SUPPLEMENTARY DATA

Theoretical interpretation of conductivity data below and above the CMC: The case of alkaline ion decanoate solutions

S. Durand-Vidal[a*], O. Bernard[a], Ž. Medoš[b], M. Bešter-Rogač[b]

[a] Sorbonne Université, Faculté des Sciences et d'Ingénierie - Campus Pierre et Marie Curie. Laboratoire PHENIX - UMR CNRS 8234. CC 51, 4 place Jussieu 75252 Paris, France.

[b] Faculty of Chemistry and Chemical Technology, Aškerčeva 5, University of Ljubljana, Sl-1000 Ljubljana, Slovenia.

[*] E-mail address: serge.durand-vidal@sorbonne-universite.fr

We present in Table S1 the specific conductivity values κ as a function of molality of sodium decanoate (NaDec) in aqueous solution, obtained in this study, between 278.15 and 328.15 K. In Table S2 are provided the parameters used to calculate the theoretical curves of conductivity of potassium and cesium decanoate (KDec, CsDec) solutions, as well as data from the literature, given for comparison. Figure S1 and S2 represent the molar conductivities of KDec and CsDec aqueous solutions from 278.15 to 328.15 K (in step of 10 K) as function of the square root of the total monomer concentration. Finally, we report in tables S3, S4 and S5 the values of molarities and molar conductivities at different temperatures used in this study, for NaDec, KDec and CsDec respectively.

Table S1: Conductivity, κ, as a function of molality, m, for aqueous solutions of NaDec at different temperatures. The measurement of conductivity were carried out for each concentration at all temperatures and p = 0.1 MPa.

	T/K					
	278.15	**288.15**	**298.15**	**308.15**	**318.15**	**328.15**
m/ mol.kg^{-1}	κ / S . m^{-1}					
0.00106	0.00436	0.00578	0.00735	0.00907	0.01092	0.01288
0.00213	0.00863	0.01144	0.01456	0.01800	0.02161	0.02544
0.00317	0.01281	0.01696	0.02155	0.02650	0.03183	0.03753
0.00425	0.01709	0.02264	0.02879	0.03550	0.04263	0.05002
0.00636	0.02521	0.03339	0.04246	0.05232	0.06284	0.07406
0.00847	0.03327	0.04410	0.05612	0.06921	0.08312	0.09790
0.01053	0.04100	0.05434	0.06911	0.08521	0.1023	0.1206
0.01585	0.06063	0.08029	0.1022	0.1261	0.1513	0.1784
0.02111	0.07955	0.1055	0.1343	0.1656	0.1989	0.2346

Then, we used density measurements of NaDec determined previously [2] and the molar mass M of the sodium decanoate, to determine molarities C from molalities m. Next, the molar conductivities Λ were deduced from C and the mesured κ, using the relation: $\Lambda = \kappa/C$. These values of molarities and molar conductivities at different temperatures are reported with the previous one in Table S3.

Table S2: Values of the fitted thermodynamic constants K, CMC, apparent charge of the micelle Z_{Mic} and dissociation degree α as a function of temperature for potassium and cesium decanoate with aggregation number of 12 for the two systems.

T (K)	278.15	288.15	298.15	308.15	318.15	328.15
KDec						
K ($dm^3.mol^{-1}$)	–	0.5	0.4	0.3	0.2	0.0
CMC ($mol.dm^{-3}$)	–	0.115^a	0.108^a	0.104^a	0.102^a	0.104^a
	–	0.109^b	0.102^b	0.097^b	0.097^b	0.099^b
	–	0.116^c	0.103^c	0.095^c	0.092^c	0.091^c
Z_{Mic}	–	-8	-8	-8	-9	-9
$\alpha = \mid Z_{Mic} \mid / n_{agg}$	–	0.67	0.67	0.67	0.75	0.75
CsDec						
K ($dm^3.mol^{-1}$)	1.8	1.7	1.3	1.2	1.1	0.9
CMC ($mol.dm^{-3}$)	0.142^a	0.130^a	0.106^a	0.101^a	0.102^a	0.105^a
	0.120^b	0.109^b	0.102^b	0.099^b	0.097^b	0.098^b
	–	0.122^c	0.106^c	0.102^c	0.097^c	0.103^c
Z_{Mic}	-8	-8	-9	-9	-9	-9
$\alpha = \mid Z_{Mic} \mid / n_{agg}$	0.67	0.67	0.75	0.75	0.75	0.75

[a]This work.

[b]From [1].

[c]From [2].

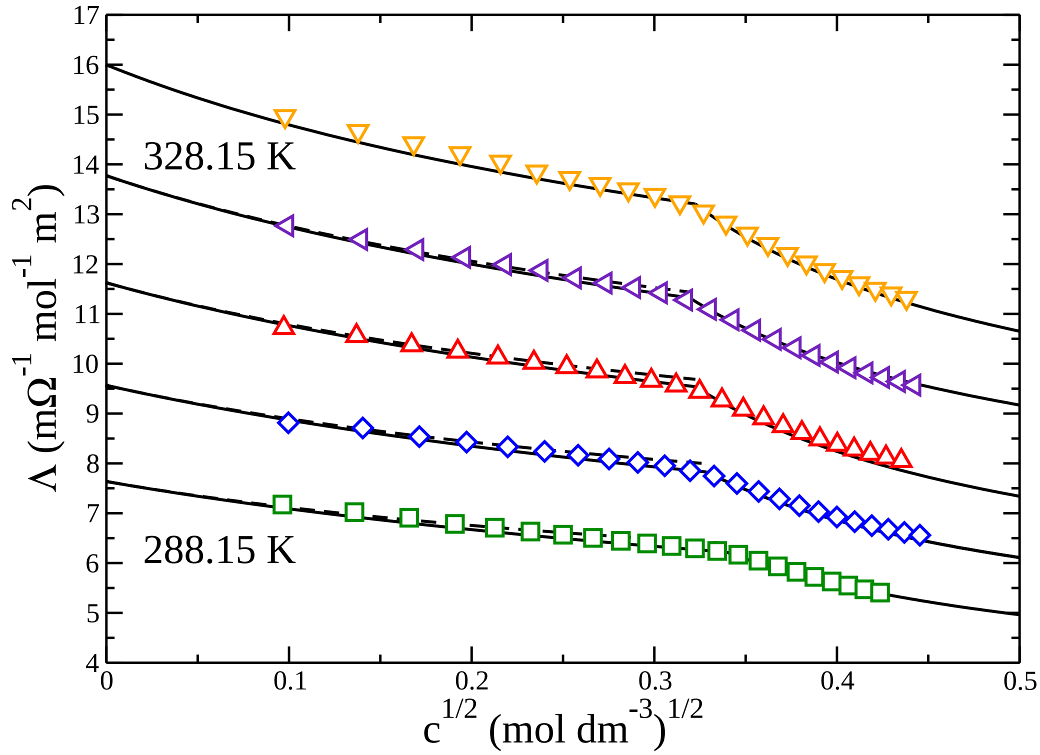

Figure S1: Molar conductivities, Λ, of KDec aqueous solutions from 278.25 K to 328.15 K (in step of 10 K) as a function of the square root of the total monomer concentration. Empty symbols from [1], Dashed line: MSA-transport calculations without association below the CMC; Solid line: MSA-transport calculations with association below the CMC and with parameters indicated in Table S2 above the CMC.

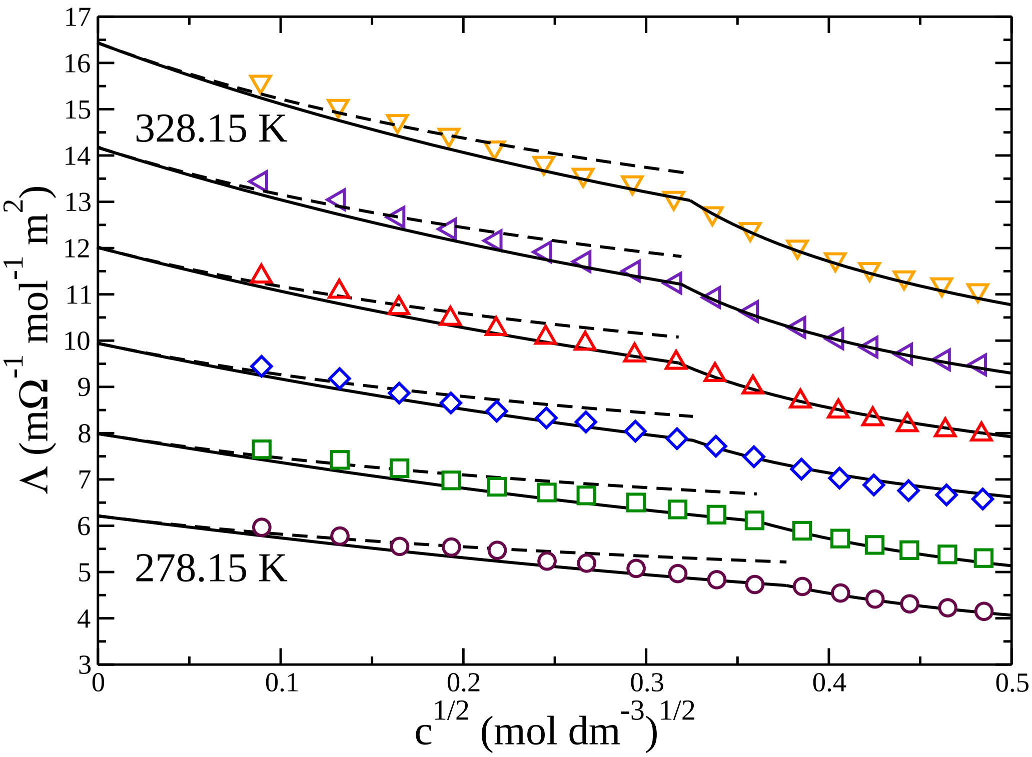

Figure S2: Molar conductivities, Λ, of CsDec aqueous solutions from 278.25 K to 328.15 K (in step of 10 K) as a function of the square root of the total monomer concentration. Empty symbols from [1], Dashed line: MSA-transport calculations without association below the CMC; Solid line: MSA-transport calculations with association below the CMC and with parameters from Table S2 above the CMC.

References

[1] Ž. Medoš, M. Bešter-Rogač, J. Chem. Thermodyn. 83 (2015) 117-122.

[2] Ž Medoš, M. Bešter-Rogač, Langmuir 33 (2017) 7722-7731.

Table S3: molarities c (/mol dm^{-3}) and molar conductivities Λ (/mS mol^{-1} m^2) of NaDec aqueous solutions at different temperatures.

T / K											
278.15		288.15		298.15		308.15		318.15		328.15	
c	Λ	c	Λ	c	Λ	c	Λ	c	Λ	c	Λ
0.0011	4.130	0.0011	5.479	0.0011	6.989	0.0011	8.647	0.0011	10.454	0.0010	12.383
0.0021	4.054	0.0021	5.380	0.0021	6.861	0.0021	8.491	0.0021	10.249	0.0021	12.125
0.0032	4.040	0.0032	5.351	0.0032	6.813	0.0032	8.404	0.0031	10.134	0.0031	12.003
0.0043	4.021	0.0043	5.331	0.0042	6.793	0.0042	8.401	0.0042	10.128	0.0042	11.937
0.0064	3.962	0.0064	5.254	0.0063	6.694	0.0063	8.275	0.0063	9.976	0.0063	11.811
0.0085	3.928	0.0085	5.211	0.0085	6.644	0.0084	8.218	0.0084	9.908	0.0084	11.724
0.0105	3.892	0.0105	5.163	0.0105	6.580	0.0105	8.137	0.0104	9.808	0.0104	11.610
0.0159	3.823	0.0158	5.068	0.0158	6.463	0.0158	7.997	0.0157	9.636	0.0156	11.412
0.0163	3.830	0.0163	5.087	0.0163	6.496	0.0162	8.032	0.0162	9.682	0.0161	11.429
0.0211	3.765	0.0211	4.999	0.0211	6.377	0.0210	7.886	0.0209	9.507	0.0208	11.265
0.0317	3.668	0.0317	4.886	0.0316	6.244	0.0315	7.723	0.0314	9.310	0.0313	10.996
0.0478	3.549	0.0478	4.729	0.0477	6.046	0.0476	7.490	0.0474	9.042	0.0472	10.683
0.0605	3.471	0.0604	4.621	0.0603	5.915	0.0601	7.332	0.0599	8.856	0.0596	10.480
0.0743	3.399	0.0742	4.526	0.0740	5.799	0.0738	7.194	0.0735	8.692	0.0732	10.287
0.0904	3.321	0.0903	4.421	0.0901	5.670	0.0899	7.032	0.0895	8.494	0.0891	10.057
0.1060	3.241	0.1059	4.330	0.1057	5.526	0.1054	6.822	0.1050	8.237	0.1045	9.772
0.1223	3.176	0.1222	4.194	0.1220	5.304	0.1216	6.536	0.1211	7.911	0.1206	9.413
0.1400	3.064	0.1399	4.000	0.1396	5.053	0.1392	6.242	0.1387	7.575	0.1380	9.046
0.1566	2.936	0.1564	3.830	0.1561	4.854	0.1556	6.015	0.1550	7.314	0.1543	8.746
0.1745	2.805	0.1743	3.674	0.1740	4.676	0.1735	5.813	0.1728	7.083	0.1720	8.482
0.1927	2.694	0.1925	3.549	0.1921	4.537	0.1915	5.655	0.1908	6.899	0.1899	8.255
0.2099	2.606	0.2097	3.452	0.2093	4.429	0.2087	5.533	0.2079	6.759	0.2069	8.094
0.2274	2.533	0.2272	3.371	0.2267	4.341	0.2260	5.434	0.2252	6.639	0.2242	7.954
0.2450	2.470	0.2448	3.304	0.2443	4.268	0.2436	5.350	0.2426	6.544	0.2415	7.837

Table S4: molarities c (/mol dm^{-3}) and molar conductivities Λ (/mS mol^{-1} m^2) of KDec aqueous solutions at different temperatures.

T / K									
278.15		298.15		308.15		318.15		328.15	
c	Λ	c	Λ	c	Λ	c	Λ	c	Λ
0.0093	7.174	0.0099	8.815	0.0094	10.719	0.0098	12.768	0.0096	14.965
0.0184	7.023	0.0197	8.710	0.0187	10.557	0.0194	12.493	0.0190	14.665
0.0275	6.909	0.0294	8.537	0.0279	10.372	0.0289	12.290	0.0283	14.421
0.0364	6.785	0.0389	8.427	0.0370	10.245	0.0383	12.134	0.0375	14.221
0.0452	6.710	0.0483	8.331	0.0460	10.127	0.0476	11.990	0.0466	14.051
0.0539	6.633	0.0576	8.240	0.0548	10.023	0.0567	11.871	0.0555	13.853
0.0625	6.569	0.0667	8.164	0.0635	9.935	0.0657	11.721	0.0644	13.723
0.0710	6.506	0.0757	8.089	0.0721	9.848	0.0747	11.617	0.0731	13.603
0.0794	6.446	0.0847	8.020	0.0806	9.738	0.0834	11.528	0.0817	13.496
0.0876	6.394	0.0934	7.953	0.0890	9.661	0.0921	11.422	0.0902	13.384
0.0958	6.343	0.1021	7.852	0.0973	9.566	0.1007	11.277	0.0986	13.236
0.1039	6.296	0.1107	7.747	0.1055	9.439	0.1091	11.091	0.1069	13.050
0.1118	6.243	0.1192	7.597	0.1136	9.266	0.1175	10.882	0.1151	12.828
0.1197	6.168	0.1275	7.437	0.1216	9.082	0.1257	10.671	0.1232	12.607
0.1275	6.048	0.1358	7.287	0.1295	8.908	0.1339	10.488	0.1312	12.398
0.1352	5.934	0.1440	7.151	0.1373	8.751	0.1419	10.320	0.1391	12.200
0.1428	5.824	0.1520	7.032	0.1450	8.612	0.1499	10.166	0.1469	12.029
0.1503	5.722	0.1600	6.924	0.1526	8.486	0.1577	10.034	0.1546	11.875
0.1577	5.630	0.1678	6.831	0.1601	8.377	0.1655	9.919	0.1623	11.737
0.1650	5.548	0.1756	6.750	0.1676	8.280	0.1731	9.815	0.1698	11.611
0.1723	5.474	0.1833	6.679	0.1749	8.194	0.1807	9.724	0.1773	11.500
0.1794	5.408	0.1909	6.615	0.1822	8.120	0.1882	9.644	0.1846	11.406
		0.1984	6.559	0.1894	8.051	0.1956	9.570	0.1919	11.318

Table S5: molarities c (/mol dm^{-3}) and molar conductivities Λ (/mS mol^{-1} m^2) of CsDec aqueous solutions at different temperatures.

T / K											
278.15		288.15		298.15		308.15		318.15		328.15	
c	Λ	c	Λ	c	Λ	c	Λ	c	Λ	c	Λ
0.0080	5.965	0.0080	7.652	0.0080	9.444	0.0080	11.389	0.0080	13.437	0.0079	15.590
0.0175	5.776	0.0175	7.423	0.0175	9.180	0.0174	11.060	0.0174	13.045	0.0173	15.069
0.0273	5.553	0.0272	7.243	0.0272	8.867	0.0271	10.706	0.0270	12.666	0.0269	14.740
0.0374	5.538	0.0374	6.979	0.0373	8.653	0.0372	10.475	0.0371	12.410	0.0369	14.444
0.0478	5.469	0.0477	6.842	0.0476	8.475	0.0475	10.254	0.0473	12.159	0.0471	14.170
0.0604	5.236	0.0603	6.719	0.0602	8.330	0.0600	10.065	0.0598	11.915	0.0595	13.839
0.0715	5.192	0.0715	6.656	0.0713	8.242	0.0711	9.937	0.0708	11.706	0.0705	13.580
0.0868	5.077	0.0867	6.501	0.0865	8.042	0.0862	9.683	0.0859	11.502	0.0855	13.416
0.1007	4.966	0.1006	6.352	0.1004	7.881	0.1001	9.524	0.0997	11.241	0.0993	13.081
0.1147	4.834	0.1146	6.239	0.1144	7.718	0.1140	9.260	0.1136	10.933	0.1131	12.748
0.1292	4.730	0.1291	6.115	0.1289	7.490	0.1285	8.991	0.1280	10.628	0.1274	12.407
0.1486	4.687	0.1485	5.891	0.1482	7.222	0.1478	8.689	0.1472	10.285	0.1466	12.027
0.1652	4.547	0.1650	5.722	0.1647	7.029	0.1642	8.472	0.1636	10.041	0.1628	11.754
0.1808	4.416	0.1807	5.584	0.1803	6.882	0.1798	8.304	0.1791	9.859	0.1783	11.543
0.1974	4.313	0.1972	5.472	0.1968	6.759	0.1962	8.175	0.1955	9.709	0.1946	11.363
0.2163	4.227	0.2161	5.380	0.2157	6.666	0.2150	8.067	0.2142	9.584	0.2133	11.212
0.2351	4.149	0.2349	5.300	0.2345	6.577	0.2338	7.975	0.2329	9.477	0.2319	11.086