

Supplementary Information to

Contrasting effect of 1-butanol and 1, 4-butanediol on the triggered micellar self-assemblies of C₁₆-type cationic surfactants

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Table S1. Interfacial descriptors for surfactants in H₂O and 1M (*fix*) BuOH and BTB at 303.15 K.

Surfactant	Solvent	CMC (mM)	γ_{CMC} (mN/m)	π_{CMC} (mN/m)	Γ_{max} ($\times 10^{-6}$ mol m ⁻²)	A_{min} (\AA^2)
CPB	H ₂ O	0.790	38.5	32.0	2.04	81.3
	1M BTB	0.279	44.0	26.5	1.19	139.8
	1M BuOH	0.013	27.1	43.4	0.79	804.9
CTPPB	H ₂ O	0.376	44.2	26.3	0.73	229.1
	1M BTB	0.052	44.3	26.2	0.62	266.6
	1M BuOH	0.008	25.0	45.5	0.17	952.7
CTAT	H ₂ O	0.327	37.4	33.1	2.65	62.7
	1M BTB	0.029	52.2	18.3	0.34	494.7
	1M BuOH	0.018	28.6	42.0	0.21	776.2

Table S2. Quantum chemical parameters obtained for cationic surfactant-alcohol templates.

System	TE (a.u.)	E_{HOMO} (eV)	E_{LUMO} (eV)	ΔE (eV)
BTB	-0.1655	-0.3858	0.0875	0.4733
BuOH	-0.1033	-0.3817	0.0975	0.4792
CPB	0.0832	-0.3007	-0.1186	0.1821
CPB + BTB	-0.2628	-0.2917	-0.0469	0.2448
CPB + BuOH	-0.2126	-0.2892	-0.0437	0.2455
CTPPB	-0.0379	-0.2644	-0.0187	0.2457
CTPPB + BTB	-0.2362	-0.2893	-0.0166	0.2727
CTPPB + BuOH	-0.1617	-0.2783	-0.0160	0.2623
CTAT	-0.2777	-0.3425	0.0084	0.3509
CTAT + BTB	-0.4719	-0.3441	0.0115	0.3556
CTAT + BuOH	-0.3960	-0.3433	0.0154	0.3587