Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Mobility and Association of Ions in Aqueous Solutions: The Case of Imidazolium Based Ionic Liquids

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Electronic Supplementary Information

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A. MD simulations

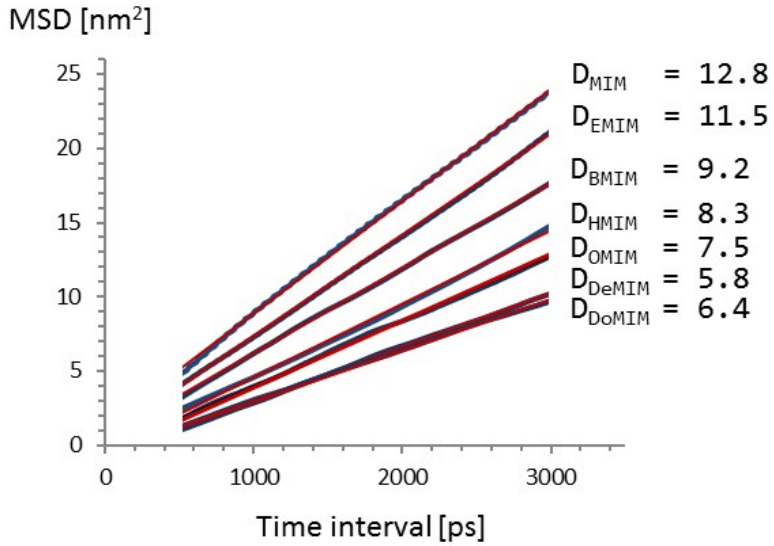


Figure A1: Mean square displacements of the center-of-mass of cations as a function of time interval, as derived from MD simulations. Diffusion coefficients for the different cations derived as slopes of these curves are shown on the right hand side in units of 10^{-10} m^2 s^{-1}. The part of the curves that is shown has been used to determine the slopes. For clarity, curves were slightly shifted vertically relative to each other. The linearity of the curves can be clearly seen.

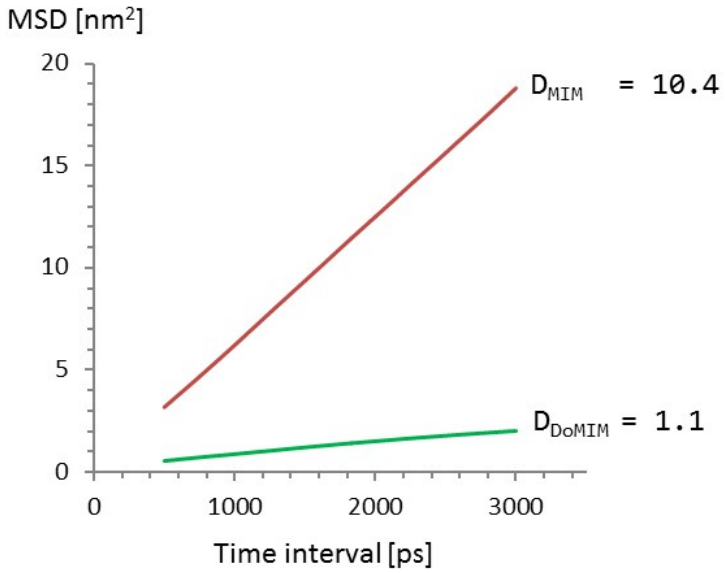


Figure A2: Mean square displacements of the center-of-mass of MIM cations (red) and 1,3-DoMIM cations (green), at very high concentrations (1.0 M and 1.2 M, respectively), as a function of time interval as derived from MD simulations. Diffusion coefficients were derived as slopes of these curves and are shown on the right hand side in units of 10^{-10} m^2 s^{-1}.

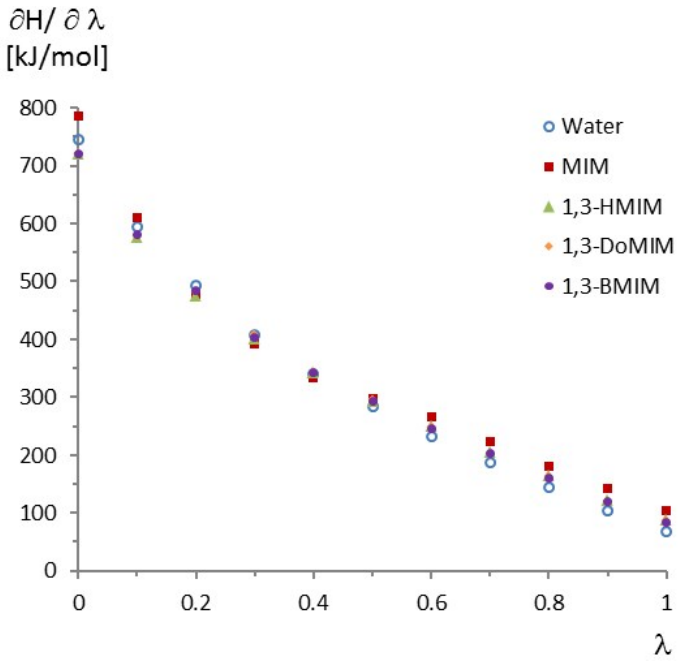


Figure A3: Derivate of enthalpy with respect to the interaction coupling parameter λ, ∂H/∂λ as a function of λ as derived from gradually switching off the Coulomb interactions of Cl^- when binding to MIM, 1,3-BMIM, 1,3-HMIM and 1,3-DoMIM in solution and in pure water.

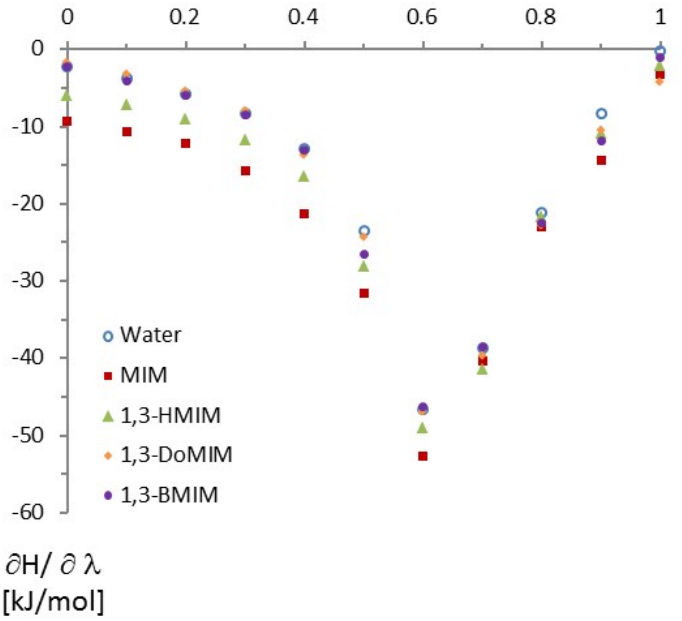
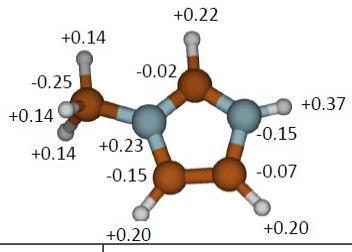


Figure A4: Derivate of enthalpy with respect to the interaction coupling parameter λ, ∂H/∂λ as a function of λ as derived from gradually switching off the Lennard-Jones interactions of uncharged Cl^- when binding to MIM, 1,3-BMIM, 1,3-HMIM and 1,3-DoMIM in solution and in pure water

B. RISM Calculations

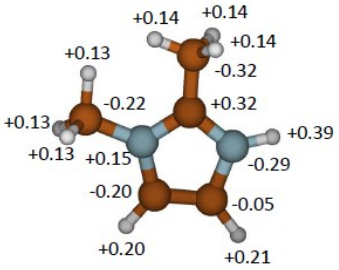
Atom charges and coordinates

Figure B1. $[MIM]^+$



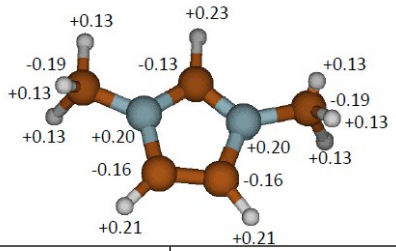
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.108	0.665	0.000
C3	-2.105	-0.696	-0.000
C4	-0.325	2.471	0.000
N1	-0.786	1.077	0.000
N2	-0.782	-1.082	-0.000
H1	1.076	-0.000	-0.000
H2	-2.922	1.367	0.000
H3	-2.912	-1.407	-0.000
H4	-0.696	2.971	-0.892
H5	-0.696	2.972	0.892
H6	0.762	2.480	0.000
H7	-0.441	-2.035	-0.000

Figure B2. $[1,2\text{-MMIM}]^+$



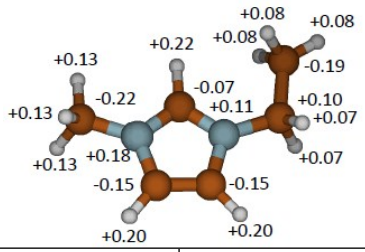
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	1.484	0.000	0.000
C3	-2.124	-0.694	0.000
C4	-2.126	0.662	-0.007
C5	-0.354	2.473	-0.047
N1	-0.803	1.076	-0.004
N2	-0.798	-1.077	0.005
H1	1.868	0.522	-0.879
H2	1.859	-1.022	-0.010
H3	1.868	0.503	0.891
H4	-1.164	3.103	0.311
H5	0.512	2.599	0.600
H6	-0.097	2.750	-1.070
H7	-2.940	1.366	-0.013
H8	-2.928	-1.407	0.007
H9	-0.464	-2.032	0.015

Figure B3. $[1,3\text{-MMIM}]^+$



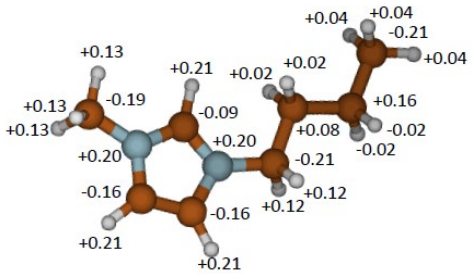
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.098	0.680	0.000
C3	-2.098	-0.680	-0.000
C4	-0.307	2.476	0.000
C5	-0.307	-2.476	-0.000
N1	-0.777	1.086	0.000
N2	-0.777	-1.086	-0.000
H1	1.076	-0.000	-0.000
H2	-2.912	1.384	0.000
H3	-2.912	-1.384	-0.000
H4	0.780	2.478	-0.002
H5	-0.676	2.981	-0.891
H6	-0.673	2.980	0.893
H7	-0.676	-2.981	-0.891
H8	-0.673	-2.980	0.893
H9	0.780	-2.478	-0.002

Figure B4. $[1,3\text{-EMIM}]^+$



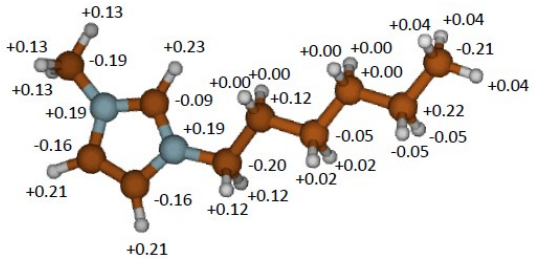
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.092	0.702	0.000
C3	-2.104	-0.658	-0.000
C4	-0.285	2.479	0.000
C5	-0.362	-2.500	-0.000
C6	1.148	-2.679	-0.000
N1	-0.768	1.094	0.000
N2	-0.787	-1.080	-0.000
H1	1.075	0.000	0.000
H2	-2.899	1.413	0.000
H3	-2.925	-1.355	-0.000
H4	-0.648	2.988	0.893
H5	-0.648	2.988	-0.892
H6	0.803	2.472	0.000
H7	-0.807	-2.960	-0.883
H8	-0.807	-2.960	0.884
H9	1.611	-2.249	0.891
H10	1.611	-2.249	-0.891
H11	1.360	-3.750	-0.000

Figure B5. $[1,3\text{-BMIM}]^+$



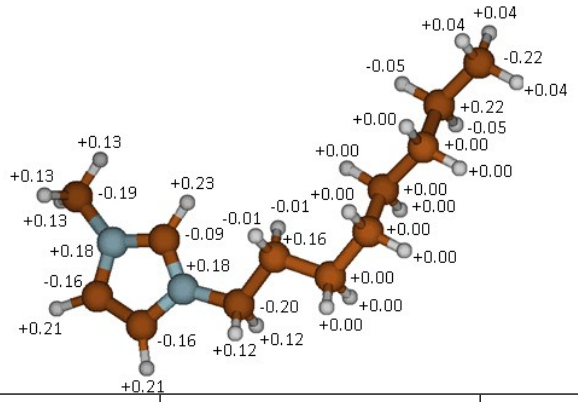
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.090	0.705	0.000
C3	-2.105	-0.654	0.000
C4	-0.282	2.481	0.003
C5	-0.368	-2.500	-0.002
C6	1.143	-2.692	0.031
C7	1.509	-4.183	0.034
C8	3.022	-4.413	0.070
N1	-0.766	1.096	-0.000
N2	-0.789	-1.078	0.001
H1	1.075	0.000	0.000
H2	-2.896	1.418	0.000
H3	-2.926	-1.349	0.000
H4	-0.650	2.993	-0.884
H5	-0.637	2.985	0.900
H6	0.806	2.471	-0.005
H7	-0.835	-2.965	0.868
H8	-0.795	-2.951	-0.899
H9	1.600	-2.211	-0.840
H10	1.559	-2.217	0.926
H11	1.043	-4.667	0.899
H12	1.085	-4.660	-0.857
H13	3.510	-3.965	-0.801
H14	3.467	-3.972	0.967
H15	3.255	-5.481	0.071

Figure B6. $[1,3\text{-HMIM}]^+$



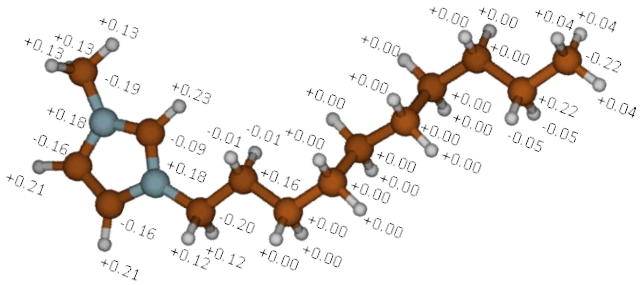
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.116	0.698	0.018
C3	-2.125	-0.660	0.020
C4	-0.305	2.467	0.019
C5	-0.366	-2.491	0.016
C6	1.121	-2.676	0.278
C7	1.480	-4.167	0.315
C8	2.978	-4.409	0.520
C9	3.351	-5.894	0.548
C10	4.854	-6.135	0.715
N1	-0.779	1.083	0.007
N2	-0.792	-1.072	0.019
H1	1.078	0.000	-0.000
H2	-2.923	1.411	0.029
H3	-2.944	-1.357	0.036
H4	-0.685	2.974	-0.866
H5	-0.668	2.957	0.921
H6	0.783	2.470	0.008
H7	-0.956	-2.974	0.795
H8	-0.649	-2.918	-0.949
H9	1.709	-2.190	-0.508
H10	1.389	-2.203	1.229
H11	0.917	-4.659	1.118
H12	1.162	-4.641	-0.622
H13	3.536	-3.912	-0.284
H14	3.300	-3.935	1.456
H15	2.809	-6.388	1.364
H16	3.008	-6.370	-0.379
H17	5.419	-5.691	-0.110
H18	5.225	-5.692	1.646
H19	5.086	-7.203	0.740

Figure B7. [1,3-OMIM]$^+$



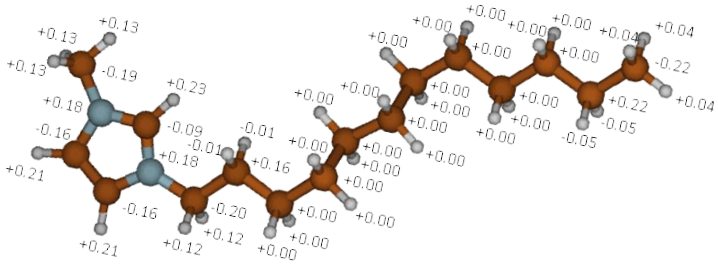
Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.091	0.703	0.001
C3	-2.104	-0.657	0.001
C4	-0.283	2.480	0.013
C5	-0.366	-2.501	-0.014
C6	1.146	-2.693	0.024
C7	1.512	-4.183	0.008
C8	3.025	-4.422	0.054
C9	3.405	-5.906	0.023
C10	4.917	-6.152	0.078
C11	5.300	-7.636	0.039
C12	6.812	-7.872	0.098
N1	-0.766	1.094	-0.000
N2	-0.787	-1.079	-0.000
H1	1.076	-0.000	0.000
H2	-2.898	1.415	0.001
H3	-2.924	-1.352	-0.001
H4	-0.729	3.022	-0.820
H5	-0.558	2.951	0.955
H6	0.800	2.476	-0.094
H7	-0.837	-2.974	0.849
H8	-0.789	-2.944	-0.917
H9	1.606	-2.200	-0.840
H10	1.557	-2.229	0.927
H11	1.039	-4.682	0.862
H12	1.098	-4.648	-0.895
H13	3.498	-3.910	-0.793
H14	3.436	-3.961	0.961
H15	2.925	-6.420	0.867
H16	2.998	-6.365	-0.886
H17	5.398	-5.635	-0.761
H18	5.325	-5.698	0.991
H19	4.817	-8.155	0.877
H20	4.896	-8.088	-0.874
H21	7.240	-7.461	1.019
H22	7.051	-8.939	0.068
H23	7.320	-7.394	-0.745

Figure B8. $[1,3\text{-DeMIM}]^+$



Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.091	0.702	0.001
C3	-2.103	-0.657	0.001
C4	-0.285	2.481	0.006
C5	-0.363	-2.500	-0.004
C6	1.149	-2.689	0.002
C7	1.520	-4.179	-0.002
C8	3.035	-4.410	0.007
C9	3.422	-5.893	0.000
C10	4.937	-6.128	0.011
C11	5.329	-7.610	0.002
C12	6.843	-7.845	0.015
C13	7.236	-9.327	0.003
C14	8.750	-9.552	0.017
N1	-0.767	1.093	0.001
N2	-0.787	-1.079	0.000
H1	1.076	-0.000	0.000
H2	-2.898	1.414	0.002
H3	-2.923	-1.354	0.000
H4	-0.682	3.002	-0.864
H5	-0.615	2.974	0.919
H6	0.802	2.475	-0.035
H7	-0.814	-2.964	0.875
H8	-0.806	-2.955	-0.892
H9	1.588	-2.206	-0.876
H10	1.579	-2.212	0.890
H11	1.072	-4.667	0.871
H12	1.085	-4.658	-0.886
H13	3.482	-3.914	-0.863
H14	3.469	-3.926	0.892
H15	2.973	-6.388	0.870
H16	2.988	-6.375	-0.885
H17	5.386	-5.630	-0.857
H18	5.371	-5.645	0.897
H19	4.878	-8.107	0.870
H20	4.896	-8.091	-0.886
H21	7.295	-7.347	-0.853
H22	7.276	-7.365	0.902
H23	6.785	-9.826	0.870
H24	6.804	-9.808	-0.884
H25	8.997	-10.617	0.008
H26	9.207	-9.113	0.911
H27	9.226	-9.092	-0.856

Figure B9. $[1,3DoDMIM]^+$



Atom	*x* (Å)	*y* (Å)	*z* (Å)
C1	0.000	0.000	0.000
C2	-2.092	0.703	-0.001
C3	-2.104	-0.655	-0.001
C4	-0.282	2.480	0.000
C5	-0.365	-2.499	0.000
C6	1.147	-2.686	0.000
C7	1.523	-4.174	0.000
C8	3.040	-4.397	0.000
C9	3.438	-5.877	-0.000
C10	4.956	-6.097	0.000
C11	5.363	-7.575	0.000
C12	6.881	-7.792	0.000
C13	7.292	-9.269	-0.000
C14	8.809	-9.484	-0.000
C15	9.223	-10.961	0.001
C16	10.741	-11.164	-0.000
N1	-0.766	1.095	-0.001
N2	-0.788	-1.079	0.000
H1	1.074	0.000	-0.000
H2	-2.897	1.416	-0.001
H3	-2.926	-1.352	-0.002
H4	-0.646	2.990	-0.890
H5	-0.641	2.987	0.894
H6	0.806	2.471	-0.003
H7	-0.811	-2.959	0.884
H8	-0.811	-2.959	-0.884
H9	1.581	-2.206	-0.884
H10	1.581	-2.206	0.883
H11	1.083	-4.660	0.879
H12	1.083	-4.661	-0.878
H13	3.476	-3.905	-0.877
H14	3.477	-3.905	0.878
H15	3.001	-6.369	0.878
H16	3.001	-6.369	-0.878
H17	5.391	-5.603	-0.878
H18	5.392	-5.603	0.878
H19	4.927	-8.070	0.879
H20	4.927	-8.071	-0.877
H21	7.316	-7.296	-0.878
H22	7.316	-7.296	0.877
H23	6.857	-9.765	0.878
H24	6.856	-9.765	-0.877
H25	9.245	-8.988	0.877
H26	9.245	-8.989	-0.878
H27	8.788	-11.456	-0.876
H28	8.789	-11.455	0.877
H29	11.003	-12.226	-0.000
H30	11.200	-10.707	0.883
H31	11.200	-10.708	-0.883

C. Experiment

Materials:

1-Methylimidazolium chloride, 98 % (IL-0094-SG-0025) Lot: J00120.1.1

1,2-Dimethylimidazolium chloride, 98 % (IL-0277-SG-0025) Lot: J00123.1.2

1,3-Dimethylimidazolium chloride, 98 % (CS-0399-HP-0050) Lot: K00133.1.1-CS-0399

1-Ethyl-3-methylimidazolium chloride, >98 % (IL-0093-HP-0050) Lot: J01321.8

1-Butyl-3-methylimidazolium chloride, 99 % (IL-0014-HP-0100) Lot: I01028.3

1-Hexyl-3-methylimidazolium chloride, >98 % (IL-0054-HP-0050) Lot: I00225.1

1-Octyl-3-methylimidazolium chloride, >98 % (IL-0072-HP-0025) Lot: J00233.1.1

1-Decyl-3-methylimidazolium chloride, >98 % (IL-0065-HP-0025) Lot: K00131.1

1-Dodecyl-3-methylimidazolium chloride, >98 % (IL-0120-HP-0025) Lot: K00141.1

Table C1. Densities, viscosities and dielectric constants of pure water and limiting ionic conductances of Cl^- in water.[a] In Supporting Maaterial

T	d_0[b]	$\eta \cdot 10^3$[c]	ε[d]	$\lambda^\infty(Cl^-)$[e]
278.15	0.999967	1.5192	85.897	47.50
283.15	0.999702	1.3069	83.945	54.33
288.15	0.999102	1.1382	82.039	61.42
293.15	0.998206	1.0020	80.176	68.77
298.15	0.997048	0.8903	78.358	76.35
303.15	0.995651	0.7975	76.581	84.17
308.15	0.994036	0.7195	74.846	92.20
313.15	0.992219	0.6530	73.157	100.46

[a]Units: T, K; d_0, $kg \cdot dm^{-3}$; η, Pa·s; λ^∞, $S \cdot cm^2 \cdot mol^{-1}$

[b]Ref.[1]; [c]Ref.[2]; [d]Ref.[3]; [e]Ref.[4]

Table C2. Molar conductivities, Λ, of investigated systems in aqueous solutions, together with density coefficient b and molar mass of solute, M_2 .[a]

	T							
$m \cdot 10^3$	278.15	283.15	288.15	293.15	298.15	303.15	308.15	313-15
[MIM][Cl], b =0.0237, M_2 = 117.59								
0.18954	75.240	86.648						
0.44403	74.774	86.062						
0.70033	74.512	85.522	97.091	109.164	121.750	134.759	147.845	160.925
0.98194	74.192	85.130	96.608	108.622	121.083	134.011	147.313	160.517
1.29376	73.887	84.723	96.166	108.107	120.478	133.274	146.352	159.057
1.63866	73.692	84.498	95.815	107.677	119.955	132.588	145.291	158.107
2.03783	73.437	84.096	95.372	107.166	119.379	131.984	144.744	157.495
2.58313	73.065	83.743	94.931	106.651	118.771	131.315	144.157	157.087
3.2472	72.732	83.354	94.451	106.090	118.141	130.584	143.372	156.219
4.10998	72.371	82.908	93.936	105.498	117.449	129.778	142.214	154.712
5.17933	71.970	82.431	93.343	104.801	116.680	128.912	141.422	153.757
[1,2-MMIM][Cl], b = 0.0193, M_2 = 132.59								
0.28945	73.125	83.757	94.889	106.500	118.498	130.840	143.466	156.362
0.55158	72.801	83.388	94.473	106.016	117.965	130.292	142.827	155.738
0.85275	72.517	83.062	94.012	105.487	117.402	129.639	142.188	155.185
1.21579	72.076	82.574	93.604	105.046	116.875	129.024	141.497	154.499
1.65136	71.866	82.303	93.213	104.590	116.363	128.442	140.936	153.743
2.1016	71.625	82.017	92.883	104.231	115.781	127.866	140.204	153.032
2.68498	71.323	81.664	92.326	103.615	115.305	127.320	139.591	152.396
3.33628	70.883	81.170	91.930	103.172	114.819	126.771	139.037	151.697
3.99769	70.594	80.897	91.625	102.808	114.409	126.350	138.677	151.167
4.70898	70.452	80.656	91.334	102.477	113.990	125.800	138.059	150.747
5.51431	70.164	80.345	91.005	102.097	113.581	125.419	137.581	150.071

Table C2. Continued.[a]

	T							
$m \cdot 10^3$	278.15	283.15	288.15	293.15	298.15	303.15	308.15	313-15
[1,3-MMIM][Cl], $b = 0.0191$, $M_2 = 132.59$								
0.45474			93.544	105.220	117.283	129.698	142.432	153.683
0.80708	71.383	82.237	93.226	104.761	116.701	128.974	141.381	153.516
1.16674	71.205	81.884	92.910	104.381	116.227	128.445	140.904	153.037
1.53916	71.164	81.634	92.638	104.004	115.858	128.040	140.743	152.490
1.92318	70.898	81.511	92.410	103.728	115.448	127.550	139.896	151.764
2.43647	70.639	81.255	92.109	103.395	115.063	127.033	139.497	151.422
3.10436	70.427	80.953	91.744	102.958	114.562	126.555	138.871	150.344
3.78026	70.167	80.665	91.394	102.543	114.111	126.029	138.208	149.657
4.62378	69.828	80.316	91.011	102.115	113.598	125.468	137.574	149.321
5.60443	71.383	79.965	90.592	101.635	113.052	124.731	137.042	153.683
[1,3-EMIM][Cl], $b = 0.0163$, $M_2 = 146.62$								
0.22563	69.997	80.278	91.032	102.257	113.774	125.783	138.156	150.687
0.49068	69.472	79.681	90.394	101.522	113.090	124.998	137.291	149.904
0.81714	69.276	79.464	90.110	101.116	112.640	124.498	136.738	149.336
1.16889	68.872	78.981	89.654	100.679	112.098	123.920	136.048	148.542
1.50939	68.594	78.658	89.205	100.204	111.607	123.364	135.471	147.932
1.89394	68.381	78.405	88.922	99.873	111.221	122.919	134.705	147.148
2.35567	68.087	78.075	88.540	99.213	110.564	122.224	134.224	146.682
2.78975	67.920	77.870	88.144	99.034	110.282	121.878	133.849	146.266
3.285	67.715	77.577	87.923	98.785	109.990	121.560	133.421	145.629
3.70504	67.354	77.254	87.641	98.429	109.655	121.223	133.058	145.238
4.3113	67.128	77.013	87.330	98.096	109.259	120.802	132.656	144.697
5.09781	66.920	76.741	87.020	97.739	108.853	120.318	132.064	144.167

Table C2. Continued.[a]

	T							
$m \cdot 10^3$	**278.15**	**283.15**	**288.15**	**293.15**	**298.15**	**303.15**	**308.15**	**313-15**
[1,3-BMIM][Cl], b= 0.0128, M_2 = 174.67								
0.21756	65.982	75.769	86.049	96.821	107.769	119.349	131.274	143.606
0.42633	65.591	75.368	85.593	96.316	107.444	118.950	130.838	143.042
0.6929	65.799	75.505	85.738	96.408	107.224	118.652	130.448	142.633
1.00327	65.336	74.805	84.994	95.579	106.611	117.938	129.608	141.668
1.34087	64.761	74.389	84.511	95.057	106.039	117.301	128.967	140.906
1.63702	64.575	74.150	84.203	94.742	105.628	116.885	128.451	140.351
1.96337	64.296	73.849	83.852	94.327	105.193	116.374	127.553	139.502
2.33837	64.079	73.584	83.570	94.006	104.565	115.690	127.160	139.085
2.66458	63.915	73.417	83.349	93.508	104.273	115.396	126.884	138.649
3.0159	63.717	73.189	82.933	93.288	104.008	115.128	126.553	138.331
3.49489	63.503	72.748	82.635	92.967	103.688	114.752	126.137	137.806
4.25795	63.109	72.460	82.286	92.535	103.183	114.209	125.558	137.206
[1,3-HMIM][Cl], b = 0.103, M_2 = 202.72								
0.234	63.493	73.007	82.967	93.390	104.000	115.192	126.664	138.509
0.52502	63.010	72.452	82.288	92.631	103.330	114.401	125.727	137.512
0.80732	62.737	72.099	81.932	91.802	102.452	113.477	124.744	136.392
1.13903	62.468	71.528	81.292	91.521	102.111	113.059	124.325	135.930
1.43416	62.037	71.333	81.079	91.262	101.827	112.685	123.929	135.397
1.7634	61.997	71.236	80.950	91.100	101.626	112.498	123.677	134.749
2.10914	61.823	71.052	80.717	90.854	101.358	111.753	122.896	134.397
2.48689	61.675	70.873	80.513	90.614	100.695	111.549	122.644	133.974
2.8585	61.523	70.697	80.309	90.063	100.445	111.245	122.320	133.795
3.39628	61.271	70.119	79.725	89.742	100.137	110.890	121.920	133.240
3.92066	60.832	69.953	79.489	89.500	99.872	110.567	121.522	132.845
4.50967	60.798	69.867	79.433	89.394	99.740	110.441	121.352	132.621

Table C2. Continued.[a]

	T							
$m \cdot 10^3$	**278.15**	**283.15**	**288.15**	**293.15**	**298.15**	**303.15**	**308.15**	**313-15**
[1,3-OMIM][Cl], b = 0.0063, M_2 = 230.78								
0.19748	62.065	71.343	81.087	91.274	101.852	112.782	123.863	135.349
0.37867	61.709	70.917	80.565	90.723	101.241	112.078	123.231	134.523
0.56877	61.396	70.571	80.186	90.262	100.701	111.501	122.540	133.614
0.76991	61.188	70.352	79.926	89.958	99.927	110.680	121.686	133.087
0.98513	61.117	70.214	79.539	89.530	99.897	110.610	121.604	132.910
1.31508	60.669	69.727	79.247	89.222	99.560	110.225	121.106	132.505
1.62773	60.476	69.537	79.007	88.924	99.207	109.798	120.708	131.867
1.96676	60.193	69.171	78.668	88.541	98.795	109.398	119.579	130.815
2.25946	60.038	69.024	78.451	88.280	98.515	108.484	119.401	130.456
2.57309	59.950	68.917	78.321	88.157	98.015	108.536	119.414	130.553
2.92974	59.798	68.743	78.126	87.552	97.717	108.219	119.057	130.056
3.29771	59.681	68.587	77.555	87.356	97.589	108.094	118.893	129.956
3.66377	59.557	68.173	77.499	87.231	97.387	107.931	118.652	129.748
4.03165	59.257	68.080	77.364	87.109	97.266	107.730	118.444	129.438
4.54382	59.012	67.839	77.100	86.855	96.952	107.372	118.106	129.158
[1,3-DeMIM][Cl], b = 0.0056, M_2 = 258.84								
0.18277	60.832	69.921	79.480	89.481	99.872	110.684	121.809	132.769
0.3737	60.636	69.435	78.882	88.841	99.149	109.887	120.839	132.089
0.55475	60.265	69.273	78.709	88.613	98.951	109.510	120.279	131.259
0.77803	60.056	69.018	78.415	88.265	97.980	108.599	119.476	130.560
0.98709	59.913	68.852	77.933	87.748	97.935	108.410	118.961	129.775
1.24515	59.570	68.449	77.755	87.532	97.703	108.187	118.932	129.816
1.54371	59.314	68.160	77.542	87.239	97.351	107.774	118.133	128.887
1.82386	59.184	68.000	77.284	86.988	97.070	107.502	118.109	128.667
2.14145	59.044	67.845	77.083	86.855	96.826	107.213	117.256	127.889
2.54195	58.835	67.613	76.821	86.544	96.209	106.657	117.105	127.644
2.93474	58.699	67.441	76.663	85.975	95.915	106.285	116.819	127.186
3.40294	58.548	67.297	76.151	85.726	95.693	106.036	116.664	127.619
3.9266	58.354	66.782	75.911	85.474	95.405	105.692	116.247	126.856
4.47114	57.967	66.628	75.709	85.425	95.159	105.398	115.955	126.775

Table C2. Continued.[a]

	T							
$m \cdot 10^3$	**278.15**	**283.15**	**288.15**	**293.15**	**298.15**	**303.15**	**308.15**	**313-15**
[1,3-DoMIM][Cl], $b = 0.034$, $M_2 = 286.88$								
0.19427	60.405	69.429	78.922	88.834	99.141	109.817	120.554	131.868
0.42567	59.821	68.759	78.174	88.016	98.228	108.806	119.725	130.904
0.64488	59.695	68.619	77.980	87.778	97.958	108.500	119.027	130.166
0.88716	59.396	68.257	77.556	87.023	97.148	107.650	118.491	129.649
1.16833	59.081	67.659	76.879	86.580	96.649	107.112	117.950	129.024
1.42864	58.684	67.444	76.664	86.295	96.316	106.692	117.464	128.513
1.73399	58.446	67.193	76.388	86.011	96.012	106.360	117.056	127.968
2.08744	58.296	66.993	76.127	85.680	95.661	105.959	116.226	127.271
2.58249	58.013	66.660	75.740	85.287	94.770	105.061	115.688	126.682
3.23238	57.707	66.321	75.043	84.531	94.421	104.614	115.143	125.892
3.84412	57.470	65.819	74.809	84.278	94.101	104.315	114.877	125.607
4.47532	57.188	65.740	74.700	84.123	93.904	104.032	114.353	125.136
5.20929	56.827	65.377	74.294	83.730	93.506	103.557	113.843	124.562

[a]Units: T, K; m, $mol \cdot kg^{-1}$; Λ, $S \cdot cm^2 \cdot mol^{-1}$; b, $kg^2 \cdot dm^{-3} \cdot mol^{-1}$, M_2, $g \cdot mol^{-1}$

Table C3. Limiting Molar Conductivities, Λ^{∞}, and Association Constants, K_A, for the Parameter R =0.786 nm for Solutions of Imidazolium ILs in water.[a]

T	Λ^{∞}	K_A	Λ^{∞}	K_A	Λ^{∞}	K_A
	[MIM][Cl]		**[1,2-MMIM][Cl]**		**[1,3-MMIM][Cl]**	
278.15	75.90 ± 0.02	3.19 ± 0.15	73.99 ±0.03	2.61 ± 0.20	73.06 ± 0.05	0.32 ± 0.25
283.15	87.26 ± 0.08	4.24 ± 0.43	84.77 ± 0.03	2.58 ± 0.17	83.84 ± 0.04	0.73 ± 0.18
288.15	98.89 ± 0.06	4.10 ± 0.27	96.03 ± 0.04	2.58 ± 0.17	95.08 ± 0.04	0.80 ± 0.19
293.15	111.24 ± 0.07	4.46 ± 0.29	107.79 ± 0.04	2.55 ± 0.16	106.89 ± 0.02	1.22 ± 0.10
298.15	124.06 ± 0.10	4.87 ± 0.37	119.94 ± 0.05	2.49 ± 0.16	119.13 ± 0.01	1.60 ± 0.05
303.15	137.34 ± 0.14	5.32 ± 0.45	132.46 ± 0.05	2.45 ± 0.16	131.74 ± 0.03	1.93 ± 0.09
308.15	150.81 ± 0.20	5.57 ± 0.61	145.26 ± 0.06	2.20 ± 0.18	144.60 ± 0.09	1.84 ± 0.25
313.15	164.24 ± 0.26	5.66 ± 0.71	158.48 ± 0.06	2.03 ± 0.16	157.32 ± 0.17	1.46 ± 0.42
	[1,3-EMIM][Cl]		**[1,3-BMIM][Cl]**		**[1,3-HMIM][Cl]**	
278.15	70.70 ± 0.04	3.28 ± 0.22	66.87 ± 0.08 66.54[b]	4.99 ± 0.69 7.2[b]	64.16 ± 0.05	3.16 ± 0.42
283.15	81.09 ± 0.04	3.23 ± 0.20	76.78 ± 0.08 76.41[b]	4.96 ± 0.55 6.9[b]	73.73 ± 0.08	3.27 ± 0.51
288.15	92.00 ± 0.04	3.28 ± 0.20	87.23 ± 0.09 86.74[b]	5.08 ± 0.55 6.7[b]	83.78 ± 0.08	3.07 ± 0.48
293.15	103.31 ± 0.06	3.12 ± 0.26	98.14 ± 0.09 97.48[b]	5.19 ± 0.53 6.4[b]	94.23 ± 0.10	2.82 ± 0.55
298.15	115.05 ± 0.05	2.95 ± 0.20	109.34 ± 0.09 108.64[b]	4.79 ± 0.48 6.2[b]	105.07 ± 0.10	2.61 ± 0.48
303.15	127.92 ± 0.06	2.86 ± 0.20	121.04 ± 0.10 120.11[b]	4.76 ± 0.44 5.6[b]	116.33 ± 0.12	2.56 ± 0.50
308.15	139.69 ± 0.07	2.90 ± 0.24	133.08 ± 0.13 131.92[b]	4.83 ± 0.51 5.1[b]	127.93 ± 0.12	2.57 ± 0.46
313.15	152.55 ± 0.06	2.87 ± 0.18	145.54 ± 0.12 143.93[b]	4.97 ± 0.45 4.5[b]	139.86 ± 0.14	2.58 ± 0.51

Table C3. Continued.[a]

T	Λ^{∞}	K_A	Λ^{∞}	K_A	Λ^{∞}	K_A
	[1,3-OMIM][Cl]		**[1,3-DeMIM][Cl]**		**[1,3-DoMIM][Cl]**	
278.15	62.65 ± 0.05	4.12 ± 0.33	61.45 ± 0.04	3.63 ± 0.38	60.91 ± 0.06	5.47 ± 0.48
283.15	72.04 ± 0.04	4.33 ± 0.29	70.61 ± 0.04	3.65 ± 0.32	69.99 ± 0.08	5.38 ± 0.56
288.15	81.84 ± 0.05	4.29 ± 0.52	80.22 ± 0.05	3.64 ± 0.31	79.57 ± 0.10	5.56 ± 0.62
293.15	92.13 ± 0.06	4.28 ± 0.35	90.31 ± 0.07	3.46 ± 0.39	89.52 ± 0.11	5.07 ± 0.61
298.15	102.71 ± 0.09	3.80 ± 0.47	100.73 ± 0.09	3.49 ± 0.47	99.90 ± 0.14	4.94 ± 0.68
303.15	113.70 ± 0.14	3.64 ± 0.60	111.59 ± 0.09	3.35 ± 0.44	110.70 ± 0.15	4.83 ± 0.63
308.15	124.93 ± 0.15	3.27 ± 0.63	122.60 ± 0.16	3.17 ± 0.69	121.72 ± 0.12	4.56 ± 0.49
313.15	136.48 ± 0.16	2.90 ± 0.58	133.78 ± 0.22	2.92 ± 0.86	133.15 ± 0.12	4.40 ± 0.44

[a]Units: T, K; Λ^{∞}, S·cm^2·mol^{-1}; K_A, dm^3·mol^{-1}
[b] from ref.[5]

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