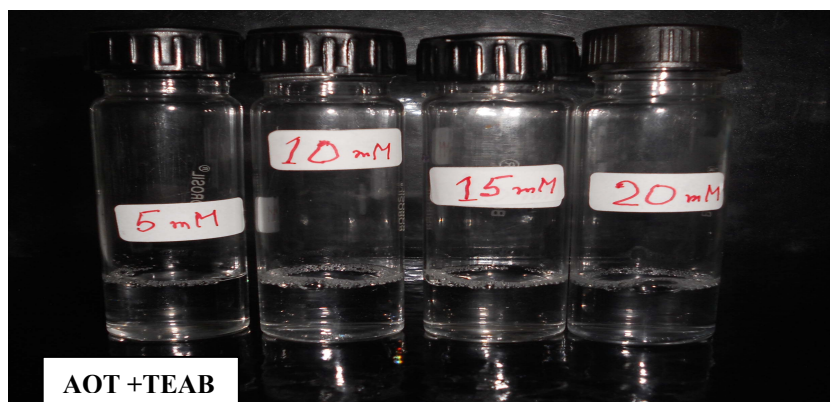


Fig. S2. Images of aqueous AOT (15 mM) + TAAB solutions as a function of TAAB amount at 25 ± 1 °C.

Table S1. Values of cmc of AOT in aqueous TAAB solutions at 25 °C obtained from surface tension data.

Salt	Salt Conc. / mmol kg ⁻¹	Cmc / mmol kg ⁻¹	Salt Conc. / mmol kg ⁻¹	Cmc / mmol kg ⁻¹
TEAB	0.65	2.50	10.0	1.10
	1.0	2.29	20.0	0.75
	3.0	1.88	30.0	0.56
	5.0	1.62	50.0	0.45
TPAB	0.65	2.01	10.0	0.50
	1.0	1.81	20.0	0.34
	3.0	1.39	30.0	0.25
	5.0	0.96	50.0	0.20
TBAB	0.1	2.30	1.0	0.70
	0.3	1.86	3.0	0.26
	0.5	1.60	5.2	0.17
	0.65	1.15		

Table S2. Values of the fitted parameters of the sigmoid equation^{a)} for I_1/I_3 data of pyrene in aqueous solutions of AOT + TAAB at 25 °C.

Salt	Salt conc. / mmol kg ⁻¹	A ₁	A ₂	10 ³ x ₀ / mol kg ⁻¹	10 ³ b/ mol kg ⁻¹
TEAB	0.65	1.8807	1.1091	1.91	0.42
	1.0	1.8586	1.0617	1.74	0.53
	3.0	1.8387	1.0651	1.88	0.25
	10.0	1.8422	1.0906	0.89	0.19
	20.0	1.8203	1.1197	0.65	0.12
	30.0	1.8826	1.1841	0.52	0.08
TPAB	0.65	1.7898	1.0530	1.78	0.25
	1.00	1.7550	1.0743	1.50	0.19
	3.0	1.7473	1.0991	1.04	0.14
	5.0	1.7800	1.1310	0.77	0.10
	10.0	1.7807	1.3030	0.53	0.04
TBAB	0.1	1.8321	1.0831	2.43	0.43
	0.3	1.8714	1.0953	1.72	0.37
	0.5	1.8290	1.1006	1.49	0.31

^{a)} $I_1/I_3 = A_2 + \{(A_1 - A_2)/[1 + \exp((c_s - x_0)/b)]\}$, where c_s is AOT concentration, x_0 is the value of c_s corresponding to the centre of the sigmoid, A_1 and A_2 are the upper and lower limits of the sigmoid, respectively, and b is a term that reflects the range of c_s where sudden change in I_1/I_3 occurs. The value of x_0 is taken as equal to cmc.

SANS data analysis.

For monodispersed particles in a medium the differential scattering cross section per unit volume is presented by the following expression^{R1-R3}

$$d\Sigma / d\Omega = nF(Q)S(Q) + B \quad (S1)$$

where n is the number density of the particles, $F(Q)$ is the single particle form factor and depends on the shape and size of the particles. $S(Q)$ is the structure factor and is decided by the spatial distribution of the particles thereby giving information about the inter-particle interaction. B is a constant term accounting for the incoherent scattering background that occurs in the case of neutrons mainly due to the presence of hydrogen in the sample. The relevant equations of the form factors of different shapes are given below:

The form factor equations used for prolate-ellipsoidal micelles are

$$F(Q) = \frac{16\pi^2}{9} (\rho_p - \rho_s)^2 (ab^2)^2 \int_0^1 [f(Q, \mu)]^2 d\mu \quad (S2)$$

$$f(Q, \mu) = 3(\sin x - x \cos x)/x^3 \quad (S3)$$

$$x = Q[a^2\mu^2 + b^2(1 - \mu^2)]^{1/2} \quad (S4)$$

where ρ_p and ρ_s are the scattering length densities of particle (micelle) and solvent, respectively. a and b are the semi-major and semi-minor axes of the ellipsoid, respectively. The term μ in the above equations refers to the cosine of the angle between the directions of a and Q .

For vesicles having inner radius R and thickness dR , the form factor equation is

$$F(Q) = \frac{16\pi^2}{9} (\rho_p - \rho_s)^2 \left[(R + dR)^3 \frac{\sin(Q(R + dR)) - Q(R + dR) \cos(Q(R + dR))}{Q^3 (R + dR)^3} - R^3 \frac{\sin(QR) - QR \cos(QR)}{Q^3 R^3} \right]^2 \quad (S5)$$

For a rod-like structure of radius R and length $2l$, equation for $F(Q)$ is

$$F(Q) = \frac{(\pi R^2 l)^2 (\rho_p - \rho_s)^2}{2} \int_0^{\pi/2} \frac{\sin^2(Ql \cos \beta)}{(Ql \cos \beta)^2} \frac{4J_1^2(QR \sin \beta)}{(QR \sin \beta)^2} \sin \beta \, d\beta \quad (S6)$$

where J_1 is the Bessel function of order unity and β is the angle between the axis of the cylinder and bisectrix.

The expression for $S(Q)$ is given by the Fourier transform of the radial distribution function $g(r)$. $g(r)$ gives the probability of finding the centre of another micelle at a distance r from the centre of a reference micelle. $S(Q)$ is calculated using the analysis as developed by Hayter and Penfold under mean spherical approximation.^{R4} In this approximation, the micelle is treated as a rigid equivalent sphere of diameter $d = 2(ab^2)^{1/3}$ interacting with another micelle through a screened coulomb potential $u(r)$ given by the relation

$$u(r) = u_0 d \exp[-\kappa(r - d)]/r \quad r > d \quad (S7)$$

where u_0 is the potential at $r = d$ and the Debye-Hückel inverse screening length κ is evaluated by using the expression

$$\kappa = \left(\frac{8\pi N_A e^2 I}{10^3 \epsilon k_B T} \right)^{1/2} \quad (S8)$$

In eqn (S8), N_A , e , ϵ , k_B and T denote Avogadro number, electronic charge, dielectric constant of the solvent, Boltzmann constant and absolute temperature, respectively.

References

- R1. S. H. Chen, E. Y. Sheu, J. Kalus and H. Hoffmann, *J. Appl. Crystallogr.*, 1988, **21**, 751.
- R2. J. S. Pedersen, *Adv. Colloid Interface Sci.*, 1997, **70**, 171.
- R3. J. B. Hayter and J. Penfold, *Colloid Polymer. Sci.*, 1983, **261**, 1022.
- R4. J. B. Hayter and J. Penfold, *Mol. Phys.* 1981, **42**, 109.