

Supporting Material

Generic nature of interfacial phenomena in solutions of nonionic hydrotropes

Andrei A. Novikov,^{*,†} Anton P. Semenov,[†] Alexandra A. Kuchierskaya,[†] Dmitry S. Kopitsyn,[†] Vladimir A. Vinokurov,[†] and Mikhail A. Anisimov^{*,‡}

[†] *Gubkin University, Moscow, 119991, Russia*

[‡] *Department of Chemical and Biomolecular Engineering, University of Maryland, College Park, MD 20742, USA*

*Email: novikov.a@gubkin.ru, anisimov@umd.edu



Figure S1 – Custom-made jacketed cell for sample preparation. Red dots inside the jacket serve as graduation marks. The circulating water bath connects by hose barbs.

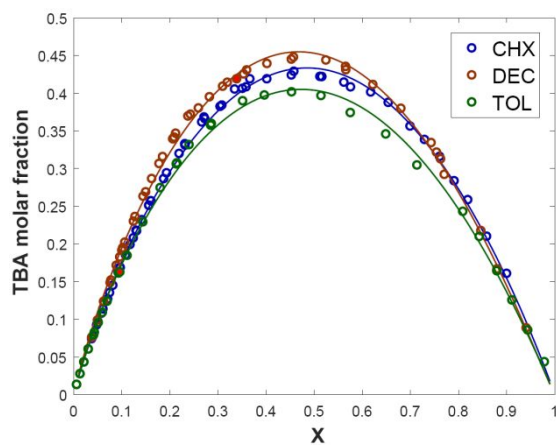


Figure S2 – Separation curves at +20 °C approximated by Hlavaty equation (Eq.1 in main manuscript)

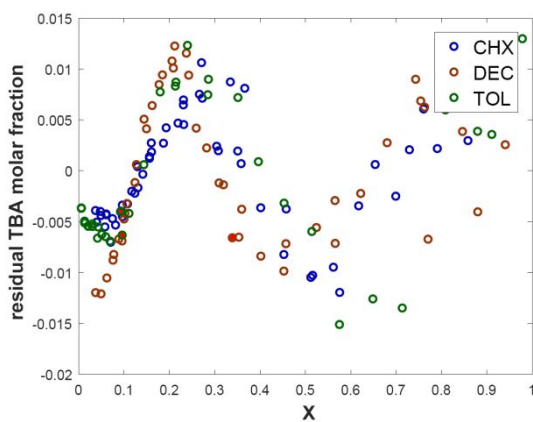


Figure S3 – Residuals for the approximation of the separation curves at +20 °C by Hlavaty equation

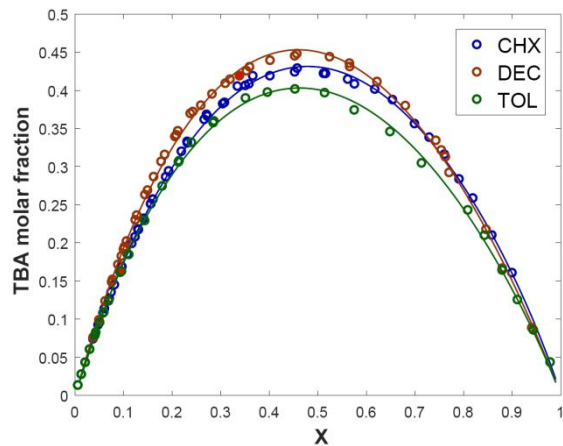


Figure S4 – Separation curves at +20 °C approximated by Letcher equation

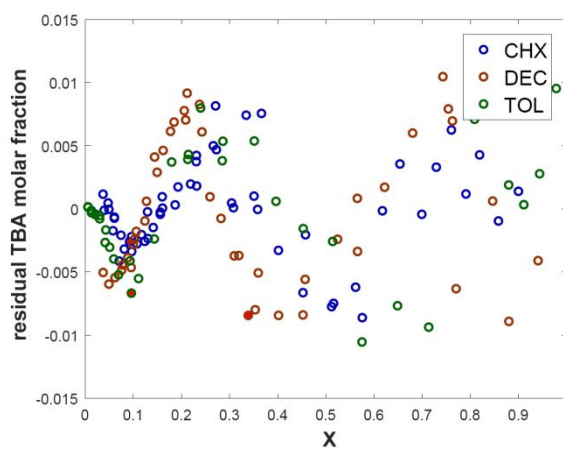


Figure S5 – Residuals for the approximation of the separation curves at +20 °C by Letcher equation

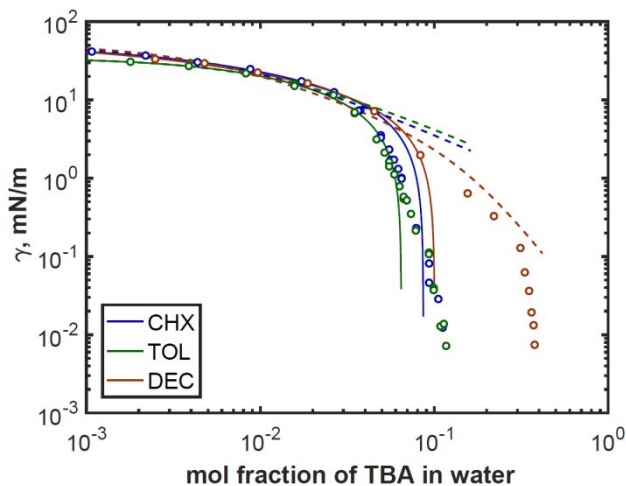


Figure S6 – Interfacial tensions for H₂O-TBA-OIL systems: OIL=cyclohexane (blue), OIL=toluene (green), OIL=*n*-decane (brown); circles – experimental data, solid lines – Langmuir isotherms, dashed lines – asymptotic functions ψ_1 for H₂O-TBA-OIL systems.

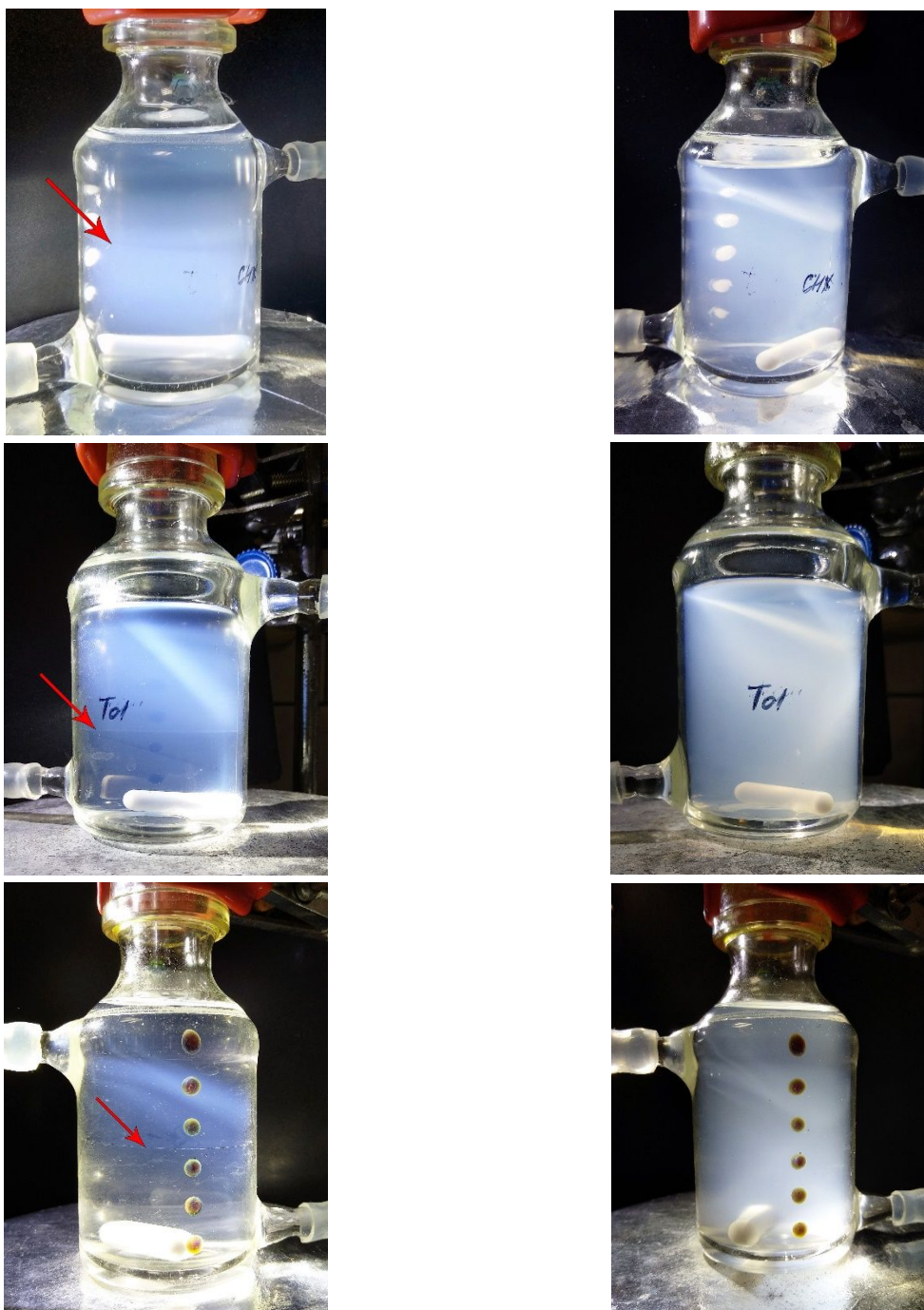


Figure S7 – Near-critical samples at the titration step when complete miscibility is achieved. Red arrows indicate the liquid-liquid interface.

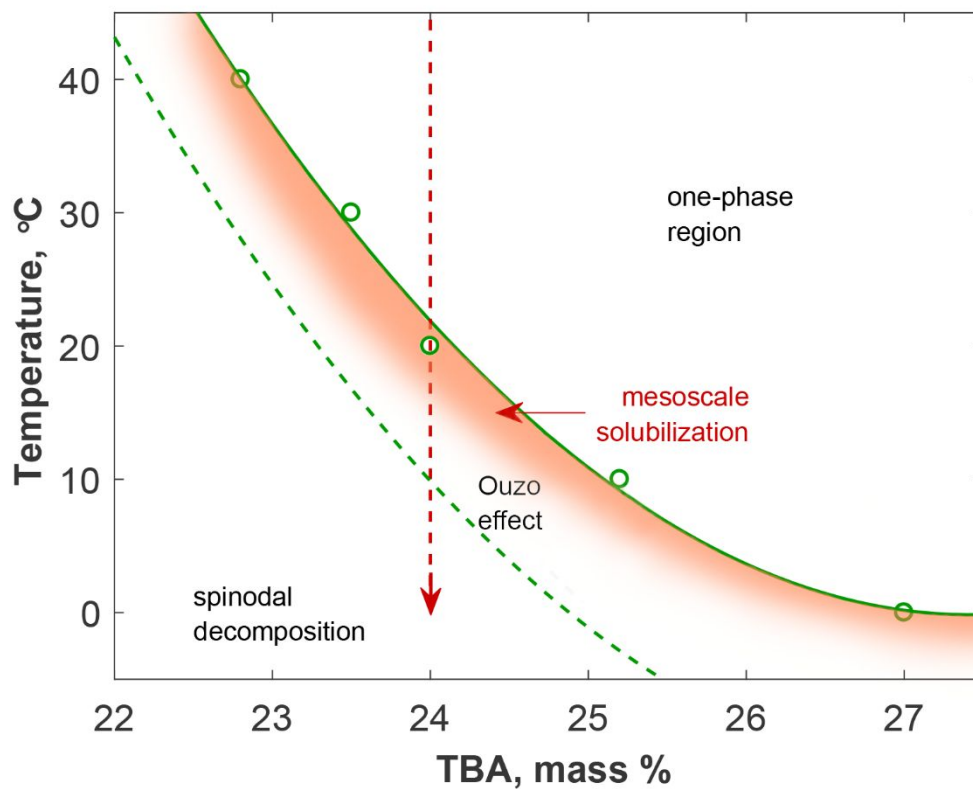


Figure S8 – Separation boundary at 0.4 mass % of CHX as function of TBA mass fraction. Solid green line – binodal curve, dashed green line – estimated location of the spinodal curve; circles – interpolated oil solubilities at 0, 10, 20, 30, and 40 °C; pink shaded area – mesoscale solubilization region; dashed red arrow – experimental path.

Table S1 – Composition of two-phase samples for interfacial tension measurements

Sample	Mass fraction			Mole fraction		
	H ₂ O	TBA	OIL	H ₂ O	TBA	OIL
CHX0	0.5002	0	0.4998	0.8238	0	0.1762
CHX1	0.5000	1.0·10 ⁻⁵	0.5000	0.8237	4.0·10 ⁻⁶	0.1763
CHX2	0.4999	0.0001	0.5000	0.8236	4.0·10 ⁻⁵	0.1763
CHX3	0.4997	0.0005	0.4998	0.8235	0.0002	0.1763
CHX4	0.4995	0.0010	0.4994	0.8234	0.0004	0.1762
CHX5	0.4987	0.0025	0.4988	0.8228	0.0010	0.1762
CHX6	0.4974	0.0051	0.4976	0.8220	0.0020	0.1760
CHX7	0.4950	0.0100	0.4950	0.8204	0.0040	0.1756
CHX8	0.4902	0.0200	0.4898	0.8171	0.0081	0.1748
CHX9	0.4800	0.0400	0.4800	0.8102	0.0164	0.1734
CHX10	0.5647	0.0725	0.3628	0.8556	0.0267	0.1177
CHX11	0.5251	0.1152	0.3597	0.8334	0.0444	0.1222
CHX12	0.4449	0.1101	0.4449	0.7848	0.0472	0.1680
CHX13	0.4561	0.2091	0.3348	0.7883	0.0878	0.1239
CHX14	0.3973	0.2889	0.3138	0.7430	0.1313	0.1256
CHX15	0.3518	0.3620	0.2862	0.7021	0.1756	0.1223
CHX16	0.3113	0.3774	0.3113	0.6628	0.1953	0.1419
CHX17	0.2849	0.4299	0.2852	0.6325	0.2320	0.1355
CHX18	0.2603	0.4798	0.2599	0.6018	0.2696	0.1286
CHX19	0.4806	0.4130	0.1064	0.7960	0.1663	0.0377
CHX20	0.5071	0.4220	0.0709	0.8116	0.1641	0.0243
CHX21	0.5208	0.4268	0.0524	0.8192	0.1632	0.0177
CHX22	0.5247	0.4280	0.0473	0.8213	0.1629	0.0159
CHX23	0.5282	0.4293	0.0425	0.8232	0.1626	0.0142
TOL0	0.5000	0	0.5000	0.8365	0.0000	0.1635
TOL1	0.4998	0.0005	0.4997	0.8363	0.0002	0.1635
TOL2	0.4995	0.0010	0.4995	0.8361	0.0004	0.1635
TOL3	0.4987	0.0025	0.4988	0.8356	0.0010	0.1634
TOL4	0.4975	0.0050	0.4975	0.8348	0.0020	0.1632
TOL5	0.4950	0.0100	0.4950	0.8330	0.0041	0.1629
TOL6	0.4900	0.0200	0.4900	0.8296	0.0082	0.1622
TOL7	0.4800	0.0400	0.4800	0.8225	0.0167	0.1608
TOL8	0.5640	0.0724	0.3636	0.8641	0.0270	0.1089
TOL9	0.4449	0.1100	0.4451	0.7964	0.0479	0.1558
TOL10	0.4561	0.2091	0.3348	0.7969	0.0888	0.1144
TOL11	0.3969	0.2884	0.3147	0.7510	0.1326	0.1164
TOL12	0.3516	0.3621	0.2863	0.7095	0.1776	0.1130

Sample	Mass fraction			Mole fraction		
	H ₂ O	TBA	OIL	H ₂ O	TBA	OIL
TOL13	0.3946	0.3782	0.2272	0.7432	0.1731	0.0837
TOL14	0.4377	0.3940	0.1683	0.7728	0.1691	0.0581
TOL15	0.4594	0.4020	0.1386	0.7864	0.1672	0.0464
TOL16	0.4724	0.4069	0.1207	0.7941	0.1662	0.0397
TOL17	0.4852	0.4117	0.1031	0.8014	0.1653	0.0333
TOL18	0.4979	0.4164	0.0856	0.8085	0.1643	0.0272
TOL19	0.4980	0.4165	0.0855	0.8085	0.1643	0.0271
TOL20	0.5142	0.4224	0.0634	0.8172	0.1631	0.0197
TOL21	0.5158	0.4230	0.0612	0.8180	0.1630	0.0190
TOL22	0.5174	0.4236	0.0590	0.8188	0.1629	0.0183
TOL23	0.5175	0.4236	0.0589	0.8189	0.1629	0.0182
TOL24	0.5191	0.4242	0.0567	0.8197	0.1628	0.0175
TOL25	0.5208	0.4247	0.0544	0.8206	0.1626	0.0168
TOL26	0.5215	0.4252	0.0532	0.8209	0.1627	0.0164
TOL27	0.5219	0.4254	0.0528	0.8211	0.1627	0.0162
DEC1	0.4974	0.0049	0.4976	0.8857	0.0021	0.1122
DEC2	0.4950	0.0100	0.4950	0.8838	0.0043	0.1119
DEC3	0.4900	0.0200	0.4900	0.8799	0.0087	0.1114
DEC4	0.4777	0.0399	0.4824	0.8710	0.0177	0.1114
DEC5	0.4350	0.1099	0.4551	0.8376	0.0514	0.1110
DEC6	0.3546	0.2350	0.4103	0.7648	0.1232	0.1120
DEC7	0.2743	0.3601	0.3656	0.6721	0.2145	0.1134
DEC8	0.2288	0.4251	0.3461	0.6086	0.2748	0.1166
DEC9	0.1834	0.4900	0.3266	0.5334	0.3464	0.1203
DEC10	0.1673	0.5084	0.3243	0.5040	0.3723	0.1237
DEC11	0.1591	0.5177	0.3233	0.4883	0.3861	0.1256
DEC12	0.1509	0.5268	0.3222	0.4720	0.4004	0.1276
DEC13	0.1486	0.5296	0.3217	0.4672	0.4047	0.1281
DEC14	0.1462	0.5324	0.3214	0.4622	0.4091	0.1287

OIL = Cyclohexane for CHX0 – CHX23 samples; OIL = Toluene for TOL0 – TOL27 samples; OIL = *n*-Decane for DEC0 – DEC14 samples

Table S2 – Interfacial tension γ in H₂O-TBA-OIL ternary systems at 20.0 °C

OIL = Cyclohexane				OIL = Toluene				OIL = <i>n</i> -Decane			
Sample	x_{TBA} in water phase (GC data)	γ , 10 ⁻³ N/m	Method	Sample	x_{TBA} in water phase (GC data)	γ , 10 ⁻³ N/m	Method	Sample	x_{TBA} in water phase (GC data)	γ , 10 ⁻³ N/m	Method
CHX0	0	48.8±0.3	WP	TOL0	0	34.5±0.3	WP	DEC0	0	52.33*	SD
CHX1	4.98·10 ⁻⁶	48.3±0.3		TOL1	1.75·10 ⁻⁴	34.5±0.3		DEC1	0.0025	32.89±0.03	
CHX2	4.01·10 ⁻⁵	48.2±0.3		TOL2	4.24·10 ⁻⁴	34.2±0.3		DEC2	0.0048	29.05±0.05	
CHX3	2.07·10 ⁻⁴	47.0±0.3		TOL3	8.99·10 ⁻⁴	32.5±0.3		DEC3	0.0097	22.17±0.03	
CHX4	4.35·10 ⁻⁴	45.0±0.3		TOL4	0.0018	30.3±0.3		DEC4	0.0188	16.10±0.03	
CHX5	0.0011	41.0±0.3		TOL5	0.0039	26.8±0.3		DEC5	0.0454	7.090±0.008	
CHX6	0.0022	36.5±0.3		TOL6	0.0083	21.6±0.3		DEC6	0.0835	1.950±0.011	
CHX7	0.0044	30.0±0.3		TOL7	0.0158	15.9±0.3		DEC7	0.1563	0.633±0.004	
CHX8	0.0088	24.5±0.3		TOL8	0.0265	11.4±0.3		DEC8	0.2213	0.324±0.001	
CHX9	0.0173	17.1±0.3		TOL9	0.0350	6.7±0.3		DEC9	0.3143	0.127±0.001	
CHX10	0.0267	12.4±0.3		TOL10	0.0468	3.1±0.3		DEC10	0.3330	0.0620±0.0007	
CHX11	0.0377	7.3±0.3		TOL11	0.0520	2.1±0.3		DEC11	0.3525	0.0359±0.003	
CHX12	0.0367	7.2±0.3		TOL12	0.0553	1.6±0.3		DEC12	0.3642	0.0191±0.0005	
CHX13	0.0495	3.5±0.3		TOL7	0.0158	14.940±0.013		DEC13	0.3742	0.0131±0.0003	
CHX14	0.0554	2.3±0.3		TOL9	0.0350	6.864±0.006		DEC14	0.3795	0.00736±0.00011	
CHX15	0.0562	1.7±0.3		TOL12	0.0553	1.400±0.002					
CHX16	0.0589	1.7±0.3		TOL13	0.0592	1.104±0.0004					
CHX17	0.0624	1.3±0.3		TOL14	0.0635	0.779±0.003					
CHX18	0.0652	1.0±0.3	TOL15	0.0670	0.539±0.001						
CHX0	0	48.3±0.19	SD	TOL15	0.0670	0.573±0.002					
CHX13	0.0495	3.26±0.14		TOL15	0.0670	0.539±0.001					
CHX18	0.0652	0.977±0.041		TOL16	0.0699	0.517±0.007					
CHX19	0.0697	0.515±0.020		TOL17	0.0738	0.346±0.0006					
CHX20	0.0791	0.228±0.013		TOL18	0.0782	0.213±0.0005					
CHX21	0.0939	0.0805±0.0011		TOL19	0.0787	0.212±0.0005					
CHX22	0.1060	0.0283±0.0005		TOL20	0.0936	0.111±0.0005					
CHX23	0.1123	0.0122±0.0003		TOL20	0.0936	0.106±0.0002					
				TOL21	0.0959	0.0526±0.0002					
				TOL22	0.0997	0.0393±0.0006					
			TOL23	0.0997	0.0368±0.0005						
			TOL24	0.1033	0.0256±0.0002						
			TOL25	0.1091	0.0127±0.0002						
			TOL26	0.1140	0.0136±0.0002						
			TOL27	0.1175	0.00713±0.00005						

* - literature data [1]

WP – Wilhelmy plate, SD – Spinning drop; the standard uncertainty $u(x_{TBA}) \leq 3$ percent of concentration value

References

- (1) Zeppieri, S.; Rodríguez, J.; López de Ramos, A. L. Interfacial Tension of Alkane + Water Systems. *J. Chem. Eng. Data* **2001**, *46* (5), 1086–1088.