Supplementary Information

The spontaneous vesicle–micelle transition in a catanionic surfactant system: A chemical trapping study

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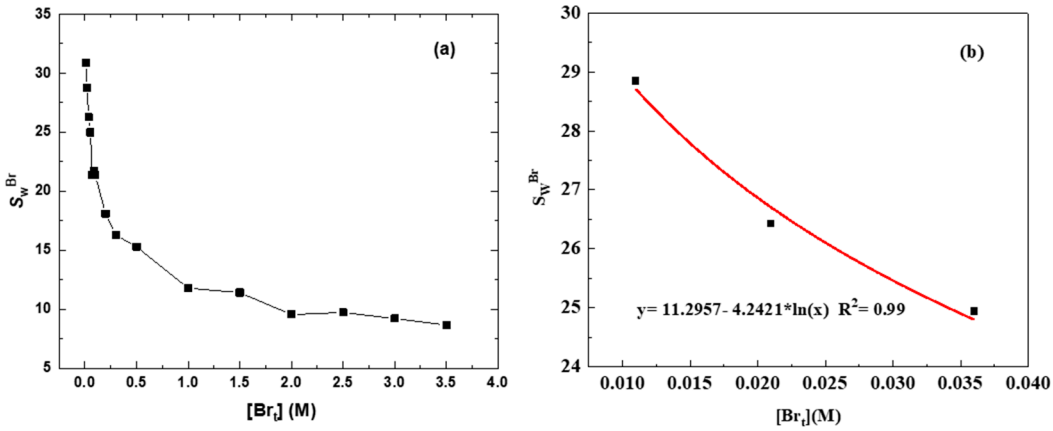
Section Ⅰ: Chemical trapping with 1-ArN_2^+ in aqueous TMABr solutions.

Figure S1 shows the plot of the selectivity between bromide ion and water, S_w^{Br} versus [Br_t] in TMABr aqueous solutions. The data was also fitted into Equation S1, which was used to estimate the selectivity, S_w^{Br}, at the interfacial region.

$$S_W^{Br} = 11.2957 - 4.2421 \times \ln([Br_t]) \quad \text{(S1)}$$

Figure S1 Plot between S_w^{Br} and [Br_t], in TMABr aqueous solutions ([HBr] = 1 mM) (a) containing 0 to 3.5 M [Br_t] ; and (b) containing 0.01 to 0.04 M [Br_t] fitted to equation $S_W^{Br} = 11.2957 - 4.2421 \times \ln([Br_t])$.



Section II Equations for calculations of chemical trapping product yields and interfacial molarities

Table S1. Calibration curves for observed product yields

Products	Calibration curves	R^2	Retention time（min）
16-ArOH	y= 1.000 × 10^8x + 77.138	0.9995	13.5
16-ArBr	y= 2.000 × 10^8x – 160.74	0.9994	30
16-ArOSOct	y= 1.459 × 10^8x	1	22

The normalized product yields were calculated by **Equation S2-S4**:

$$\%\text{16-ArOH}_N = 100 \times \frac{\%\text{16-ArOH}}{\%\text{16-ArOH}+\%\text{16-ArOSOct}+\%\text{16-ArBr}} \quad \text{(S2)}$$

$$\%\text{16-ArBr}_N = 100 \times \frac{\%\text{16-ArBr}}{\%\text{16-ArOH}+\%\text{16-ArOSOct}+\%\text{16-ArBr}} \quad \text{(S3)}$$

$$\%\text{16-ArOSOct}_N = 100 \times \frac{\%\text{16-ArOSOct}}{\%\text{16-ArOH}+\%\text{16-ArOSOct}+\%\text{16-ArBr}} \quad \text{(S4)}$$

Equations S1 and S5-S6 were employed for interfacial molarity calculation [1]:

$$\%\text{16-ArOSOct}_N = 9.036\,[SO_{3m}] - 0.103 \quad \text{(S5)}$$

$$\%16\text{-ArOH}_N = 0.914\,[H_2O_m] + 49.72 \quad (S6)$$

Section III: Interfacial molarities

Table S2 Estimated values of interfacial molarities of Br_m, H_2O_m, and SO_{3m}, in aqueous solutions of 20 – 500 mM CTAB/SOS solutions at 25ºC. [HBr] = 1 mM.

[CTAB]+[SOS]	Normalized yields (%)			Interfacial molarities(M)		
(mM)	16-$ArOH_N$	16-$ArOSOct_N$	16-$ArBr_N$	H_2O_m	SO_{3m}	Br_m
20	80.9	17.1	2.1	34.08	1.90	0.05
50	80.2	17.3	2.5	33.39	1.92	0.06
80	79.2	18.4	2.4	32.27	2.05	0.06
100	78.4	19.3	2.4	31.33	2.14	0.06
200	76.8	20.6	2.6	29.63	2.29	0.06
500	74.0	22.9	3.1	26.57	2.55	0.08

Table S3 Estimated values of interfacial molarities of Br_m, H_2O_m, and SO_{3m}, in aqueous solutions of 200 – 500 mM NaBr/SOS solutions at 25ºC. [HBr] = 1 mM.

[NaBr]+[SOS]	Normalized yields (%)			Interfacial molarities(M)		
(mM)	16-$ArOH_N$	16-$ArOSOct_N$	16-$ArBr_N$	H_2O_m	SO_{3m}	Br_m
200	85.3	12.1	2.5	38.95	1.36	0.06
300	85.7	11.6	2.7	39.41	1.29	0.06
400	84.4	12.7	2.9	37.92	1.42	0.07
500	85.7	11.4	2.9	39.34	1.28	0.07

Reference

[1] C. Liu, Y. Wang, Y. Gao, Y. Zhang, L. Zhao, B. Xu, L.S. Romsted, Effects of interfacial specific cations and water molarities on AOT micelle-to-vesicle transitions by chemical trapping: the specific ion-pair/hydration model, Phys. Chem. Chem. Phys., 21 (2019) 8633-8644.