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The role of ion-water interactions in determining the Soret coefficient of LiCl aqueous solutions

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$T\ [K]$	$b\ [kg\ mol^{-1}]$	$s_T \times 10^3\ [K^{-1}]$
250	0.964 ± 0.033	-3.023 ± 0.273
	1.472 ± 0.036	-4.140 ± 0.323
	1.989 ± 0.047	-4.060 ± 0.181
	2.524 ± 0.036	-4.641 ± 0.118
	3.016 ± 0.038	-4.163 ± 0.154
	3.582 ± 0.065	-3.237 ± 0.559
	4.166 ± 0.062	-2.398 ± 0.464
	4.722 ± 0.052	-2.604 ± 0.070
	5.359 ± 0.053	-2.293 ± 0.032
260	0.992 ± 0.031	-2.427 ± 0.262
	1.527 ± 0.032	-2.978 ± 0.302
	2.059 ± 0.043	-2.627 ± 0.303
	2.622 ± 0.036	-2.822 ± 0.075
	3.132 ± 0.042	-3.079 ± 0.013
	3.692 ± 0.050	-2.565 ± 0.327
	4.265 ± 0.047	-2.101 ± 0.291
	4.842 ± 0.050	-2.206 ± 0.053
	5.480 ± 0.053	-1.995 ± 0.024

Table S1 Soret coefficient as a function of LiCl molality and temperature (at 250 K and 260 K), obtained with the method implemented in GROMACS. The NEMD simulations were performed using the system equilibrated at an average pressure of 600 bar.

$T\ [K]$	$b\ [kg\ mol^{-1}]$	$s_T \times 10^3\ [K^{-1}]$
280	1.029 ± 0.027	-1.329 ± 0.242
	1.590 ± 0.026	-1.315 ± 0.199
	2.129 ± 0.033	-1.026 ± 0.250
	2.715 ± 0.032	-1.009 ± 0.092
	3.274 ± 0.039	-1.643 ± 0.119
	3.842 ± 0.038	-1.608 ± 0.086
	4.419 ± 0.034	-1.592 ± 0.083
	5.023 ± 0.048	-1.609 ± 0.030
	5.669 ± 0.053	-1.538 ± 0.014
300	1.045 ± 0.023	-0.187 ± 0.221
	1.612 ± 0.022	-0.082 ± 0.118
	2.153 ± 0.026	-0.183 ± 0.088
	2.744 ± 0.029	-0.194 ± 0.063
	3.349 ± 0.032	-0.685 ± 0.109
	3.938 ± 0.036	-0.904 ± 0.004
	4.541 ± 0.032	-1.114 ± 0.020
	5.162 ± 0.047	-1.138 ± 0.015
	5.824 ± 0.053	-1.169 ± 0.006

Table S2 Same as Table S1 for the temperatures 280 K and 300 K.

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T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
310	1.044 ± 0.021	0.360 ± 0.211
	1.609 ± 0.022	0.374 ± 0.106
	2.154 ± 0.025	0.055 ± 0.012
	2.747 ± 0.027	0.008 ± 0.047
	3.366 ± 0.029	-0.360 ± 0.082
	3.968 ± 0.037	-0.646 ± 0.013
	4.585 ± 0.034	-0.902 ± 0.036
	5.214 ± 0.047	-0.955 ± 0.010
	5.886 ± 0.054	-1.023 ± 0.005
320	1.037 ± 0.018	0.951 ± 0.201
	1.599 ± 0.023	0.789 ± 0.129
	2.151 ± 0.025	0.237 ± 0.061
	2.744 ± 0.026	0.150 ± 0.032
	3.374 ± 0.027	-0.079 ± 0.046
	3.990 ± 0.038	-0.411 ± 0.006
	4.623 ± 0.036	-0.683 ± 0.035
	5.262 ± 0.047	-0.783 ± 0.005
	5.945 ± 0.054	-0.883 ± 0.004
330	1.024 ± 0.016	1.497 ± 0.191
	1.585 ± 0.026	1.111 ± 0.212
	2.145 ± 0.027	0.356 ± 0.118
	2.739 ± 0.025	0.236 ± 0.020
	3.373 ± 0.026	0.127 ± 0.011
	4.002 ± 0.038	-0.230 ± 0.010
	4.649 ± 0.038	-0.492 ± 0.021
	5.298 ± 0.047	-0.645 ± 0.002
	5.993 ± 0.054	-0.770 ± 0.004

Table S3 Same as Table S1 for temperature interval between 310 K and 330 K.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
340	1.024 ± 0.016	1.497 ± 0.191
	1.585 ± 0.026	1.111 ± 0.212
	2.145 ± 0.027	0.356 ± 0.118
	2.739 ± 0.025	0.236 ± 0.020
	3.373 ± 0.026	0.127 ± 0.011
	4.002 ± 0.038	-0.230 ± 0.010
	4.649 ± 0.038	-0.492 ± 0.021
	5.298 ± 0.047	-0.645 ± 0.002
	5.993 ± 0.054	-0.770 ± 0.004
350	0.983 ± 0.012	2.631 ± 0.170
	1.541 ± 0.034	1.631 ± 0.379
	2.126 ± 0.034	0.506 ± 0.208
	2.723 ± 0.025	0.332 ± 0.009
	3.353 ± 0.027	0.436 ± 0.063
	4.008 ± 0.035	0.061 ± 0.063
	4.678 ± 0.037	-0.123 ± 0.060
	5.354 ± 0.048	-0.412 ± 0.002
	6.074 ± 0.055	-0.575 ± 0.003
360	0.956 ± 0.010	3.174 ± 0.161
	1.516 ± 0.040	1.824 ± 0.455
	2.115 ± 0.038	0.548 ± 0.239
	2.714 ± 0.024	0.356 ± 0.016
	3.337 ± 0.030	0.541 ± 0.096
	4.003 ± 0.032	0.168 ± 0.093
	4.680 ± 0.034	0.041 ± 0.090
	5.373 ± 0.048	-0.321 ± 0.004
	6.105 ± 0.056	-0.498 ± 0.002

Table S4 Same as Table S1 for temperature interval between 340 K and 360 K.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
240	0.960 ± 0.035	-3.740 ± 0.281
	2.419 ± 0.028	-6.514 ± 0.664
	4.087 ± 0.06	-3.867 ± 0.505
250	0.993 ± 0.033	-3.189 ± 0.260
	2.553 ± 0.040	-4.774 ± 0.256
	4.229 ± 0.046	-3.215 ± 0.317
260	1.023 ± 0.032	-2.592 ± 0.236
	2.663 ± 0.045	-3.329 ± 0.029
	4.359 ± 0.036	-2.611 ± 0.17
270	1.046 ± 0.030	-2.042 ± 0.215
	2.736 ± 0.044	-2.306 ± 0.128
	4.460 ± 0.032	-2.133 ± 0.077
280	1.064 ± 0.029	-1.493 ± 0.194
	2.786 ± 0.041	-1.514 ± 0.183
	4.543 ± 0.030	-1.721 ± 0.014
290	1.078 ± 0.027	-0.899 ± 0.170
	2.820 ± 0.036	-0.856 ± 0.190
	4.616 ± 0.031	-1.340 ± 0.027
300	1.084 ± 0.026	-0.352 ± 0.162
	2.837 ± 0.031	-0.390 ± 0.168
	4.669 ± 0.033	-1.038 ± 0.045

Table S5 Same as Table S1 for the temperature interval between 240 K and 300 K and using the LAMMPS implementation.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
310	1.085 ± 0.024	0.196 ± 0.162
	2.843 ± 0.027	-0.029 ± 0.129
	4.710 ± 0.036	-0.779 ± 0.049
320	1.080 ± 0.023	0.787 ± 0.162
	2.839 ± 0.024	0.271 ± 0.079
	4.743 ± 0.038	-0.538 ± 0.042
330	1.069 ± 0.022	1.333 ± 0.163
	2.828 ± 0.022	0.483 ± 0.070
	4.763 ± 0.022	-0.347 ± 0.027
340	1.05 ± 0.02	1.923 ± 0.163
	2.811 ± 0.022	0.659 ± 0.059
	4.776 ± 0.041	-0.171 ± 0.005
350	1.028 ± 0.020	2.467 ± 0.163
	2.792 ± 0.023	0.784 ± 0.068
	4.780 ± 0.041	-0.031 ± 0.019
360	1.002 ± 0.164	3.011 ± 0.019
	2.769 ± 0.110	0.880 ± 0.025
	4.779 ± 0.045	0.089 ± 0.039

Table S6 Same as Table S5 for the temperature interval between 310 K and 360 K.

T [K]	b [kg mol^{-1}]	$s_T \times 10^3$ [K^{-1}]
250	0.966 ± 0.029	-2.867 ± 0.235
	2.468 ± 0.036	-4.387 ± 0.182
	4.098 ± 0.067	-3.145 ± 0.267
260	0.993 ± 0.027	-2.305 ± 0.226
	2.568 ± 0.040	-3.203 ± 0.007
	4.223 ± 0.058	-2.618 ± 0.206
280	1.028 ± 0.024	-1.271 ± 0.209
	2.688 ± 0.037	-1.683 ± 0.120
	4.407 ± 0.047	-1.833 ± 0.123
300	1.043 ± 0.020	-0.196 ± 0.191
	2.752 ± 0.032	-0.711 ± 0.078
	4.543 ± 0.040	-1.221 ± 0.066
310	1.042 ± 0.018	0.319 ± 0.182
	2.766 ± 0.031	-0.391 ± 0.034
	4.591 ± 0.038	-0.985 ± 0.046
320	1.036 ± 0.016	0.876 ± 0.173
	2.773 ± 0.031	-0.121 ± 0.020
	4.633 ± 0.037	-0.765 ± 0.029
330	1.024 ± 0.014	1.390 ± 0.164
	2.774 ± 0.032	0.073 ± 0.071
	4.664 ± 0.036	-0.589 ± 0.016
340	1.007 ± 0.012	1.946 ± 0.155
	2.769 ± 0.035	0.237 ± 0.124
	4.688 ± 0.036	-0.425 ± 0.009
350	0.986 ± 0.010	2.458 ± 0.147
	2.761 ± 0.039	0.355 ± 0.170
	4.704 ± 0.036	-0.294 ± 0.012
360	0.960 ± 0.009	2.970 ± 0.138
	2.751 ± 0.043	0.448 ± 0.212
	4.715 ± 0.036	-0.181 ± 0.015

Table S7 Same as Table S1 for average pressure 100 bar for temperature interval between 250 K and 360 K.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
240	1.007 ± 0.030	-2.733 ± 0.171
	2.002 ± 0.054	-6.624 ± 0.628
	3.125 ± 0.055	-4.407 ± 0.425
	4.130 ± 0.076	-4.131 ± 0.608
250	1.030 ± 0.030	-1.993 ± 0.202
	2.099 ± 0.047	-3.470 ± 0.378
	3.220 ± 0.056	-2.082 ± 0.226
	4.271 ± 0.059	-2.891 ± 0.360
260	1.048 ± 0.028	-1.269 ± 0.288
	2.152 ± 0.041	-1.460 ± 0.218
	3.266 ± 0.057	-0.768 ± 0.094
	4.378 ± 0.048	-1.912 ± 0.194
270	1.058 ± 0.025	-0.666 ± 0.310
	2.170 ± 0.038	-0.373 ± 0.131
	3.280 ± 0.057	-0.138 ± 0.021
	4.445 ± 0.043	-1.254 ± 0.103
280	1.062 ± 0.022	-0.120 ± 0.291
	2.171 ± 0.036	0.280 ± 0.079
	3.278 ± 0.057	0.199 ± 0.023
	4.488 ± 0.040	-0.768 ± 0.050
290	1.060 ± 0.019	0.414 ± 0.232
	2.159 ± 0.034	0.695 ± 0.046
	3.268 ± 0.057	0.389 ± 0.050
	4.515 ± 0.039	-0.385 ± 0.021
300	1.054 ± 0.017	0.859 ± 0.152
	2.142 ± 0.033	0.920 ± 0.032
	3.254 ± 0.057	0.480 ± 0.065
	4.526 ± 0.038	-0.127 ± 0.009

Table S8 Soret coefficient as a function of LiCl molality for the system with cation size $\sigma_{Li^+,+0.05} = 0.1006\ nm$, and temperature range 240 K – 300 K. NEMD simulation were performed using the system equilibrated at an average pressure of 600 bar.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
310	1.043 ± 0.015	1.262 ± 0.052
	2.122 ± 0.032	1.055 ± 0.036
	3.238 ± 0.057	0.529 ± 0.073
	4.527 ± 0.038	0.063 ± 0.005
320	1.027 ± 0.015	1.656 ± 0.071
	2.098 ± 0.032	1.141 ± 0.038
	3.220 ± 0.056	0.556 ± 0.078
	4.520 ± 0.037	0.214 ± 0.007
330	1.009 ± 0.016	1.985 ± 0.195
	2.074 ± 0.031	1.187 ± 0.040
	3.202 ± 0.056	0.569 ± 0.081
	4.508 ± 0.037	0.315 ± 0.012
340	0.987 ± 0.019	2.306 ± 0.336
	2.048 ± 0.031	1.217 ± 0.041
	3.183 ± 0.056	0.577 ± 0.083
	4.492 ± 0.036	0.395 ± 0.018
350	0.964 ± 0.022	2.573 ± 0.471
	2.024 ± 0.030	1.233 ± 0.042
	3.165 ± 0.056	0.580 ± 0.083
	4.473 ± 0.035	0.448 ± 0.024
360	0.939 ± 0.026	2.815 ± 0.607
	2.000 ± 0.030	1.243 ± 0.042
	3.148 ± 0.055	0.582 ± 0.084
	4.453 ± 0.034	0.488 ± 0.029

Table S9 Same as Table S8 for for temperatures between 310 K and 360 K.

T [K]	b [$kg\,mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
240	1.054 ± 0.038	-1.562 ± 0.714
	2.148 ± 0.041	-2.772 ± 0.323
	3.237 ± 0.061	-2.253 ± 0.443
	4.491 ± 0.070	-3.394 ± 1.128
250	1.067 ± 0.032	-1.023 ± 0.593
	2.193 ± 0.035	-1.506 ± 0.281
	3.297 ± 0.049	-1.562 ± 0.330
	4.590 ± 0.041	-1.308 ± 0.370
260	1.076 ± 0.026	-0.440 ± 0.461
	2.214 ± 0.030	-0.423 ± 0.227
	3.340 ± 0.040	-0.898 ± 0.228
	4.620 ± 0.032	-0.098 ± 0.078
270	1.077 ± 0.022	0.098 ± 0.340
	2.215 ± 0.025	0.368 ± 0.175
	3.360 ± 0.035	-0.355 ± 0.151
	4.610 ± 0.031	0.498 ± 0.061
280	1.074 ± 0.019	0.635 ± 0.219
	2.200 ± 0.022	0.998 ± 0.122
	3.363 ± 0.031	0.128 ± 0.088
	4.580 ± 0.032	0.824 ± 0.048
290	1.063 ± 0.017	1.216 ± 0.088
	2.171 ± 0.019	1.538 ± 0.069
	3.350 ± 0.029	0.592 ± 0.076
	4.536 ± 0.032	1.013 ± 0.035
300	1.048 ± 0.017	1.752 ± 0.100
	2.134 ± 0.018	1.932 ± 0.023
	3.325 ± 0.028	0.971 ± 0.074
	4.490 ± 0.031	1.106 ± 0.027

Table S10 Same as Table S8 for $\sigma_{Li^+,+0.05} = 0.2006$ *nm* in the temperature interval between 240 K and 300 K.

T [K]	b [$kg\,mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
310	1.028 ± 0.017	2.287 ± 0.161
	2.092 ± 0.018	2.246 ± 0.019
	3.289 ± 0.028	1.309 ± 0.065
	4.441 ± 0.029	1.157 ± 0.046
320	1.001 ± 0.019	2.865 ± 0.283
	2.040 ± 0.018	2.515 ± 0.059
	3.238 ± 0.030	1.633 ± 0.062
	4.387 ± 0.026	1.186 ± 0.061
330	0.971 ± 0.022	3.399 ± 0.404
	1.989 ± 0.019	2.712 ± 0.092
	3.183 ± 0.031	1.899 ± 0.078
	4.336 ± 0.023	1.201 ± 0.071
340	0.934 ± 0.026	3.976 ± 0.534
	1.932 ± 0.021	2.880 ± 0.123
	3.117 ± 0.034	2.153 ± 0.090
	4.282 ± 0.019	1.209 ± 0.078
350	0.897 ± 0.030	4.509 ± 0.653
	1.878 ± 0.023	3.002 ± 0.147
	3.049 ± 0.036	2.361 ± 0.096
	4.232 ± 0.016	1.214 ± 0.083
360	0.856 ± 0.035	5.040 ± 0.773
	1.823 ± 0.025	3.100 ± 0.168
	2.978 ± 0.038	2.547 ± 0.098
	4.183 ± 0.012	1.216 ± 0.086

Table S11 Same as Table S10 for temperatures between 310 K and 360 K.

T [K]	b [$kg\,mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
240	0.994 ± 0.055	-7.262 ± 0.761
	1.901 ± 0.070	-10.560 ± 0.757
	2.999 ± 0.163	-6.723 ± 1.907
	4.316 ± 0.103	-2.788 ± 0.087
250	1.052 ± 0.051	-4.561 ± 0.682
	2.067 ± 0.084	-7.025 ± 0.142
	3.175 ± 0.124	-5.165 ± 1.284
	4.424 ± 0.102	-2.336 ± 0.086
260	1.090 ± 0.046	-2.278 ± 0.569
	2.190 ± 0.086	-4.160 ± 0.291
	3.325 ± 0.095	-3.683 ± 0.786
	4.522 ± 0.100	-1.847 ± 0.085
270	1.105 ± 0.042	-0.635 ± 0.455
	2.257 ± 0.080	-2.183 ± 0.431
	3.425 ± 0.077	-2.482 ± 0.457
	4.594 ± 0.098	-1.395 ± 0.084
280	1.104 ± 0.037	0.658 ± 0.340
	2.288 ± 0.072	-0.687 ± 0.444
	3.490 ± 0.068	-1.422 ± 0.229
	4.646 ± 0.095	-0.945 ± 0.083
290	1.090 ± 0.034	1.752 ± 0.221
	2.289 ± 0.062	0.526 ± 0.374
	3.523 ± 0.063	-0.414 ± 0.074
	4.680 ± 0.092	-0.457 ± 0.082
300	1.068 ± 0.031	2.538 ± 0.120
	2.268 ± 0.055	1.363 ± 0.311
	3.523 ± 0.062	0.403 ± 0.003
	4.690 ± 0.088	-0.008 ± 0.081

Table S12 Soret coefficient as a function of LiCl molality for the system with anion size $\sigma_{Cl^-,-0.05} = 0.3901\ nm$, and temperature range between 240 K and 300 K. NEMD simulation were performed using the system equilibrated at an average pressure of 600 bar.

T [K]	b [$kg\,mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
310	1.039 ± 0.030	3.158 ± 0.064
	2.231 ± 0.050	1.996 ± 0.273
	3.497 ± 0.062	1.125 ± 0.026
	4.681 ± 0.084	0.441 ± 0.080
320	1.002 ± 0.029	3.681 ± 0.059
	2.179 ± 0.047	2.509 ± 0.217
	3.443 ± 0.062	1.811 ± 0.010
	4.647 ± 0.080	0.927 ± 0.078
330	0.965 ± 0.029	4.058 ± 0.130
	2.123 ± 0.048	2.863 ± 0.160
	3.374 ± 0.060	2.367 ± 0.040
	4.596 ± 0.075	1.375 ± 0.077
340	0.923 ± 0.029	4.376 ± 0.196
	2.057 ± 0.051	3.150 ± 0.278
	3.283 ± 0.056	2.896 ± 0.118
	4.519 ± 0.070	1.859 ± 0.076
350	0.884 ± 0.030	4.605 ± 0.248
	1.994 ± 0.056	3.348 ± 0.391
	3.186 ± 0.049	3.324 ± 0.209
	4.429 ± 0.066	2.306 ± 0.075
360	0.845 ± 0.031	4.786 ± 0.293
	1.929 ± 0.063	3.497 ± 0.493
	3.079 ± 0.040	3.703 ± 0.312
	4.322 ± 0.061	2.753 ± 0.075

Table S13 Same as Table S1 for temperature interval between 310 K and 360 K.

$T\ [K]$	$b\ [kg\ mol^{-1}]$	$s_T \times 10^3\ [K^{-1}]$	$T\ [K]$	$b\ [kg\ mol^{-1}]$	$s_T \times 10^3\ [K^{-1}]$
240	0.845 ± 0.034	-5.255 ± 1.376	310	1.075 ± 0.024	-1.725 ± 0.292
	1.733 ± 0.024	-6.309 ± 0.037		2.192 ± 0.019	-1.563 ± 0.087
	2.690 ± 0.055	-6.421 ± 0.557		3.375 ± 0.025	-1.381 ± 0.134
	3.829 ± 0.036	-3.897 ± 0.030		4.639 ± 0.025	-1.758 ± 0.011
250	0.887 ± 0.031	-4.760 ± 0.593	320	1.092 ± 0.025	-1.195 ± 0.058
	1.831 ± 0.025	-5.193 ± 0.031		2.225 ± 0.018	-1.266 ± 0.082
	2.845 ± 0.052	-5.182 ± 0.381		3.419 ± 0.021	-1.095 ± 0.118
	3.969 ± 0.036	-3.559 ± 0.058		4.718 ± 0.026	-1.487 ± 0.028
260	0.929 ± 0.028	-4.225 ± 0.351	330	1.102 ± 0.025	-0.706 ± 0.213
	1.923 ± 0.025	-4.206 ± 0.062		2.249 ± 0.016	-1.042 ± 0.076
	2.985 ± 0.048	-4.108 ± 0.242		3.451 ± 0.018	-0.884 ± 0.104
	4.112 ± 0.034	-3.208 ± 0.075		4.781 ± 0.028	-1.248 ± 0.070
270	0.966 ± 0.027	-3.732 ± 0.304	340	1.107 ± 0.025	-0.177 ± 0.552
	1.995 ± 0.025	-3.461 ± 0.079		2.272 ± 0.015	-0.844 ± 0.068
	3.094 ± 0.043	-3.315 ± 0.194		3.480 ± 0.014	-0.700 ± 0.091
	4.235 ± 0.032	-2.897 ± 0.080		4.837 ± 0.034	-1.000 ± 0.122
280	0.999 ± 0.026	-3.240 ± 0.471	350	1.106 ± 0.025	0.311 ± 0.899
	2.057 ± 0.024	-2.849 ± 0.088		2.289 ± 0.013	-0.694 ± 0.062
	3.184 ± 0.039	-2.675 ± 0.181		3.501 ± 0.011	-0.565 ± 0.079
	4.349 ± 0.030	-2.600 ± 0.076		4.879 ± 0.041	-0.781 ± 0.174
290	1.030 ± 0.025	-2.707 ± 0.510	360	1.100 ± 0.026	0.798 ± 1.273
	2.113 ± 0.022	-2.307 ± 0.092		2.302 ± 0.012	-0.572 ± 0.055
	3.265 ± 0.034	-2.121 ± 0.164		3.518 ± 0.009	-0.456 ± 0.069
	4.461 ± 0.027	-2.292 ± 0.061		4.911 ± 0.051	-0.570 ± 0.232
300	1.055 ± 0.025	-2.216 ± 0.442			
	2.156 ± 0.021	-1.899 ± 0.091			
	3.325 ± 0.029	-1.711 ± 0.149			
	4.555 ± 0.026	-2.019 ± 0.040			

Table S15 Same as Table S14 for temperatures between 310 K and 360 K.

Table S14 Same as Table S12 for $\sigma_{Cl^-,+0.05}$ = 0.4901 nm in the temperature interval between 240 K and 300 K.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
240	0.885 ± 0.026	-4.622 ± 0.301
	2.200 ± 0.029	-6.545 ± 0.188
	3.841 ± 0.043	-3.536 ± 0.056
250	0.923 ± 0.024	-4.072 ± 0.267
	2.329 ± 0.033	-5.267 ± 0.020
	3.969 ± 0.044	-3.262 ± 0.046
260	0.961 ± 0.023	-3.477 ± 0.230
	2.446 ± 0.034	-4.141 ± 0.083
	4.100 ± 0.045	-2.965 ± 0.034
270	0.991 ± 0.022	-2.929 ± 0.196
	2.535 ± 0.032	-3.297 ± 0.126
	4.213 ± 0.045	-2.691 ± 0.035
280	1.016 ± 0.020	-2.381 ± 0.162
	2.608 ± 0.030	-2.605 ± 0.134
	4.318 ± 0.044	-2.417 ± 0.047
290	1.039 ± 0.019	-1.789 ± 0.125
	2.671 ± 0.027	-1.997 ± 0.117
	4.422 ± 0.043	-2.121 ± 0.061
300	1.054 ± 0.018	-1.242 ± 0.091
	2.717 ± 0.025	-1.541 ± 0.086
	4.508 ± 0.041	-1.848 ± 0.073
310	1.064 ± 0.018	-0.697 ± 0.104
	2.752 ± 0.023	-1.167 ± 0.046
	4.583 ± 0.038	-1.575 ± 0.085

Table S16 Soret coefficient as a function of LiCl molality of the system with the molar mass inverted, $M_{Li^+} = 35.453\ g\ mol^{-1}$ and $M_{Cl^-} = 6.941\ g\ mol^{-1}$, in the temperature range between 240 K and 310 K. NEMD simulation were performed using the system equilibrated at an average pressure of 500 bar.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
320	1.068 ± 0.018	-0.106 ± 0.138
	2.781 ± 0.023	-0.838 ± 0.003
	4.651 ± 0.034	-1.280 ± 0.099
330	1.067 ± 0.017	0.438 ± 0.168
	2.800 ± 0.024	-0.591 ± 0.049
	4.703 ± 0.030	-1.007 ± 0.111
340	1.059 ± 0.018	1.027 ± 0.202
	2.814 ± 0.026	-0.374 ± 0.098
	4.746 ± 0.024	-0.713 ± 0.124
350	1.045 ± 0.018	1.570 ± 0.233
	2.822 ± 0.029	-0.211 ± 0.142
	4.772 ± 0.018	-0.441 ± 0.137
360	1.027 ± 0.019	2.112 ± 0.263
	2.826 ± 0.034	-0.078 ± 0.183
	4.786 ± 0.012	-0.170 ± 0.149

Table S17 Same as Table S16 for temperatures between 320 K and 360 K.

T [K]	b [kg mol^{-1}]	$s_T \times 10^3$ [K^{-1}]
240	1.001 ± 0.032	-1.910 ± 0.569
	2.541 ± 0.067	-2.185 ± 0.862
	4.041 ± 0.078	-4.579 ± 0.573
250	1.018 ± 0.027	-1.555 ± 0.475
	2.590 ± 0.050	-1.817 ± 0.609
	4.199 ± 0.062	-3.446 ± 0.350
260	1.032 ± 0.023	-1.171 ± 0.372
	2.635 ± 0.037	-1.436 ± 0.387
	4.331 ± 0.052	-2.501 ± 0.191
270	1.042 ± 0.020	-0.817 ± 0.278
	2.667 ± 0.030	-1.099 ± 0.225
	4.422 ± 0.047	-1.832 ± 0.098
280	1.049 ± 0.018	-0.463 ± 0.184
	2.691 ± 0.026	-0.776 ± 0.098
	4.489 ± 0.045	-1.312 ± 0.041
290	1.052 ± 0.016	-0.080 ± 0.082
	2.709 ± 0.025	-0.442 ± 0.007
	4.540 ± 0.045	-0.879 ± 0.037
300	1.051 ± 0.016	0.272 ± 0.074
	2.716 ± 0.026	-0.147 ± 0.074
	4.572 ± 0.045	-0.572 ± 0.040
310	1.046 ± 0.016	0.624 ± 0.107
	2.716 ± 0.029	0.137 ± 0.119
	4.592 ± 0.046	-0.333 ± 0.039

Table S18 Same as Table S16 for $M_{Li^+} = M_{Cl^-} = 35.453\ g\ mol^{-1}$, in the range of temperature between 240 K and 310 K.

T [K]	b [kg mol^{-1}]	$s_T \times 10^3$ [K^{-1}]
320	1.037 ± 0.018	1.005 ± 0.208
	2.708 ± 0.033	0.430 ± 0.145
	4.603 ± 0.046	-0.134 ± 0.033
330	1.026 ± 0.020	1.357 ± 0.302
	2.694 ± 0.036	0.689 ± 0.151
	4.605 ± 0.046	0.007 ± 0.025
340	1.009 ± 0.024	1.736 ± 0.404
	2.671 ± 0.040	0.958 ± 0.141
	4.602 ± 0.046	0.124 ± 0.016
350	0.991 ± 0.028	2.087 ± 0.497
	2.643 ± 0.043	1.195 ± 0.140
	4.595 ± 0.045	0.207 ± 0.028
360	0.969 ± 0.032	2.436 ± 0.591
	2.610 ± 0.045	1.422 ± 0.178
	4.584 ± 0.043	0.272 ± 0.040

Table S19 Same as Table S18 for temperatures between 320 K and 360 K.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
240	0.838 ± 0.031	-5.077 ± 0.574
	2.195 ± 0.039	-5.619 ± 0.248
	3.707 ± 0.065	-4.124 ± 0.200
250	0.878 ± 0.028	-4.603 ± 0.492
	2.307 ± 0.041	-4.771 ± 0.183
	3.850 ± 0.060	-3.717 ± 0.173
260	0.919 ± 0.025	-4.090 ± 0.404
	2.415 ± 0.042	-3.996 ± 0.127
	3.994 ± 0.056	-3.321 ± 0.149
270	0.954 ± 0.023	-3.618 ± 0.324
	2.502 ± 0.039	-3.393 ± 0.175
	4.117 ± 0.052	-2.993 ± 0.129
280	0.985 ± 0.021	-3.146 ± 0.243
	2.579 ± 0.036	-2.881 ± 0.205
	4.232 ± 0.049	-2.697 ± 0.111
290	1.016 ± 0.019	-2.635 ± 0.155
	2.651 ± 0.031	-2.413 ± 0.217
	4.346 ± 0.045	-2.410 ± 0.095
300	1.039 ± 0.018	-2.164 ± 0.075
	2.709 ± 0.026	-2.049 ± 0.214
	4.443 ± 0.042	-2.172 ± 0.082
310	1.059 ± 0.018	-1.694 ± 0.010
	2.759 ± 0.021	-1.740 ± 0.202
	4.533 ± 0.040	-1.957 ± 0.070

Table S20 Same as Table S18 for $M_{Li^+} = M_{Cl^-} = 6.941\ g\ mol^{-1}$, in the range of temperature between 240 K and 310 K.

T [K]	b [$kg\ mol^{-1}$]	$s_T \times 10^3$ [K^{-1}]
320	1.075 ± 0.019	-1.185 ± 0.093
	2.805 ± 0.016	-1.457 ± 0.182
	4.621 ± 0.038	-1.749 ± 0.060
330	1.085 ± 0.021	-0.716 ± 0.173
	2.842 ± 0.011	-1.237 ± 0.160
	4.696 ± 0.036	-1.576 ± 0.051
340	1.090 ± 0.023	-0.209 ± 0.259
	2.875 ± 0.007	-1.036 ± 0.132
	4.770 ± 0.034	-1.408 ± 0.043
350	1.090 ± 0.027	0.259 ± 0.339
	2.902 ± 0.006	-0.880 ± 0.106
	4.831 ± 0.033	-1.269 ± 0.037
360	1.085 ± 0.030	0.727 ± 0.419
	2.925 ± 0.009	-0.747 ± 0.110
	4.888 ± 0.031	-1.144 ± 0.031

Table S21 Same as Table S20 for temperatures between 320 K and 360 K.

b_{ave} [kg mol^{-1}]	T [K]	b [kg mol^{-1}]	b_{ave} [kg mol^{-1}]	T [K]	b [kg mol^{-1}]
0.97	247.304 ± 0.104	0.963 ± 0.031	3.12	247.402 ± 0.113	2.989 ± 0.035
	261.645 ± 0.096	0.993 ± 0.033		261.802 ± 0.110	3.138 ± 0.046
	275.807 ± 0.078	1.013 ± 0.034		276.079 ± 0.099	3.258 ± 0.039
	289.851 ± 0.081	1.039 ± 0.019		290.258 ± 0.076	3.329 ± 0.032
	303.880 ± 0.062	1.049 ± 0.019		304.395 ± 0.088	3.361 ± 0.031
	317.901 ± 0.067	1.045 ± 0.020		318.495 ± 0.086	3.366 ± 0.028
	331.922 ± 0.078	1.022 ± 0.015		332.617 ± 0.088	3.369 ± 0.027
	346.069 ± 0.080	0.986 ± 0.014		346.839 ± 0.088	3.360 ± 0.026
1.49	247.326 ± 0.417	1.456 ± 0.035	3.70	247.395 ± 0.142	3.557 ± 0.072
	260.961 ± 1.511	1.531 ± 0.035		261.778 ± 0.134	3.701 ± 0.041
	275.001 ± 1.687	1.580 ± 0.025		276.007 ± 0.132	3.819 ± 0.038
	288.978 ± 1.832	1.606 ± 0.021		290.186 ± 0.121	3.901 ± 0.042
	302.954 ± 1.922	1.609 ± 0.022		304.291 ± 0.121	3.965 ± 0.042
	316.979 ± 1.907	1.605 ± 0.024		318.376 ± 0.099	3.977 ± 0.031
	331.027 ± 1.885	1.581 ± 0.028		332.497 ± 0.085	4.002 ± 0.034
	345.150 ± 1.883	1.552 ± 0.032		346.725 ± 0.075	4.012 ± 0.039
2.01	247.341 ± 0.079	1.966 ± 0.048	4.31	247.169 ± 0.109	4.135 ± 0.074
	261.712 ± 0.077	2.073 ± 0.042		261.553 ± 0.104	4.286 ± 0.040
	275.910 ± 0.070	2.123 ± 0.031		275.798 ± 0.105	4.395 ± 0.036
	290.006 ± 0.064	2.133 ± 0.032		289.994 ± 0.084	4.476 ± 0.040
	304.048 ± 0.069	2.156 ± 0.028		304.126 ± 0.077	4.561 ± 0.025
	318.091 ± 0.073	2.157 ± 0.022		318.275 ± 0.065	4.624 ± 0.034
	332.153 ± 0.083	2.148 ± 0.026		332.441 ± 0.052	4.660 ± 0.041
	346.346 ± 0.074	2.123 ± 0.034		346.697 ± 0.051	4.673 ± 0.035
2.56	247.402 ± 0.455	2.495 ± 0.036	4.94	247.163 ± 0.165	4.692 ± 0.051
	261.113 ± 1.149	2.624 ± 0.035		261.561 ± 0.150	4.851 ± 0.053
	274.957 ± 1.606	2.715 ± 0.034		275.840 ± 0.139	4.988 ± 0.038
	288.766 ± 1.858	2.718 ± 0.030		290.034 ± 0.111	5.098 ± 0.043
	302.483 ± 2.132	2.748 ± 0.029		304.197 ± 0.112	5.170 ± 0.032
	316.286 ± 2.606	2.745 ± 0.025		318.357 ± 0.105	5.243 ± 0.041
	330.884 ± 2.210	2.748 ± 0.024		332.549 ± 0.098	5.310 ± 0.047
	345.608 ± 1.920	2.720 ± 0.026		346.823 ± 0.089	5.347 ± 0.048

Table S22 Salt concentrations as a function of temperature for solutions in the concentrations range between 0.97 – 2.56 mol kg^{-1}. The data are obtained with the method implemented in GROMACS. The NEMD simulations were performed using the system equilibrated at an average pressure of 600 bar.

Table S23 Same as Table S22 for the the solutions at average concentrations range between 3.12 – 4.9 mol kg^{-1}.

b_{ave} $[kg\ mol^{-1}]$	T $[K]$	b $[kg\ mol^{-1}]$
5.60	247.372 ± 0.168	5.346 ± 0.072
	261.718 ± 0.164	5.502 ± 0.050
	275.955 ± 0.153	5.628 ± 0.055
	290.083 ± 0.128	5.761 ± 0.036
	304.228 ± 0.116	5.839 ± 0.039
	318.382 ± 0.097	5.935 ± 0.040
	332.567 ± 0.094	6.012 ± 0.052
	346.794 ± 0.090	6.080 ± 0.060

Table S24 Same as Table S22 for the solution at average concentration 5.6 mol kg^{-1}.