

Supplementary Information (4 pages)

Catalytic Hydrogenation of Dimethyl Itaconate in Nonionic Microemulsions: Influence of the Size of Micelle

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Table A Original data of the cosurfactant partitioning study: molar percentage (%) of 1-pentanol concentrated in the aqueous phase of a biphasic system PEG 400/cyclohexane/water at 25°C.

Sample	$m_{\text{H}_2\text{O}}$ /g	$m_{\text{C}_6\text{H}_{12}}$ /g	$m_{\text{PEG}400}$ /g	$m_{\text{C}_5\text{H}_{12}\text{O}}$ /g	Peak area	$n_{\text{C}_5\text{H}_{12}\text{O}}^{\text{C}_6\text{H}_{12}}$ /mmol	$n_{\text{C}_5\text{H}_{12}\text{O}}^{\text{H}_2\text{O}}$ /mmol	% $_{\text{C}_5\text{H}_{12}\text{O}}^{\text{H}_2\text{O}}$
ME 1	0.43	6.42	0.47	0.57	14061112.9	5.53	0.95	14.62
ME 2	0.32	6.52	0.47	0.57	14152069.2	5.64	0.81	12.65
ME 3	0.21	6.61	0.47	0.57	13696833.8	5.56	0.90	13.89
ME 4	0.42	6.27	0.46	0.74	18677920.0	7.04	1.38	16.43
ME 5	0.31	6.37	0.46	0.74	18678078.8	7.16	1.26	15.00
ME 6	0.21	6.46	0.46	0.74	17986361.8	7.00	1.40	16.65
ME 7	0.41	6.14	0.45	0.91	22927464.7	8.38	1.93	18.75
ME 8	0.30	6.23	0.45	0.91	22271529.3	8.27	2.02	19.63
ME 9	0.20	6.30	0.45	0.90	21859081.2	8.22	2.03	19.77
ME 10	0.40	6.00	0.44	1.07	27487785.3	9.75	2.35	19.42
ME 11	0.30	6.09	0.44	1.06	27145658.0	9.77	2.30	19.03
ME 12	0.20	6.18	0.44	1.06	26272920.4	9.61	2.44	20.27

Table B Original data of the cosurfactant partitioning study: molar percentage (%) of 1-pentanol concentrated in the aqueous phase of a biphasic system cyclohexane/water at 25°C.

Sample	$m_{\text{H}_2\text{O}}$ /g	$m_{\text{C}_6\text{H}_{12}}$ /g	$m_{\text{C}_5\text{H}_{12}\text{O}}$ /g	Peak area	$n_{\text{C}_5\text{H}_{12}\text{O}}^{\text{C}_6\text{H}_{12}}$ /mmol	$n_{\text{C}_5\text{H}_{12}\text{O}}^{\text{H}_2\text{O}}$ /mmol	% $_{\text{C}_5\text{H}_{12}\text{O}}^{\text{H}_2\text{O}}$
ME 1	0.43	6.42	0.57	14584854.0	5.72	0.76	11.67
ME 2	0.32	6.52	0.57	14703252.0	5.85	0.61	9.49
ME 3	0.21	6.61	0.57	14251234.0	5.76	0.69	10.65
ME 4	0.42	6.27	0.74	19266890.0	7.25	1.17	13.93
ME 5	0.31	6.37	0.74	19351388.0	7.41	1.02	12.11
ME 6	0.21	6.46	0.74	18731613.0	7.27	1.12	13.39
ME 7	0.41	6.14	0.91	24072494.0	8.78	1.53	14.87
ME 8	0.30	6.23	0.91	23008840.0	8.54	1.75	17.09
ME 9	0.20	6.30	0.90	23151346.0	8.68	1.56	15.25
ME 10	0.40	6.00	1.07	27833765.0	9.87	2.23	18.45
ME 11	0.30	6.09	1.06	27367684.0	9.85	2.22	18.40
ME 12	0.20	6.17	1.06	27567972.0	10.06	1.99	16.49

Table C Original data of the cosurfactant partitioning study: molar percentage (%) of 1-pentanol concentrated in the aqueous phase of a biphasic system PEG 1000/cyclohexane/water at 25°C.

Sample	$m_{\text{H}_2\text{O}}$ /g	$m_{\text{C}_6\text{H}_{12}}$ /g	$m_{\text{PEG}400}$ /g	$m_{\text{C}_5\text{H}_{12}\text{O}}$ /g	Peak area	$n_{\text{C}_5\text{H}_{12}\text{O}}/\text{C}_6\text{H}_{12}$ /mmol	$n_{\text{C}_5\text{H}_{12}\text{O}}/\text{H}_2\text{O}$ mmol	% $_{\text{C}_5\text{H}_{12}\text{O}}\text{H}_2\text{O}$
ME 1	0.43	6.42	1.18	0.57	13008825.4	5.14	1.33	20.56
ME 2	0.32	6.52	1.17	0.57	12374776.9	4.99	1.48	22.85
ME 3	0.21	6.61	1.17	0.57	11234869.8	4.63	1.82	28.25
ME 4	0.42	6.27	1.15	0.74	16099999.6	6.12	2.30	27.34
ME 5	0.31	6.37	1.15	0.74	16336232.7	6.31	2.11	25.08
ME 6	0.21	6.46	1.14	0.74	15439785.9	6.06	2.33	27.79
ME 7	0.41	6.14	1.12	0.91	22140432.2	8.10	2.21	21.42
ME 8	0.30	6.23	1.12	0.91	21843548.8	8.12	2.17	21.10
ME 9	0.20	6.30	1.12	0.90	19194788.2	7.26	2.98	29.09
ME 10	0.40	6.00	1.10	1.07	25533580.8	9.08	3.02	24.94
ME 11	0.30	6.09	1.10	1.06	26195294.1	9.44	2.63	21.76
ME 12	0.20	6.18	1.09	1.06	22933571.5	8.43	3.62	30.01

Table D Absolute intensity of the SANS measurements from the Triton X-100 microemulsions, volume fraction of the polar components, contrast factor and volume of the Triton X-100 micelles calculated using the macroscopic scattering cross section, considering the limits of no and full penetration of pentanol in the core of the micelles.

Sample	ω	δ	I_0 /cm ⁻¹	\square_0	\square_1	Δp_0 /cm ⁻²	Δp_1 /cm ⁻²	$V_{10,0}$ /nm ⁻³	$V_{10,-1}$ /nm ⁻³
ME 1	20	0.75	138.61	0.09	0.17	-2.69E+10	-4.87E+10	2046.17	341.16
ME 2	15	0.75	37.14	0.08	0.16	-3.13E+10	-5.20E+10	461.91	85.86
ME 3	10	0.75	18.42	0.07	0.15	-3.67E+10	-5.57E+10	191.24	39.93
ME 4	20	1.00	55.11	0.09	0.19	-2.52E+10	-5.12E+10	952.51	109.19
ME 5	15	1.00	28.97	0.08	0.18	-2.96E+10	-5.42E+10	412.88	54.41
ME 6	10	1.00	15.15	0.07	0.17	-3.50E+10	-5.75E+10	177.14	26.94
ME 7	20	1.25	43.26	0.09	0.21	-2.35E+10	-5.32E+10	884.29	72.22
ME 8	15	1.25	25.24	0.08	0.20	-2.80E+10	-5.59E+10	411.91	40.12
ME 9	10	1.25	9.45	0.07	0.19	-3.34E+10	-5.88E+10	124.41	14.33
ME 10	20	1.50	34.60	0.09	0.23	-2.20E+10	-5.47E+10	823.00	50.05
ME 11	15	1.50	21.77	0.08	0.22	-2.64E+10	-5.72E+10	408.25	30.18
ME 12	10	1.50	11.38	0.07	0.21	-3.19E+10	-5.99E+10	168.28	15.13

Table E Radius of gyration, radius of the micelles, volume of the corresponding homogeneous micelles with the assumption of spherical shape and volume ratio considering no penetration of pentanol in the core of the micelles.

Sample	R_{g_1} /nm	R_1 /nm	V_{Sph} /nm ³	V_{Sph}/V_{10_1}
ME 1	11.18	14.43	12588.94	6.15
ME 2	5.41	6.99	1429.35	3.09
ME 3	3.33	4.30	332.39	1.74
ME 4	7.09	9.16	3216.55	3.38
ME 5	5.04	6.50	1152.32	2.79
ME 6	3.24	4.18	306.02	1.73
ME 7	6.37	8.23	2332.92	2.64
ME 8	5.00	6.45	1125.36	2.73
ME 9	2.73	3.52	183.01	1.47
ME 10	5.59	7.22	1575.70	1.91
ME 11	4.37	5.65	754.56	1.85
ME 12	3.49	4.51	383.53	2.28

Table F Radius of gyration, radius of the micelles, volume of the corresponding homogeneous micelles with the assumption of ellipsoidal shape and volume ratio considering no penetration of pentanol in the core of the micelles.

Sample	R_{g_2} /nm	a /nm	b /nm	V_{Ellip} /nm ³	V_{Ellip}/V_{10_1}	<i>Ellipticity</i>
ME 1	4.00	5.16	23.90	2670.19	1.30	4.63
ME 2	3.67	4.74	10.08	947.79	2.05	2.13
ME 3	3.09	3.99	4.86	323.63	1.69	1.22
ME 4	3.80	4.91	14.26	1437.86	1.51	2.91
ME 5	3.57	4.61	9.19	817.48	1.98	1.99
ME 6	2.89	3.73	4.96	289.13	1.63	1.33
ME 7	3.40	4.39	12.83	1035.23	1.17	2.92
ME 8	3.45	4.45	9.23	767.15	1.86	2.07
ME 9	2.39	3.09	4.26	170.00	1.37	1.38
ME 10	3.11	4.01	11.14	752.19	0.91	2.77
ME 11	3.31	4.27	7.69	588.35	1.44	1.80
ME 12	2.54	3.28	6.28	282.86	1.68	1.92

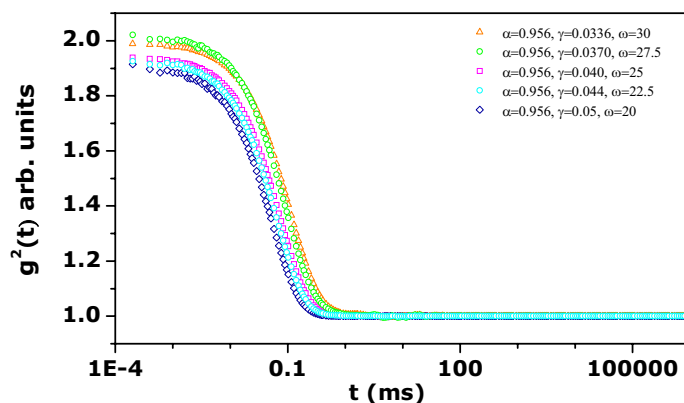


Figure A Autocorrelation functions $g^2(\tau)$ of the DLS measurements of Igepal microemulsions with different concentrations of Igepal CA-520 (γ) and constant cyclohexane-to-water ratios ($\alpha = 0.956$) at 25°C .

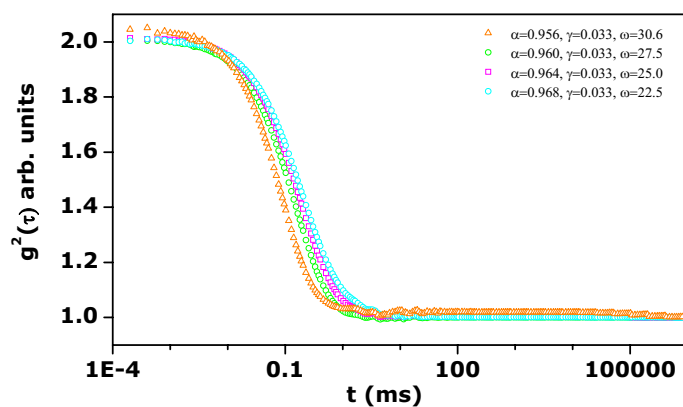


Figure B Autocorrelation functions $g^2(\tau)$ of the DLS measurements of Igepal microemulsions with different cyclohexane-to-water ratios (α) and constant concentration of Igepal CA-520 ($\gamma = 0.033$) at 25°C .