

Micellization and Related Behavior of Sodium Dodecylsulfate in Mixed Binary Solvent Media of Tetrahydrofuran (Tf) and Formamide (Fa) with Water: A Detailed Physicochemical Investigation

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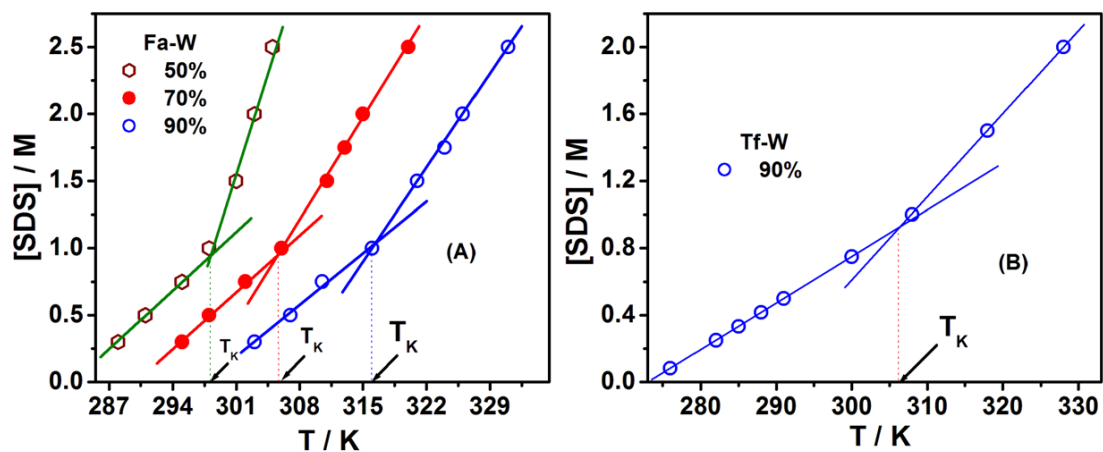


Figure S1: Temperature solubility diagram of SDS in (A) Fa-W and (B) Tf-W medium.

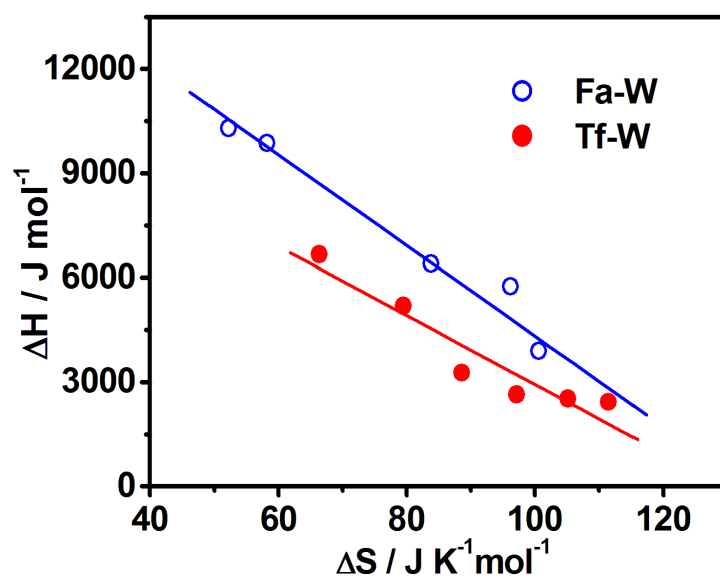


Figure S2: Enthalpy-entropy compensation plots for the micellization of SDS in Tf-W and Fa-W mixed media. The plots are least squared.

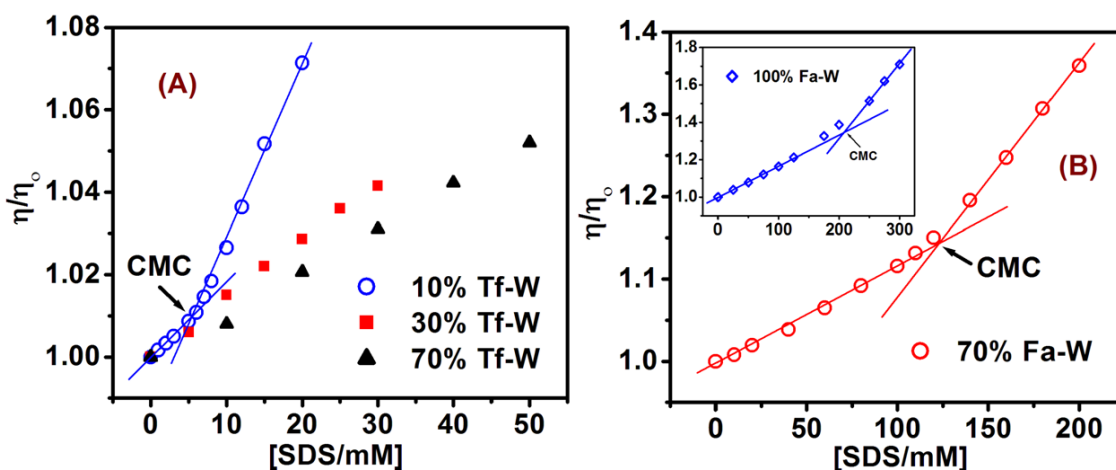


Figure S3: Relative viscosity of SDS solution in Tf-W and Fa-W mixed solvent media at 303 K., (A): 10, 30 and 70 vol% of Tf and (B): 70 v% of Fa in main plot, (Inset): 100 v% Fa.

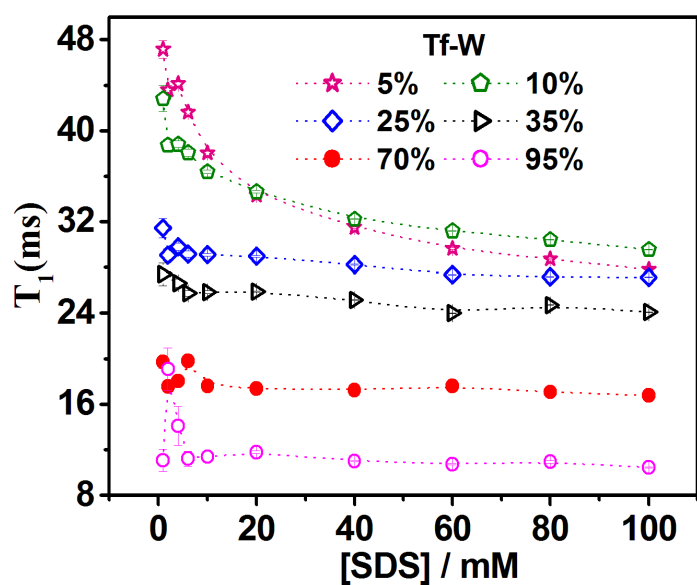


Figure S4: ^{23}Na relaxation (T_1) vs $[SDS]$ in different Tf-D₂O (5, 10, 25, 35, 70 and 95 v%) mixed systems.

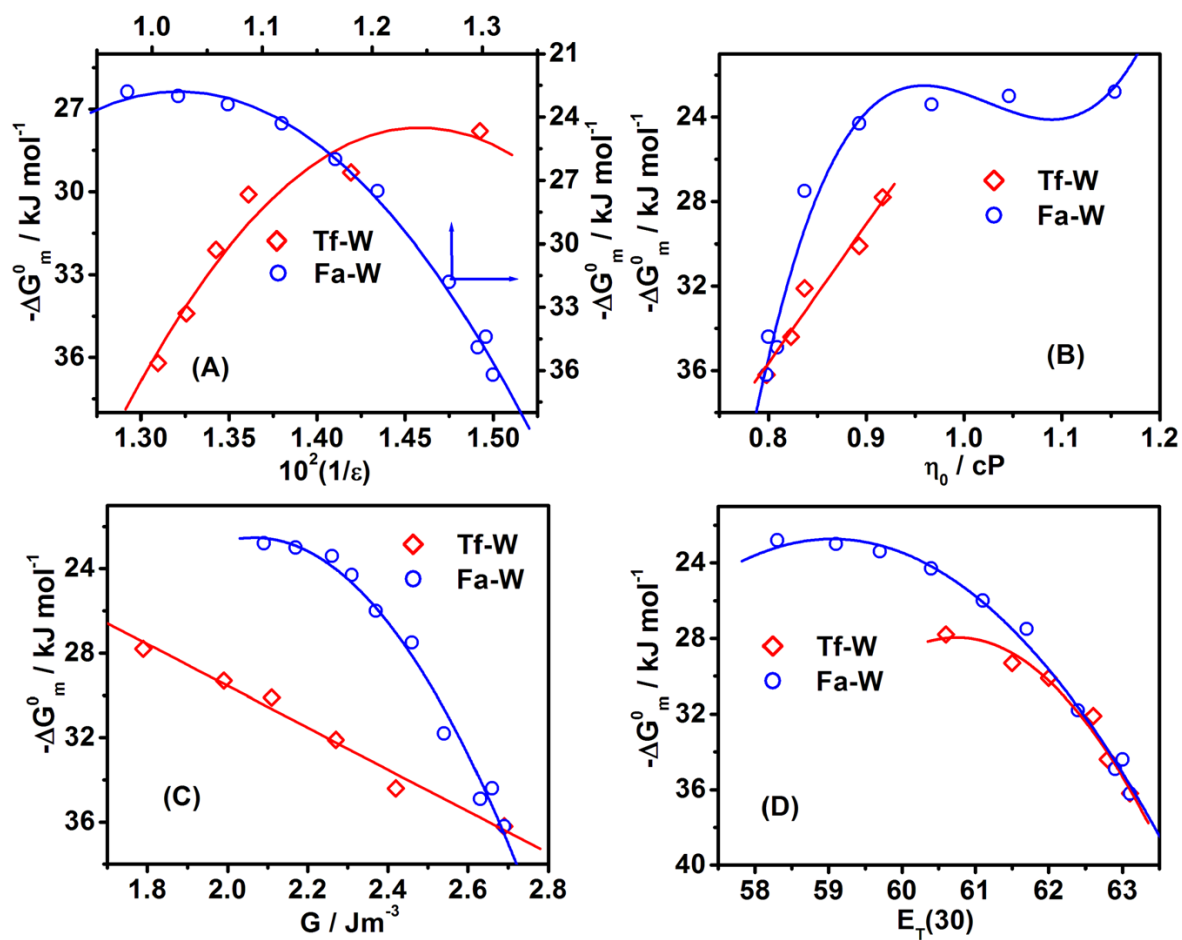


Figure S5: Free energy of micellization (ΔG_m^0) vs solvent parameters in different Tf-W and Fa-W mixed solvent media at 303 K. **(A):** Dependence on $1/\epsilon$; **(B):** Dependence on η_0 ; **(C):** Dependence on G ; **(D):** Dependence on $E_T(30)$.

Text S1: All the thermodynamic calculations were done in the rational scale. The rational activity coefficient, f_{\pm}' for electrolyte in mixed solvent is defined by the following relation;

$$\ln f_{\pm}' = \ln f_{\pm} + \frac{n}{\nu} \ln a_w + \ln \frac{S+T+\nu-n}{S+T+\nu}$$

Where, n = Solvation number, here taken as 6 for SDS molecule

ν = Number of ionic species formed in solution, here $\nu = 2$

a_w = Mole fraction of water of the mixed solvent

S = Mole of water, and T = Mole of the other liquid

The required $\ln f_{\pm}$ has been obtained from the Debye-Hückel equation modified by

Guggenheim: $\left(\log f_{\pm} = -\frac{A|Z_+Z_-|\sqrt{I}}{1+\sqrt{I}} + bI \right)$, where $A = (1.8246 \times 10^6) / (\epsilon T)^{3/2} \text{ mol}^{-1/2} \text{ L}^{1/2} \text{ K}^{3/2}$,

Z_+ and Z_- are the ionic charges of Na^+ and DS^- , respectively, I is the ionic strength of the solution and b is an adjustable parameters taken as $0.1|Z_+Z_-|$ according to Davies.

(Reference: Robinson, R. A. and Stokes, R. H. *Electrolyte Solutions*, Butterworths Scientific Publications: London, 1955. pp – 229-230; 251-252)

Table S1: Various physicochemical parameters of the mixed solvents (Tf-W and Fa-W) media at 303 K.^a

Solvent composition (V %)	Dielectric constant ^a (ϵ)		Reichardt's parameter ($E_{T30} / \text{kcal mol}^{-1}$)		Gordon parameter ^b (G / Jm^{-3})		Viscosity (η_o / cp)	
	W / Tf	W / Fa	W / Tf	W / Fa	W / Tf	W / Fa	W / Tf	W / Fa
0	76.36	76.36	63.1	63.1	2.69	2.69	0.798	0.798
1	75.43	76.74	62.8	63.0	2.42	2.66	0.823	0.800
2	74.48	-	62.6	-	2.27	-	0.837	-
3	-	77.17	-	62.9	-	2.63	-	0.809
4	73.47	-	62.0	-	2.09	-	0.893	-
5	-	77.59	-	62.7	-	2.59	-	0.818
6	70.46	-	61.5	-	1.99	-	0.917	-
10	67.01	78.74	60.6	62.4	1.79	2.54	1.002	0.837
15	63.56	-	-	-	1.65	-	-	-
20	59.39	82.98	58.1	61.7	1.47	2.46	1.220	0.893
30	55.09	85.73	55.7	61.1	1.25	2.37	1.383	0.967
40	47.84	89.44	53.1	60.4	1.18	-	1.474	1.046
50	39.08	93.57	51.1	59.7	1.05	2.26	1.524	1.154
60	30.62	97.69	-	59.1	0.98	2.17	1.339	1.291
70	23.63	102.28	45.7	58.3	0.91	2.09	1.144	1.473
80	17.67	105.16	-	57.5	0.85	1.98	0.885	1.739
90	9.84	-	40.1	56.6	0.79	-	0.649	2.147
100	7.27	107.97	37.4	55.4	0.67	1.71	0.454	2.846

^a Dielectric constant values of solvent mixtures are obtained from literature.¹²

^bThe Gordon parameter was calculated from the relation $G = \gamma/\bar{V}_m^{1/3}$ (\bar{V}_m is the molar volume of the mixed solvents). $\bar{V}_m = \sum X_i V_{m,i}$, where X_i and $V_{m,i}$ represent mole fraction and molar volume of i th solvent, respectively.