Supporting Information

The Solid–Liquid Equilibrium and Crystal Habit of l-Carnitine Fumarate

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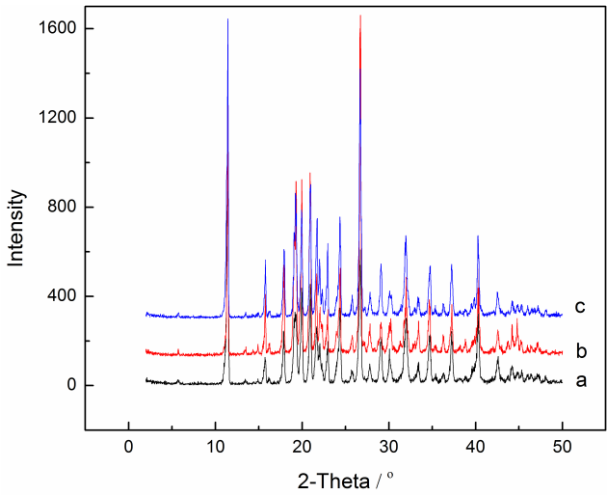

Fig. S1 X-ray power diffraction pattern of l-carnitine fumarate (T = 288.15 K, methanol + ethanol (x_2^0 = 0.5): (a) raw material; (b) solid filtered in solvents after stirring; (c) dry product.

Table S1

Parameters of the modified Apelblat equation for 1-carnitine fumarate in different binary solvent mixtures at different temperature. (P = 0.1 MPa). [a,b]

x_2^0	A	B	C	10^2ARD
		(methanol + ethanol)		
0.00	1400.407	-70094.184	-205.868	7.358
0.10	1156.394	-58592.564	-169.771	5.268
0.20	1212.896	-61075.618	-178.189	6.333
0.30	1066.803	-54006.624	-156.661	5.746
0.40	1118.393	-56249.981	-164.349	7.401
0.50	1077.029	-54101.277	-158.304	7.785
0.60	824.994	-42307.356	-120.959	6.617
0.70	756.376	-39031.316	-110.797	6.606
0.80	526.814	-28441.859	-76.694	4.898
0.90	5.668	-4456.379	0.699	1.326
1.00	-359.187	12271.245	54.925	1.261
		(methanol +1-propanol)		
0.00	906.507	-47251.518	-132.773	6.370
0.10	935.635	-48921.106	-136.873	6.659
0.20	553.568	-31002.354	-80.306	3.690
0.30	469.556	-26873.165	-67.932	2.295
0.40	404.646	-23502.857	-58.461	1.754
0.50	748.404	-38942.912	-109.642	2.581
0.60	876.254	-44552.539	-128.717	4.015
0.70	796.284	-40762.640	-116.847	4.345
0.80	275.222	-16807.824	-39.430	2.773
0.90	-213.053	5513.539	33.190	1.081
1.00	-359.187	12271.245	54.925	1.261
		(methanol + 2-propanol)		
0.00	354.014	-22058.745	-50.685	7.826
0.10	750.202	-40353.789	-109.401	5.891
0.20	666.601	-36092.710	-97.183	5.705
0.30	422.389	-25005.269	-60.801	2.464
0.40	679.633	-36661.803	-99.030	5.128
0.50	421.728	-24559.466	-60.822	3.314

0.60	641.124	-34497.095	-93.425	4.777
0.70	454.311	-25786.328	-65.699	4.204
0.80	110.271	-9676.233	-14.726	0.910
0.90	72.641	-7740.657	-9.184	2.229
1.00	-359.187	12271.245	54.925	1.261
		(methanol + 1-butanol)		
0.00	-303.266	8790.857	46.508	7.257
0.10	313.654	-19964.755	-44.803	7.108
0.20	-474.678	16944.776	71.899	10.014
0.30	73.401	-8583.047	-9.230	5.677
0.40	-466.827	16568.225	70.840	8.222
0.50	297.216	-18913.258	-42.327	6.319
0.60	238.344	-15862.012	-33.722	5.310
0.70	495.477	-27728.876	-71.804	5.321
0.80	423.465	-24047.643	-61.249	1.737
0.90	-57.719	-1996.106	10.304	1.673
1.00	-825.487	33862.727	124.062	3.766

[a] x_2^0 denotes the mole fraction of methanol in a mixed solvent.

[b] ARD is the relative average deviation.

Table S2

Parameters of the CNIBS/R–K equation for l-carnitine fumarate in different binary solvent mixtures at different temperatures. (P = 0.1 MPa). [a]

T/K	B_1	B_2	B_3	B_4	B_5	10^2ARD
			(methanol + ethanol)			
288.15	-8.425	1.729	4.298	-4.519	1.342	0.983
293.15	-8.011	1.654	4.361	-5.392	2.068	0.510
298.15	-7.643	2.008	1.524	-1.251	0.274	0.569
303.15	-7.181	1.882	-0.478	2.859	-1.927	0.450
308.15	-6.892	1.734	1.015	0.189	-0.641	0.397
313.15	-6.516	1.522	1.656	-0.959	-0.057	0.525
318.15	-6.190	1.182	2.512	-1.944	0.312	0.172
323.15	-6.010	1.374	0.848	0.606	-0.678	1.030
328.15	-5.923	2.176	-2.652	5.320	-2.502	1.150
			(methanol + 1-propanol)			
288.15	-9.280	2.578	0.334	3.387	-2.594	0.904

293.15	-8.942	3.654	-1.463	2.523	-1.093	2.121
298.15	-8.497	2.222	3.051	-3.085	1.222	0.873
303.15	-8.069	1.664	4.404	-4.698	1.854	0.540
308.15	-7.798	2.175	2.713	-2.715	1.028	0.423
313.15	-7.367	1.022	5.690	-6.089	2.389	1.411
318.15	-6.967	0.811	5.270	-5.114	1.874	1.631
323.15	-7.082	6.056	-14.757	21.131	-9.205	2.992
328.15	-6.869	6.648	-18.151	26.211	-11.420	4.260
			(methanol + 2-propanol)			
288.15	-9.857	5.572	-5.990	6.086	-1.387	3.394
293.15	-8.970	0.616	9.567	-13.410	6.876	3.168
298.15	-8.718	1.904	5.029	-7.618	4.316	2.945
303.15	-8.231	0.585	8.421	-11.238	5.617	2.589
308.15	-7.946	1.488	5.057	-6.981	3.784	1.245
313.15	-7.741	2.209	4.038	-6.767	3.909	2.867
318.15	-7.355	2.324	2.101	-3.249	2.054	1.778
323.15	-7.009	0.881	7.910	-12.047	6.405	2.735
328.15	-6.804	0.910	7.315	-10.905	5.900	2.818
			(methanol + 1-butanol)			
293.15	-8.930	-3.412	26.606	-37.554	17.967	9.422
298.15	-8.796	1.305	7.381	-10.653	5.675	4.040
303.15	-8.380	0.942	6.420	-7.827	3.998	5.079
308.15	-8.127	3.289	-2.749	3.863	-0.873	0.824
313.15	-7.874	2.988	-0.983	1.871	-0.357	1.532
318.15	-7.598	2.820	-1.701	4.050	-1.698	3.137
323.15	-7.225	2.725	-0.373	0.344	0.672	2.877
328.15	-7.230	5.225	-7.965	9.017	-2.628	4.786
333.15	-7.140	8.809	-22.942	29.690	-11.786	8.964

[a] ARD is the relative average deviation.

Table S3

Parameters of the Solubility-Polarity Model for l-carnitine fumarate in different binary solvent mixtures at different temperatures. (P = 0.1 MPa). [a]

T /K	k	E_x / kJ·mol^{-1}	10^2 ARD
	(methanol + ethanol)		
288.15	13.709	2.325	15.606
293.15	13.070	2.185	11.345
298.15	14.777	2.104	6.445
303.15	13.795	1.971	4.284
308.15	12.238	1.831	6.576
313.15	9.773	1.677	6.093
318.15	9.093	1.571	5.963
323.15	19.323	1.670	2.079
328.15	54.268	1.833	5.742
	(methanol + 1-propanol)		
288.15	1.669	1.727	21.306
293.15	1.531	1.594	11.076
298.15	1.354	1.459	10.275
303.15	1.160	1.320	9.212
308.15	1.096	1.211	9.685
313.15	1.089	1.125	6.208
318.15	0.984	1.023	3.678
323.15	1.592	1.059	6.918
328.15	2.232	1.060	12.967
	(methanol + 2-propanol)		
288.15	2.725	1.879	9.410
293.15	2.172	1.700	14.346
298.15	1.614	1.514	10.449
303.15	1.351	1.368	10.593
308.15	1.177	1.239	10.090
313.15	0.973	1.104	7.235
318.15	0.830	0.987	6.483
323.15	1.017	0.959	13.476
328.15	1.376	0.951	17.477
	(methanol + 1-butanol)		
293.15	0.559	1.325	15.409
298.15	0.464	1.175	6.565
303.15	0.491	1.098	7.712

308.15	0.528	1.029	10.548
313.15	0.476	0.919	3.256
318.15	0.525	0.869	4.096
323.15	0.600	0.825	10.178
328.15	0.799	0.816	13.912
333.15	0.902	0.782	18.814

[a] ARD is the relative average deviation.

Table S4

Parameters of the Jouyban–Acree equation for l-carnitine fumarate in different binary solvent mixtures at different temperatures. (P = 0.1 MPa). [a]

parameters	(methanol + ethanol)	(methanol + 1-propanol)	(methanol + 2-propanol)	(methanol + 1-butanol)
A_1	813.941	590.72	567.118	128.614
A_2	-42636.158	-32690.343	-31871.404	-11382.425
A_3	-119.083	-85.919	-82.311	-17.425
A_4	-947.721	-596.78	-722.02	-131.685
A_5	44628.212	28807.328	34551.988	7106.338
A_6	539.647	390.23	285.97	-378.770
A_7	-304.833	-78.852	-553.63	505.145
A_8	-3.733	-20.692	494.919	26.239
A_9	140.368	88.213	106.89	19.498
10^2ARD	4.309	3.978	3.512	4.362

[a] ARD is the relative average deviation.