Dynamic Properties of Aqueous Electrolyte Solutions from Non-polarizable, Polarizable, and Scaled-Charge Models Supplemental Information

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1. Jones-Dole Viscosity B-coefficient Calculations

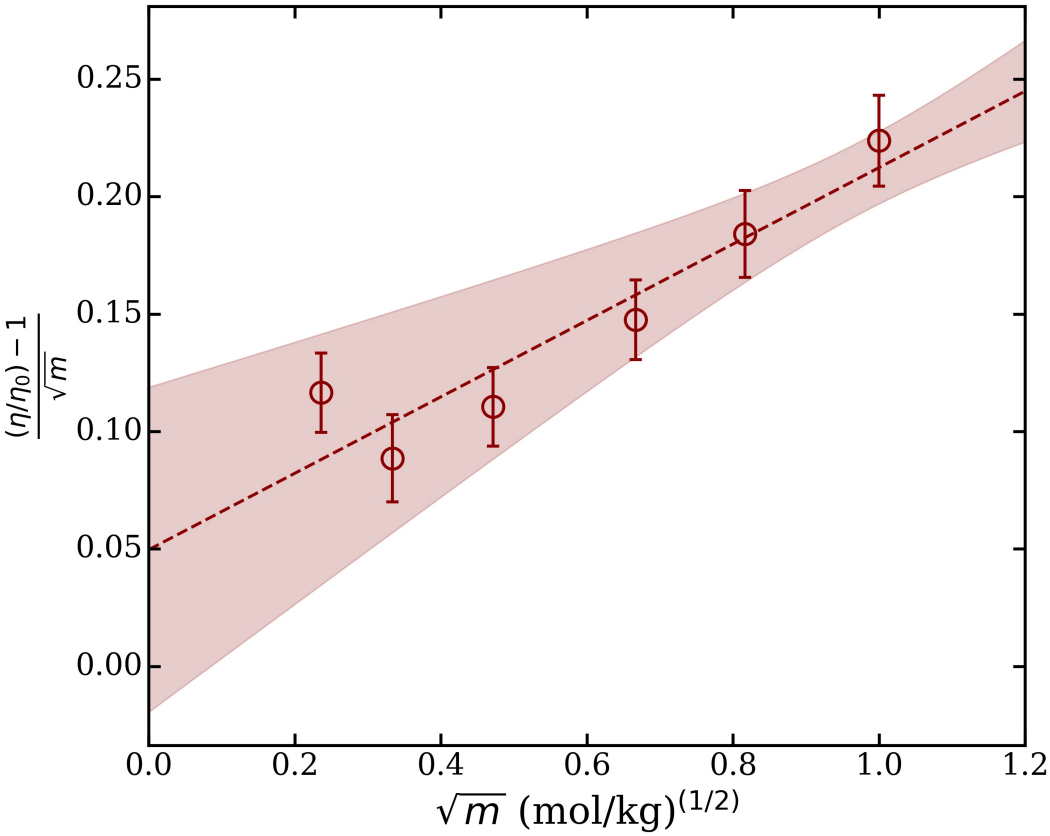

Figure 1. Jones-Dole regression for NaCl using SPC/E water [1] + SD ion [2] models at T=298.15 K and P=1 bar. The slope of this line represents the B-coefficient and y-intercept represents the A-coefficient. A linear regression with bootstrapping error analysis was performed, resulting an average (dashed line) and uncertainty (shaded) of the regression line. The plotted points and error bars represent the average and uncertainty given as 95% confidence intervals, respectively, of the viscosity calculations at each concentration.

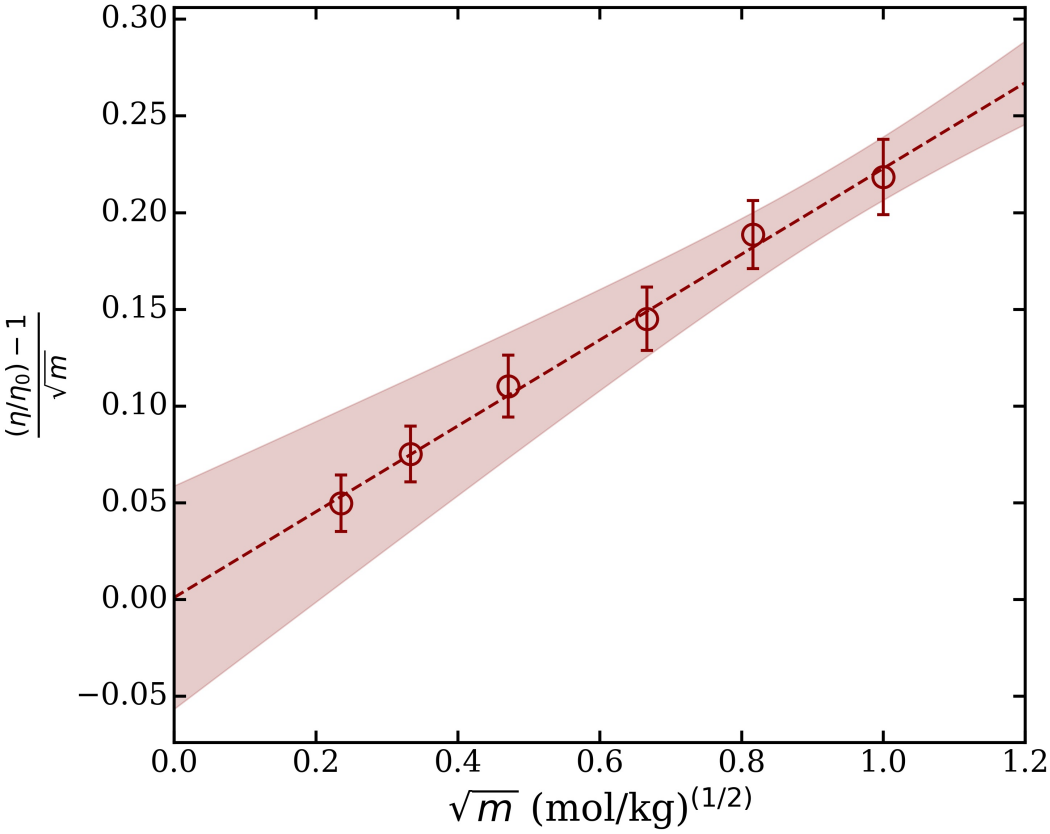

Figure 2. Jones-Dole regression for NaCl using SPC/E water [1] + KBFF ion[3] models at T=298.15 K and P=1 bar. The dashed line and shaded region are described in the caption of Figure 1.

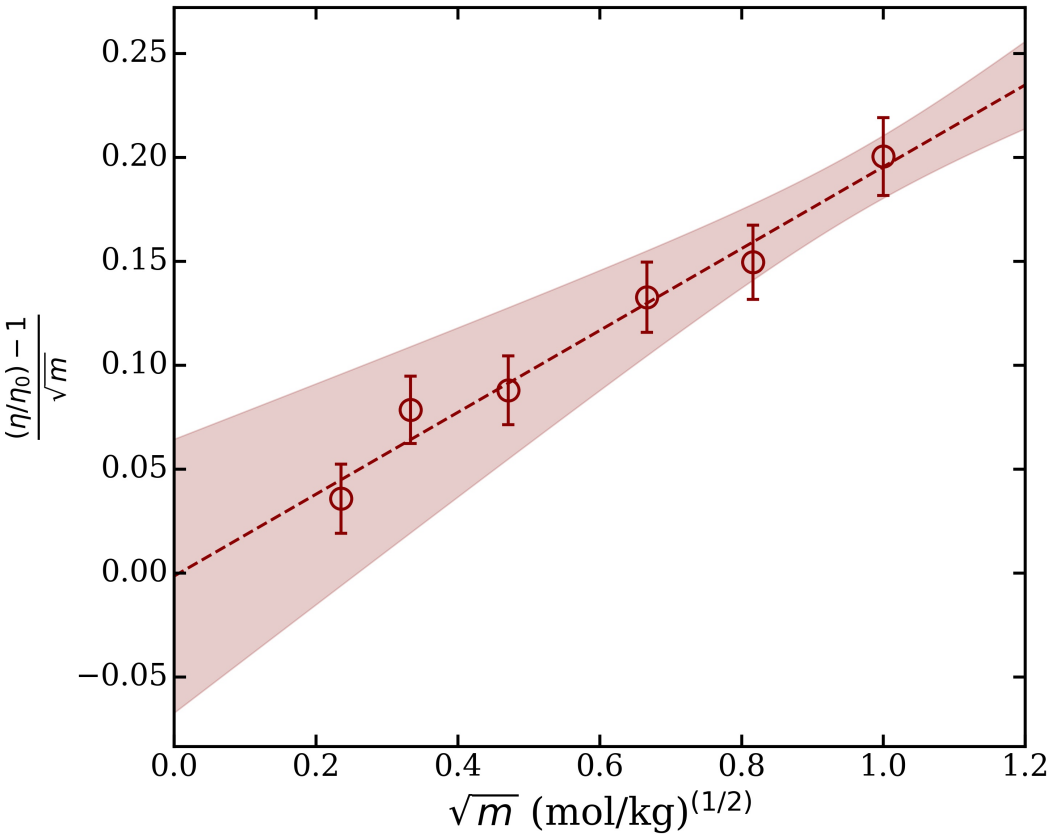

Figure 3. Jones-Dole regression for NaCl using SPC/E water [1] + RDVH ion [4] models at T=298.15 K and P=1 bar. The dashed line and shaded region are described in the caption of Figure 1.

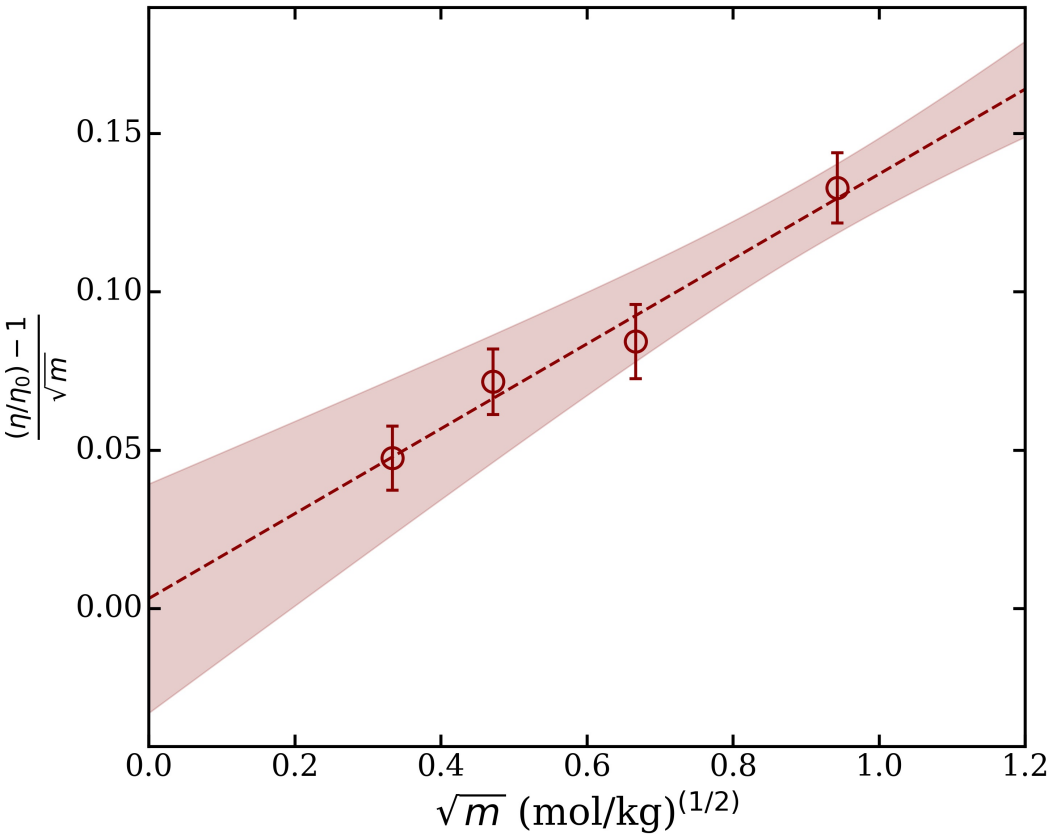

Figure 4. Jones-Dole regression for NaCl using BK3 water [5, 6] + MAHBK3 ion [7] models at T=298.15 K and P=1 bar. The dashed line and shaded region are described in the caption of Figure 1.

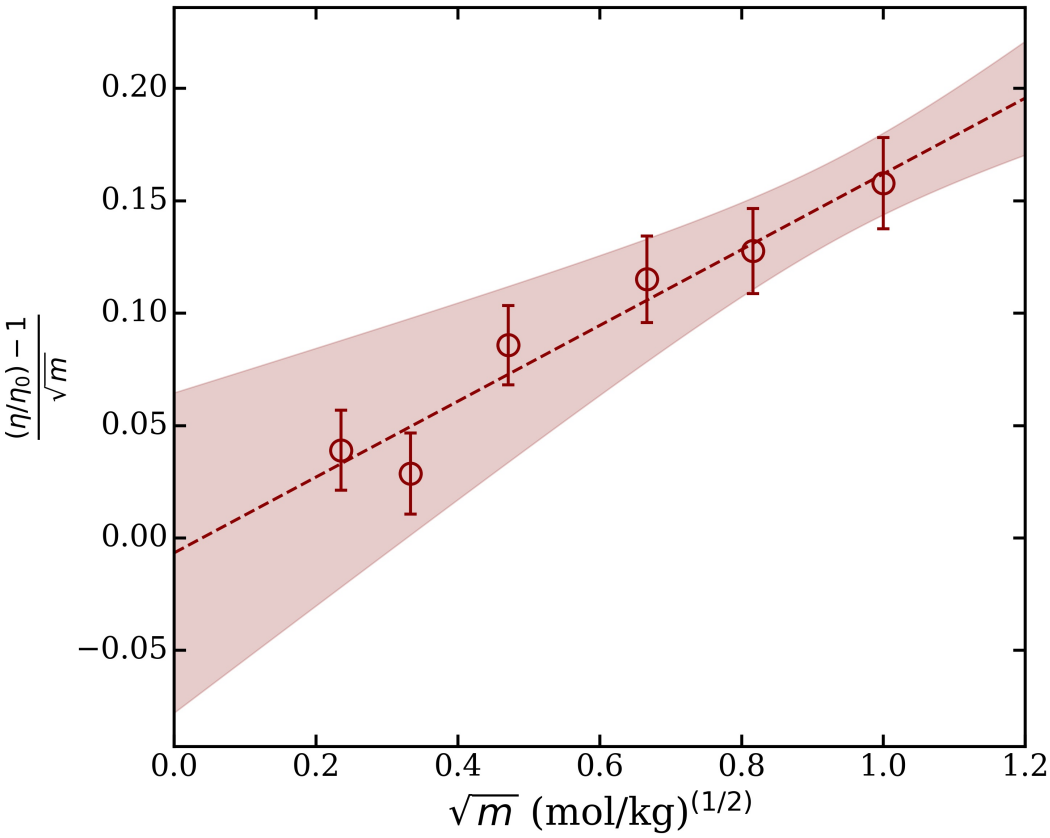

Figure 5. Jones-Dole regression for NaCl using TIP4P/2005 water [8] + MM ion [9] models at T=298.15 K and P=1 bar. The dashed line and shaded region are described in the caption of Figure 1.

2. Solution density calculations

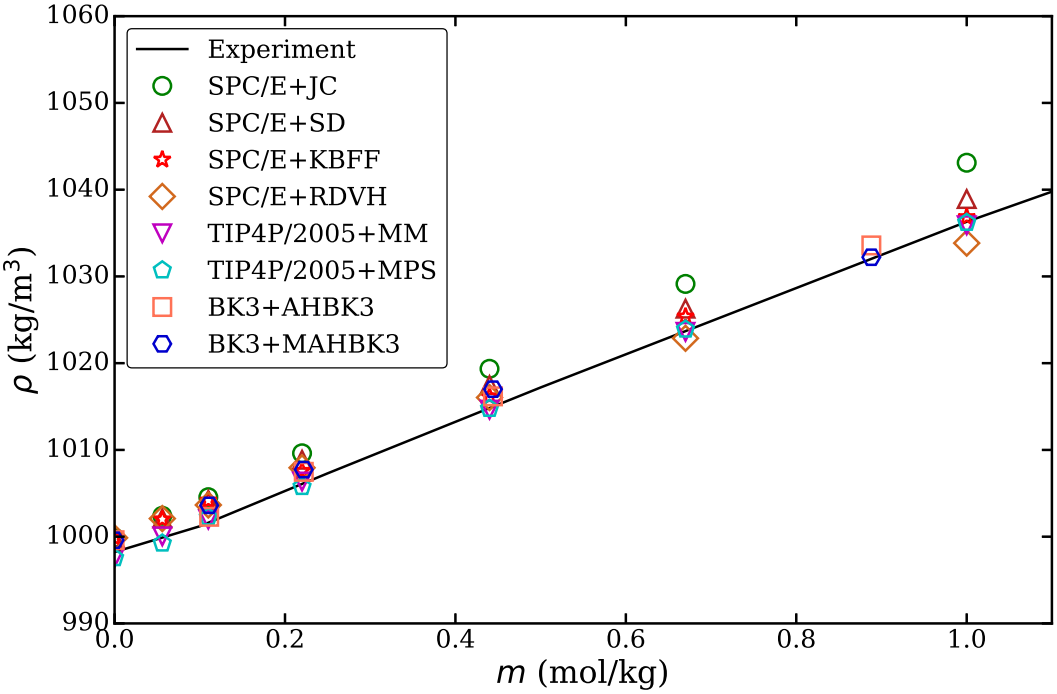

Figure 6. Calculated densities ρ (in kg/m^3) for NaCl models as functions of concentration m (mol/kg) at T=298.15 K and P=1 bar. Experimental densities were obtained from Stearn [10]. For simulation values, statistical uncertainty bars are smaller than the points and are not displayed. Tabulated density and uncertainty is found in Table 1 of the Supporting Information.

Table 1. Calculated densities (in kg/m^3) for NaCl models as functions of concentration m (mol/kg) at T=298.15 K and P=1 bar. The reported uncertainties are given as 95% confidence intervals.

m **(mol/kg)**	**SPC/E+JC**	**SPC/E+SD**	**SPC/E+KBFF**
0.00	999.9 ± 0.9	999.9 ± 0.9	999.9 ± 0.9
0.06	1002.4 ± 0.8	1002.1 ± 0.8	1002.0 ± 0.8
0.11	1004.6 ± 0.8	1004.2 ± 0.8	1004.2 ± 0.8
0.22	1009.6 ± 0.7	1008.9 ± 0.8	1007.6 ± 0.8
0.44	1019.3 ± 0.8	1017.5 ± 0.7	1016.2 ± 0.9
0.66	1029.1 ± 0.8	1026.3 ± 0.8	1025.4 ± 0.8
1.00	1043.1 ± 0.9	1038.9 ± 0.8	1036.8 ± 0.9
m **(mol/kg)**	**SPCE-RDVH**	**TIP4P/2005-MM**	**TIP4P/2005+MPS**
0.00	999.9 ± 0.9	997.6 ± 0.9	997.6 ± 0.9
0.06	1002.1 ± 0.8	1000.0 ± 0.9	999.2 ± 0.8
0.11	1003.7 ± 0.8	1002.0 ± 0.8	1002.2 ± 0.9
0.22	1007.9 ± 0.9	1006.4 ± 0.7	1005.8 ± 0.9
0.44	1016.0 ± 0.8	1014.6 ± 0.9	1014.8 ± 0.8
0.66	1022.9 ± 0.7	1024 ± 1	1023.9 ± 0.8
1.00	1033.8 ± 0.9	1035.9 ± 0.9	1036 ± 1
m **(mol/kg)**	**BK3-AHBK3**	**BK3-MAHBK3**	
0.00	1000 ± 1	1000 ± 1	
0.11	1002 ± 1	1004 ± 1	
0.22	1008 ± 1	1008 ± 1	
0.44	1016 ± 1	1017 ± 1	
0.88	1034 ± 1	1032 ± 1	

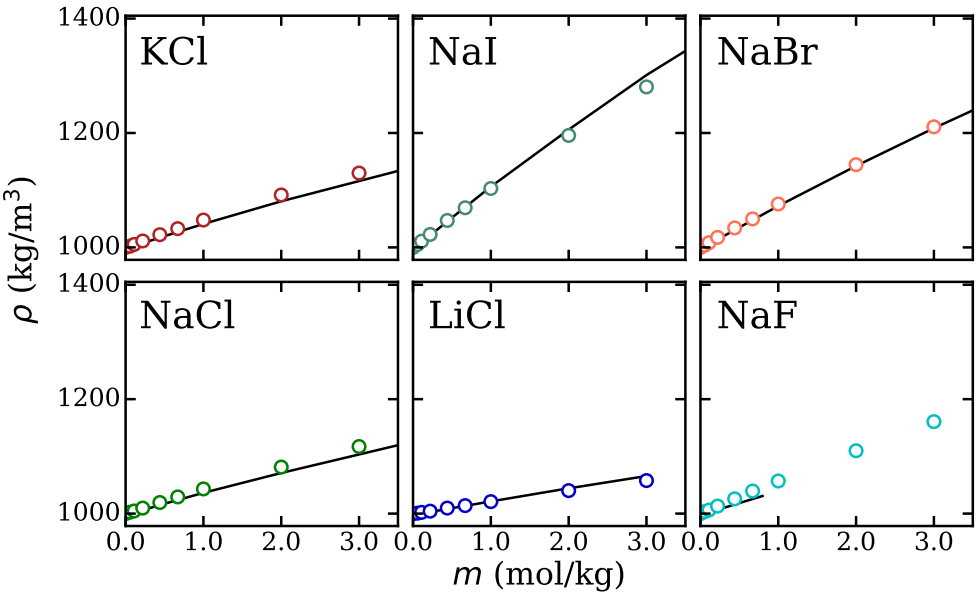

Figure 7. Calculated densities (in kg/m^3) of various alkali halide ions using SPC/E+JC models as functions of concentration m (mol/kg) at T=298.15 K and P=1 bar. Black lines represent experimental values [10–12] and colored points represent simulation values. For simulation values, statistical uncertainty bars are smaller than the points and are not displayed. Tabulated density and uncertainty is found in Table 2 of the Supporting Information.

Table 2. Calculated densities (in kg/m^3) of various alkali halide ions using SPC/E+JC models as functions of concentration m (mol/kg) at T=298.15 K and P=1 bar. The reported uncertainties are given as 95% confidence intervals.

m **(mol/kg)**	**NaCl**	**KCl**	**LICl**
0.00	999.9 ± 0.9	999.9 ± 0.9	999.9 ± 0.9
0.06	1002.4 ± 0.8	1002.0 ± 0.9	1000.7 ± 0.8
0.11	1004.6 ± 0.8	1005.2 ± 0.8	1002.1 ± 0.8
0.22	1009.6 ± 0.7	1011.2 ± 0.9	1004.2 ± 0.8
0.44	1019.3 ± 0.8	1022.2 ± 0.8	1009.6 ± 0.8
0.66	1029.1 ± 0.8	1032.8 ± 0.9	1013.9 ± 0.9
1.00	1043.1 ± 0.9	1047.8 ± 0.8	1020.9 ± 0.9
2.00	1081 ± 2	1092 ± 1	1040 ± 2
3.00	1117 ± 1	1130 ± 1	1058 ± 1
m **(mol/kg)**	**NaBr**	**NaI**	**NaF**
0.00	999.9 ± 0.9	999.9 ± 0.9	999.9 ± 0.9
0.06	1003.8 ± 0.9	1004.9 ± 0.7	1003.5 ± 0.7
0.11	1008.2 ± 0.9	1010.9 ± 0.9	1006.2 ± 0.8
0.22	1017.5 ± 0.9	1022.7 ± 0.8	1013.1 ± 0.9
0.44	1034.0 ± 0.8	1047.1 ± 0.9	1025.8 ± 0.8
0.66	1049.9 ± 0.8	1069.3 ± 0.8	1039.4 ± 0.8
1.00	1075.9 ± 0.8	1103.0 ± 0.9	1057.0 ± 0.9
2.00	1144.6 ± 0.9	1196 ± 1	1110 ± 3
3.00	1210.7 ± 0.9	1280.5 ± 0.8	1161 ± 3

3. Shear viscosity calculations

Table 3. Calculated shear viscosity (in cP) for NaCl models as functions of concentration m (mol/kg) at T=298.15 K and P=1 bar. The reported uncertainties are given as 95% confidence intervals.

m **(mol/kg)**	**SPC/E+JC**	**SPC/E+SD**	**SPC/E+KBFF**
0.00	0.728 ± 0.008	0.728 ± 0.008	0.728 ± 0.008
0.06	0.740 ± 0.008	0.746 ± 0.008	0.735 ± 0.008
0.11	0.751 ± 0.008	0.747 ± 0.008	0.744 ± 0.008
0.22	0.77 ± 0.01	0.763 ± 0.008	0.764 ± 0.008
0.44	0.810 ± 0.008	0.797 ± 0.008	0.796 ± 0.008
0.66	0.86 ± 0.01	0.84 ± 0.01	0.838 ± 0.008
1.00	0.91 ± 0.01	0.89 ± 0.01	0.88 ± 0.01
m **(mol/kg)**	**SPC/E+RDVH**	**TIP4P/2005+MM**	**TIP4P/2005+MPS**
0.00	0.728 ± 0.008	0.88 ± 0.01	0.88 ± 0.01
0.06	0.732 ± 0.008	0.88 ± 0.01	0.89 ± 0.01
0.11	0.745 ± 0.008	0.88 ± 0.01	0.89 ± 0.01
0.22	0.756 ± 0.008	0.91 ± 0.01	0.91 ± 0.01
0.44	0.790 ± 0.008	0.94 ± 0.01	0.95 ± 0.01
0.66	0.814 ± 0.008	0.97 ± 0.01	0.97 ± 0.01
1.00	0.87 ± 0.01	1.01 ± 0.01	1.02 ± 0.01
m **(mol/kg)**	**BK3+AHBK3**	**BK3+MAHBK3**	
0.00	0.980 ± 0.008	0.980 ± 0.008	
0.06	0.996 ± 0.008	0.994 ± 0.006	
0.11	1.009 ± 0.006	1.012 ± 0.008	
0.22	1.036 ± 0.006	1.033 ± 0.008	
0.44	1.107 ± 0.008	1.101 ± 0.008	

Table 4. Calculated shear viscosity (in cP) of various alkali halide ions using SPC/E+JC models as functions of concentration m (mol/kg) at T=298.15 K and P=1 bar. The reported uncertainties are given as 95% confidence intervals.

m **(mol/kg)**	**NaCl**	**KCl**	**LiCl**
0.00	0.728 ± 0.008	0.728 ± 0.008	0.728 ± 0.008
0.06	0.740 ± 0.008	0.732 ± 0.006	0.737 ± 0.008
0.11	0.751 ± 0.008	0.739 ± 0.008	0.750 ± 0.008
0.22	0.77 ± 0.01	0.757 ± 0.006	0.760 ± 0.008
0.44	0.810 ± 0.008	0.777 ± 0.008	0.81 ± 0.01
0.66	0.86 ± 0.01	0.802 ± 0.008	0.841 ± 0.008
1.00	0.91 ± 0.01	0.842 ± 0.008	0.90 ± 0.01
m **(mol/kg)**	**NaBr**	**NaI**	**NaF**
0.00	0.728 ± 0.008	0.728 ± 0.008	0.728 ± 0.008
0.06	0.740 ± 0.008	0.732 ± 0.008	0.740 ± 0.006
0.11	0.752 ± 0.008	0.740 ± 0.008	0.749 ± 0.008
0.22	0.764 ± 0.008	0.755 ± 0.008	0.778 ± 0.008
0.44	0.81 ± 0.01	0.780 ± 0.008	0.842 ± 0.008
0.66	0.841 ± 0.008	0.811 ± 0.008	0.90 ± 0.01
1.00	0.90 ± 0.01	0.85 ± 0.01	1.02 ± 0.01

4. Self-diffusion coefficients

Self-diffusion coefficients of water and ions were obtained from three different system sizes for extrapolation toward infinite finite size. The finite-size corrected diffusion coefficient is reported for nine concentrations, m, for water. For ions, due to poor sampling at lower concentrations, the finite-size corrected self-diffusion coefficient is reported only for concentrations above 0.44 mol/kg.

Table 5. Calculated densities ρ and self-diffusion coefficients for water D_W, cations D_C, and anions D_A in solutions of NaCl using the SPC/E water + JC ion models at T=298.15 K and P=1 bar. Diffusion coefficients (in units of 10^{-5} cm^2/s) and solution densities (in units of kg/m^3) are shown for three system sizes, where cubic box lengths are displayed as L (nm). The finite-size corrected diffusion coefficient is determined from extrapolation over these three values and reported at $L = \infty$. No significant finite-size effects were observed for density. The reported uncertainties are given as 95% confidence intervals.

m **(mol/kg)**	L **(nm)**	D_W	D_C	D_A	ρ
0.00	3.10	2.53 ± 0.01			999.9 ± 0.9
	3.91	2.59 ± 0.01			999.0 ± 0.6
	5.31	2.65 ± 0.01			999.3 ± 0.4
	∞	2.84 ± 0.03			
0.06	3.10	2.52 ± 0.03	1.1 ± 0.2	1.5 ± 0.3	1002.4 ± 0.8
	3.91	2.55 ± 0.02	1.1 ± 0.1	1.5 ± 0.2	1001.8 ± 0.6
	5.31	2.63 ± 0.02	1.2 ± 0.1	1.6 ± 0.1	1001.8 ± 0.4
	∞	2.72 ± 0.05			
0.11	3.11	2.48 ± 0.03	1.0 ± 0.1	1.5 ± 0.2	1004.6 ± 0.8
	3.91	2.55 ± 0.02	1.1 ± 0.1	1.5 ± 0.1	1004.6 ± 0.5
	5.31	2.60 ± 0.02	1.14 ± 0.06	1.52 ± 0.09	1004.3 ± 0.3
	∞	2.84 ± 0.06			
0.22	3.11	2.43 ± 0.03	1.0 ± 0.1	1.4 ± 0.1	1009.6 ± 0.7
	3.92	2.47 ± 0.02	1.04 ± 0.07	1.5 ± 0.1	1009.6 ± 0.5
	5.31	2.54 ± 0.01	1.11 ± 0.05	1.48 ± 0.06	1009.2 ± 0.3
	∞	2.69 ± 0.06	1.2 ± 0.2	1.7 ± 0.2	
0.44	3.11	2.32 ± 0.03	0.97 ± 0.06	1.36 ± 0.09	1019.3 ± 0.8
	3.92	2.38 ± 0.02	1.00 ± 0.05	1.37 ± 0.07	1019.0 ± 0.5
	5.32	2.44 ± 0.02	1.07 ± 0.03	1.41 ± 0.04	1018.9 ± 0.3
	∞	2.63 ± 0.05	1.2 ± 0.1	1.5 ± 0.2	
0.66	3.11	2.24 ± 0.03	0.94 ± 0.05	1.28 ± 0.07	1029.1 ± 0.8
	3.92	2.28 ± 0.02	0.95 ± 0.04	1.30 ± 0.05	1028.7 ± 0.6
	5.33	2.33 ± 0.02	1.02 ± 0.03	1.34 ± 0.03	1028.8 ± 0.4
	∞	2.55 ± 0.05	1.1 ± 0.1	1.5 ± 0.1	
1.00	3.12	2.12 ± 0.03	0.88 ± 0.04	1.22 ± 0.05	1043.1 ± 0.9
	3.93	2.16 ± 0.02	0.92 ± 0.03	1.26 ± 0.04	1042.8 ± 0.6
	5.33	2.20 ± 0.01	0.96 ± 0.02	1.28 ± 0.03	1042.7 ± 0.4
	∞	2.34 ± 0.05	1.07 ± 0.08	1.4 ± 0.1	
2.00	3.14	1.76 ± 0.02	0.74 ± 0.03	1.01 ± 0.03	1081 ± 2
	3.95	1.78 ± 0.02	0.77 ± 0.02	1.02 ± 0.03	1081.8 ± 0.7
	5.37	1.79 ± 0.01	0.80 ± 0.01	1.05 ± 0.01	1081 ± 2
	∞	1.85 ± 0.04	0.90 ± 0.05	1.12 ± 0.07	
3.00	3.16	1.41 ± 0.02	0.62 ± 0.02	0.83 ± 0.02	1117 ± 1
	3.98	1.46 ± 0.01	0.65 ± 0.01	0.86 ± 0.02	1117 ± 1
	5.40	1.46 ± 0.01	0.65 ± 0.01	0.86 ± 0.01	1116 ± 1
	∞	1.53 ± 0.04	0.71 ± 0.04	0.90 ± 0.05	

Table 6. Calculated self-diffusion coefficients of water D_W, cations D_C, and anions D_A in solutions of KCl using SPC/E water + JC ion models at T=298.15 K and P=1 bar. Labels and units are described in the caption for Table 5.

m **(mol/kg)**	L **(nm)**	D_W	D_C	D_A
0.00	3.10	2.53 ± 0.03		
	3.91	2.59 ± 0.02		
	5.31	2.65 ± 0.02		
	∞	2.84 ± 0.05		
0.06	3.11	2.52 ± 0.03	1.7 ± 0.3	1.5 ± 0.3
	3.91	2.55 ± 0.02	1.7 ± 0.2	1.3 ± 0.2
	5.31	2.63 ± 0.02	1.8 ± 0.1	1.5 ± 0.1
	∞	2.78 ± 0.07		
0.11	3.11	2.52 ± 0.03	1.7 ± 0.2	1.5 ± 0.2
	3.91	2.61 ± 0.03	1.8 ± 0.2	1.5 ± 0.2
	5.32	2.63 ± 0.01	1.7 ± 0.1	1.49 ± 0.09
	∞	2.82 ± 0.06		
0.22	3.11	2.45 ± 0.03	1.7 ± 0.2	1.4 ± 0.1
	3.92	2.53 ± 0.02	1.8 ± 0.1	1.4 ± 0.1
	5.32	2.56 ± 0.01	1.79 ± 0.07	1.55 ± 0.06
	∞	2.74 ± 0.05	2.0 ± 0.3	1.7 ± 0.3
0.44	3.12	2.44 ± 0.03	1.7 ± 0.1	1.39 ± 0.09
	3.92	2.47 ± 0.02	1.62 ± 0.08	1.42 ± 0.07
	5.33	2.56 ± 0.02	1.72 ± 0.05	1.49 ± 0.04
	∞	2.77 ± 0.06	1.8 ± 0.2	1.6 ± 0.2
0.66	3.12	2.37 ± 0.03	1.57 ± 0.08	1.39 ± 0.07
	3.93	2.44 ± 0.02	1.63 ± 0.07	1.39 ± 0.05
	5.34	2.46 ± 0.02	1.64 ± 0.04	1.43 ± 0.04
	∞	2.55 ± 0.06	1.8 ± 0.2	1.4 ± 0.1
1.00	3.13	2.30 ± 0.03	1.50 ± 0.07	1.34 ± 0.06
	3.94	2.34 ± 0.02	1.54 ± 0.05	1.35 ± 0.04
	5.35	2.40 ± 0.01	1.61 ± 0.03	1.41 ± 0.03
	∞	2.50 ± 0.05	1.8 ± 0.1	1.5 ± 0.1
2.00	3.16	2.04 ± 0.03	1.32 ± 0.04	1.18 ± 0.04
	3.98	2.09 ± 0.02	1.36 ± 0.03	1.21 ± 0.03
	5.40	2.14 ± 0.01	1.40 ± 0.02	1.26 ± 0.02
	∞	2.27 ± 0.05	1.52 ± 0.08	1.37 ± 0.08
3.00	3.19	1.81 ± 0.03	1.16 ± 0.04	1.04 ± 0.03
	4.02	1.91 ± 0.02	1.22 ± 0.02	1.11 ± 0.02
	5.45	1.92 ± 0.01	1.25 ± 0.02	1.13 ± 0.02
	∞	2.09 ± 0.04	1.38 ± 0.07	1.27 ± 0.05

Table 7. Calculated self-diffusion coefficients of water D_W, cations D_C, and anions D_A in solutions of LiCl using SPC/E water + JC ion models at T=298.15 K and P=1 bar. Labels and units are described in the caption for Table 5.

m **(mol/kg)**	L **(nm)**	D_W	D_C	D_A
0.00	3.1	2.53 ± 0.03		
	3.91	2.59 ± 0.02		
	5.31	2.65 ± 0.02		
	∞	2.84 ± 0.05		
0.06	3.11	2.51 ± 0.03	1.2 ± 0.2	1.6 ± 0.3
	3.91	2.58 ± 0.02	1.2 ± 0.1	1.5 ± 0.2
	5.31	2.61 ± 0.02	1.3 ± 0.1	1.6 ± 0.1
	∞	2.77 ± 0.06		
0.11	3.11	2.48 ± 0.03	1.1 ± 0.1	1.4 ± 0.2
	3.91	2.53 ± 0.02	1.2 ± 0.1	1.5 ± 0.2
	5.31	2.61 ± 0.01	1.16 ± 0.07	1.60 ± 0.09
	∞	2.75 ± 0.07		
0.22	3.11	2.43 ± 0.03	1.07 ± 0.09	1.4 ± 0.1
	3.92	2.49 ± 0.02	1.11 ± 0.08	1.49 ± 0.09
	5.32	2.55 ± 0.02	1.13 ± 0.04	1.50 ± 0.07
	∞	2.73 ± 0.06	1.3 ± 0.2	1.8 ± 0.3
0.44	3.17	2.37 ± 0.03	1.05 ± 0.07	1.36 ± 0.09
	3.92	2.39 ± 0.03	1.12 ± 0.06	1.34 ± 0.06
	5.32	2.46 ± 0.01	1.12 ± 0.03	1.39 ± 0.05
	∞	2.62 ± 0.06	1.3 ± 0.2	1.5 ± 0.2
0.66	3.17	2.27 ± 0.03	0.98 ± 0.06	1.26 ± 0.07
	3.93	2.30 ± 0.02	1.02 ± 0.04	1.30 ± 0.05
	5.33	2.35 ± 0.02	1.09 ± 0.03	1.35 ± 0.03
	∞	2.38 ± 0.06	1.2 ± 0.1	1.5 ± 0.1
1.00	3.13	2.13 ± 0.03	0.92 ± 0.04	1.20 ± 0.05
	3.94	2.19 ± 0.02	0.95 ± 0.03	1.25 ± 0.04
	5.34	2.22 ± 0.01	1.00 ± 0.02	1.27 ± 0.03
	∞	2.35 ± 0.05	1.13 ± 0.09	1.3 ± 0.1
2.00	3.15	1.81 ± 0.02	0.80 ± 0.03	1.03 ± 0.03
	3.97	1.80 ± 0.02	0.81 ± 0.02	1.01 ± 0.03
	5.38	1.86 ± 0.01	0.85 ± 0.01	1.07 ± 0.02
	∞	1.92 ± 0.04	0.92 ± 0.05	1.11 ± 0.07
3.00	3.17	1.49 ± 0.02	0.65 ± 0.02	0.84 ± 0.03
	4.00	1.50 ± 0.02	0.65 ± 0.01	0.86 ± 0.02
	5.42	1.53 ± 0.01	0.69 ± 0.01	0.87 ± 0.01
	∞	1.58 ± 0.04	0.74 ± 0.04	0.91 ± 0.05

Table 8. Calculated self-diffusion coefficients of water D_W, cations D_C, and anions D_A in solutions of NaBr using SPC/E water + JC ion models at T=298.15 K and P=1 bar. Labels and units are described in the caption for Table 5.

m **(mol/kg)**	L **(nm)**	D_W	D_C	D_A
0.00	3.10	2.53 ± 0.03		
	3.91	2.59 ± 0.02		
	5.31	2.65 ± 0.02		
	∞	2.84 ± 0.05		
0.06	3.11	2.51 ± 0.03	1.1 ± 0.2	1.6 ± 0.3
	3.91	2.58 ± 0.04	1.3 ± 0.2	1.6 ± 0.2
	5.31	2.64 ± 0.02	1.2 ± 0.1	1.6 ± 0.2
	∞	2.83 ± 0.06		
0.11	3.11	2.51 ± 0.03	1.1 ± 0.1	1.4 ± 0.2
	3.92	2.56 ± 0.02	1.1 ± 0.1	1.5 ± 0.1
	5.31	2.61 ± 0.01	1.18 ± 0.07	1.6 ± 0.1
	∞	2.69 ± 0.05		
0.22	3.11	2.46 ± 0.03	1.02 ± 0.09	1.5 ± 0.1
	3.92	2.47 ± 0.03	1.01 ± 0.07	1.5 ± 0.1
	5.32	2.55 ± 0.01	1.08 ± 0.04	1.55 ± 0.06
	∞	2.56 ± 0.06	1.2 ± 0.2	1.6 ± 0.3
0.44	3.11	2.36 ± 0.03	0.97 ± 0.07	1.4 ± 0.09
	3.92	2.39 ± 0.02	1.00 ± 0.05	1.41 ± 0.06
	5.33	2.48 ± 0.02	1.09 ± 0.03	1.51 ± 0.04
	∞	2.63 ± 0.05	1.2 ± 0.1	1.6 ± 0.2
0.66	3.12	2.29 ± 0.03	0.96 ± 0.05	1.34 ± 0.08
	3.93	2.32 ± 0.02	0.97 ± 0.04	1.42 ± 0.06
	5.33	2.36 ± 0.01	1.05 ± 0.03	1.40 ± 0.04
	∞	2.45 ± 0.05	1.1 ± 0.1	1.5 ± 0.1
1.00	3.13	2.13 ± 0.03	0.89 ± 0.04	1.27 ± 0.06
	3.94	2.17 ± 0.02	0.96 ± 0.03	1.28 ± 0.04
	5.35	2.26 ± 0.01	0.98 ± 0.02	1.37 ± 0.03
	∞	2.42 ± 0.05	1.09 ± 0.08	1.4 ± 0.1
2.00	3.16	1.82 ± 0.02	0.78 ± 0.03	1.06 ± 0.04
	3.98	1.85 ± 0.02	0.80 ± 0.02	1.10 ± 0.03
	5.40	1.91 ± 0.01	0.85 ± 0.01	1.16 ± 0.02
	∞	2.05 ± 0.04	0.94 ± 0.05	1.29 ± 0.07
3.00	3.19	1.53 ± 0.02	0.66 ± 0.02	0.90 ± 0.02
	4.02	1.56 ± 0.01	0.68 ± 0.02	0.92 ± 0.02
	5.45	1.59 ± 0.01	0.72 ± 0.01	0.94 ± 0.01
	∞	1.67 ± 0.04	0.81 ± 0.04	1.00 ± 0.05

Table 9. Calculated self-diffusion coefficients of water D_W, cations D_C, and anions D_A in solutions of NaI using SPC/E water + JC ion models at T=298.15 K and P=1 bar. Labels and units are described in the caption for Table 5.

m **(mol/kg)**	L **(nm)**	D_W	D_C	D_A
0.00	3.10	2.53 ± 0.03		
	3.91	2.59 ± 0.02		
	5.31	2.65 ± 0.02		
	∞	2.84 ± 0.05		
0.06	3.11	2.53 ± 0.03	1.0 ± 0.2	1.7 ± 0.3
	3.91	2.62 ± 0.02	1.1 ± 0.2	1.6 ± 0.2
	5.31	2.64 ± 0.01	1.2 ± 0.1	1.7 ± 0.2
	∞	2.73 ± 0.07		
0.11	3.11	2.49 ± 0.03	1.0 ± 0.1	1.6 ± 0.2
	3.92	2.58 ± 0.02	1.0 ± 0.1	1.7 ± 0.2
	5.32	2.62 ± 0.02	1.13 ± 0.07	1.67 ± 0.09
	∞	2.82 ± 0.05		
0.22	3.12	2.46 ± 0.03	0.98 ± 0.09	1.6 ± 0.1
	3.92	2.54 ± 0.03	1.05 ± 0.07	1.8 ± 0.1
	5.33	2.59 ± 0.01	1.13 ± 0.04	1.69 ± 0.07
	∞	2.80 ± 0.06	1.5 ± 0.2	1.9 ± 0.3
0.44	3.12	2.41 ± 0.03	0.98 ± 0.07	1.6 ± 0.1
	3.94	2.47 ± 0.02	1.02 ± 0.05	1.61 ± 0.06
	5.34	2.50 ± 0.02	1.10 ± 0.03	1.58 ± 0.05
	∞	2.62 ± 0.07	1.4 ± 0.1	1.7 ± 0.2
0.66	3.13	2.33 ± 0.03	0.97 ± 0.06	1.43 ± 0.08
	3.95	2.35 ± 0.02	1.00 ± 0.04	1.49 ± 0.06
	5.36	2.44 ± 0.01	1.03 ± 0.02	1.53 ± 0.04
	∞	2.54 ± 0.05	1.1 ± 0.1	1.6 ± 0.1
1.00	3.15	2.23 ± 0.03	0.94 ± 0.05	1.39 ± 0.06
	3.97	2.30 ± 0.02	0.99 ± 0.03	1.42 ± 0.04
	5.38	2.33 ± 0.02	1.04 ± 0.02	1.44 ± 0.03
	∞	2.47 ± 0.07	1.18 ± 0.09	1.5 ± 0.1
2.00	3.19	2.00 ± 0.02	0.86 ± 0.03	1.20 ± 0.04
	4.02	2.00 ± 0.02	0.87 ± 0.02	1.19 ± 0.03
	5.46	2.04 ± 0.01	0.91 ± 0.02	1.23 ± 0.02
	∞	2.09 ± 0.04	0.99 ± 0.06	1.25 ± 0.07
3.00	3.23	1.78 ± 0.02	0.78 ± 0.02	1.02 ± 0.03
	4.07	1.76 ± 0.02	0.76 ± 0.02	1.03 ± 0.02
	5.53	1.79 ± 0.01	0.82 ± 0.01	1.05 ± 0.01
	∞	1.80 ± 0.05	0.87 ± 0.05	1.10 ± 0.06

Table 10. Calculated self-diffusion coefficients of water D_W, cations D_C, and anions D_A in solutions of NaF using SPC/E water + JC ion models at T=298.15 K and P=1 bar. Labels and units are described in the caption for Table 5.

m **(mol/kg)**	L **(nm)**	D_W	D_C	D_A
0.00	3.10	2.53 ± 0.03		
	3.91	2.59 ± 0.02		
	5.31	2.65 ± 0.02		
	∞	2.84 ± 0.05		
0.06	3.10	2.51 ± 0.03	1.1 ± 0.2	1.0 ± 0.2
	3.91	2.55 ± 0.02	1.1 ± 0.2	1.0 ± 0.1
	5.31	2.61 ± 0.01	1.09 ± 0.09	1.17 ± 0.09
	∞	2.75 ± 0.05		
0.11	3.10	2.48 ± 0.03	1.0 ± 0.1	1.0 ± 0.1
	3.91	2.52 ± 0.03	0.99 ± 0.09	1.0 ± 0.1
	5.31	2.57 ± 0.02	1.11 ± 0.06	1.11 ± 0.07
	∞	2.68 ± 0.05		
0.22	3.10	2.41 ± 0.03	0.99 ± 0.09	0.94 ± 0.09
	3.90	2.48 ± 0.02	1.01 ± 0.08	1.05 ± 0.06
	5.30	2.51 ± 0.02	1.04 ± 0.05	1.07 ± 0.05
	∞	2.68 ± 0.06	1.1 ± 0.2	1.2 ± 0.2
0.44	3.10	2.25 ± 0.03	0.90 ± 0.06	0.91 ± 0.06
	3.90	2.28 ± 0.02	0.93 ± 0.04	0.96 ± 0.04
	5.30	2.35 ± 0.01	0.98 ± 0.03	1.01 ± 0.03
	∞	2.41 ± 0.04	1.1 ± 0.1	1.1 ± 0.1
0.66	3.09	2.15 ± 0.03	0.85 ± 0.05	0.86 ± 0.05
	3.90	2.17 ± 0.02	0.86 ± 0.04	0.89 ± 0.04
	5.29	2.23 ± 0.01	0.93 ± 0.02	0.93 ± 0.02
	∞	2.29 ± 0.05	1.0 ± 0.1	1.05 ± 0.09
1.00	3.09	1.92 ± 0.02	0.76 ± 0.03	0.75 ± 0.03
	3.89	1.97 ± 0.02	0.78 ± 0.02	0.83 ± 0.03
	5.28	2.00 ± 0.02	0.83 ± 0.02	0.84 ± 0.02
	∞	2.09 ± 0.05	0.90 ± 0.06	0.98 ± 0.06
2.00	3.08	1.42 ± 0.02	0.55 ± 0.02	0.57 ± 0.02
	3.88	1.46 ± 0.02	0.58 ± 0.02	0.59 ± 0.02
	5.27	1.50 ± 0.01	0.61 ± 0.01	0.62 ± 0.01
	∞	1.61 ± 0.03	0.70 ± 0.04	0.70 ± 0.04
3.00	3.07	1.03 ± 0.02	0.42 ± 0.01	0.41 ± 0.01
	3.87	1.03 ± 0.01	0.42 ± 0.01	0.42 ± 0.01
	5.26	1.06 ± 0.01	0.44 ± 0.01	0.45 ± 0.01
	∞	1.11 ± 0.03	0.48 ± 0.03	0.50 ± 0.03

Table 11. Infinite-dilution self-diffusion coefficients, D_{inf}, and mobilities, μ_{inf} at T=298.15 K and P=1 bar. Self-diffusion coefficients for Na^+ and Cl^- were extrapolated from systems of NaCl solutions. Experimental infinite dilution ion mobilities, μ_{Expt}, were obtained from Haynes [13]. The reported uncertainties are given as 95% confidence intervals.

Ions	D_{inf}	μ_{inf}	μ_{Expt}
K^+	1.9 ± 0.1	72 ± 6	74
Na^+	1.26 ± 0.08	47 ± 4	50
Li^+	1.4 ± 0.1	51 ± 4	39
I^-	1.7 ± 0.1	65 ± 4	77
Br^-	1.6 ± 0.1	61 ± 4	78
Cl^-	1.6 ± 0.1	61 ± 4	76
F^-	1.22 ± 0.08	46 ± 2	56

5. Viscosity finite-size effect

Table 12. Shear viscosity η of a 1 M NaCl solution using SPC/E+JC models. Three system sizes are shown, represented by the number of water molecules in the system N and the box length L. The reported uncertainties are given as 95% confidence intervals. For the system sizes used in this study, finite-size effects are within the statistical uncertainties.

N	L **(nm)**	η **(cP)**
1000	3.12	0.914 (0.005)
2000	3.93	0.915 (0.004)
5000	5.33	0.917 (0.003)

6. Comparison of dynamic property calculations to previous literature

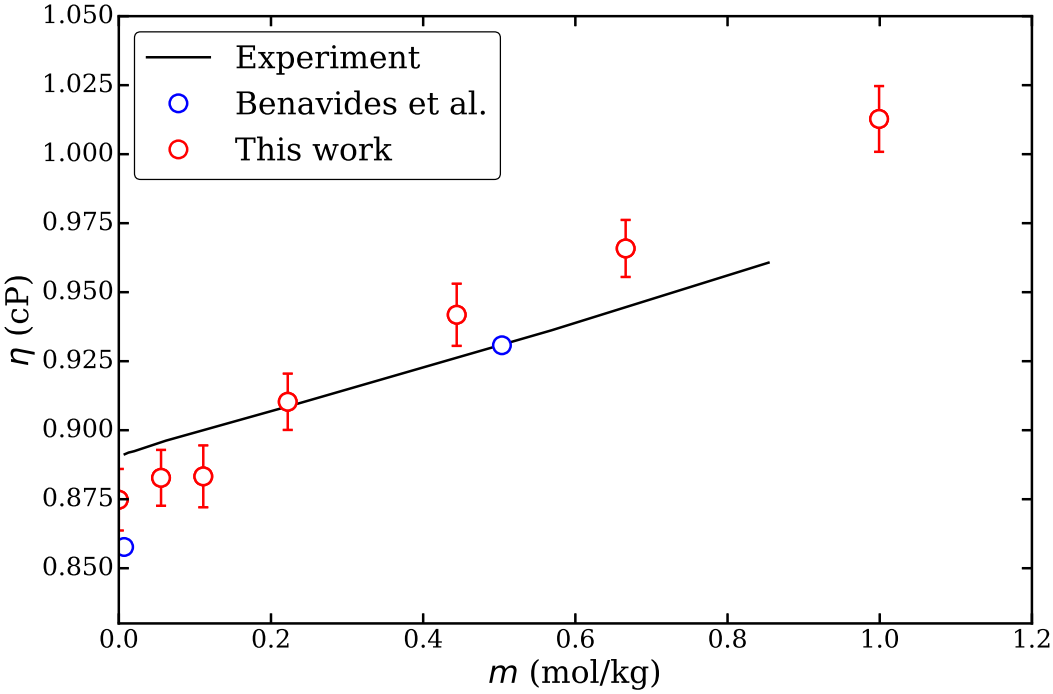

Figure 8. Comparison of viscosity, η, calculations using the TIP4P/2005 water + MM ion models in this work with that of Benavides et al. [9] for various concentrations, m, at T=298.15 K and P=1 bar. Statistical uncertainties for 'This work' are given as 95% confidence intervals. No uncertainties were provided for the data from Benavides et al. and from experiment [14].

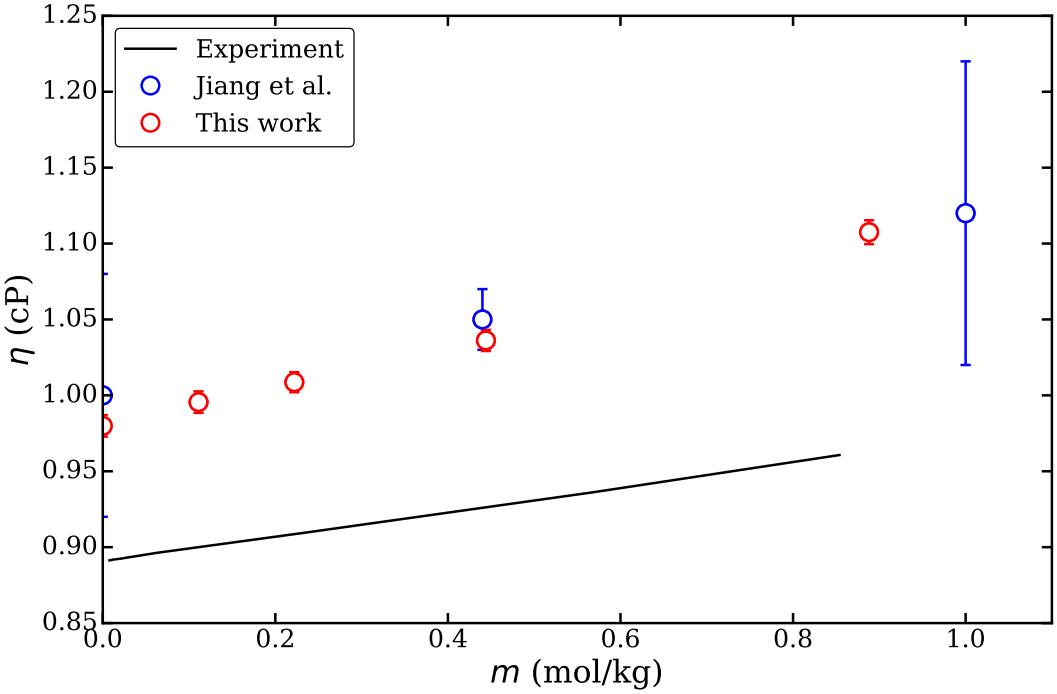

Figure 9. Comparison of viscosity, η, calculations using the BK3 water + AHBK3 ion models in this work with that of Jiang et al.[15] at various concentrations, m, at T=298.15 K and P=1 bar. Statistical uncertainties for 'This work' are given as 95% confidence intervals. Experimental values were obtained from Goncalves et al. [14] with no uncertainties provided.

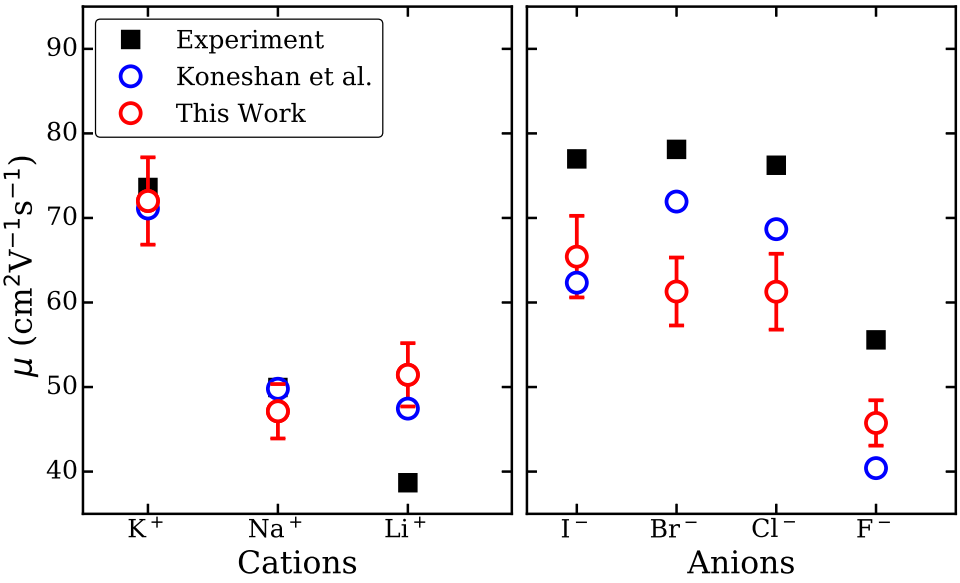

Figure 10. Comparison of ion mobility, μ, calculations using the SPC/E water + SD ion models in this work with that of Koneshan et al. [16], at T=298.15 K and P=1 bar. Statistical uncertainties for 'This work' are given as 95% confidence intervals. No uncertainties were presented for the viscosity data in Koneshan et al. and from experiment [16].

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