

Supplementary material

A force field of Li^+ , Na^+ , K^+ , Mg^{2+} , Ca^{2+} , Cl^- , and SO_4^{2-} in aqueous solution based on the TIP4P/2005 water model and scaled charges for the ions

I. M. Zeron, J. L. F. Abascal, and C. Vega

*Depto. Química Física I, Fac. Ciencias Químicas, Universidad
Complutense de Madrid, 28040 Madrid, Spain*

Here are presenting all the results of this work in tabular form so that they can be reproduced.

TABLE I. Comparison between Lennard-Jones parameters for NaCl solutions in TIP4P/2005 water for the previous NaCl model (Madrid model¹) and the current model (Madrid-2019 model). Changes are highlighted.

Interaction	Madrid model		Madrid-2019 model	
	$\sigma_{LJ}/(\text{nm})$	$\epsilon_{LJ}/(\text{kJ/mol})$	$\sigma_{LJ}/(\text{nm})$	$\epsilon_{LJ}/(\text{kJ/mol})$
Na^+-Na^+	0.221 737	1.472 356	0.221 737	1.472 356
Cl^--Cl^-	0.484 906	0.076 923	0.469 906	0.076 923
Na^+-Cl^-	0.290 512	1.438 894	0.300 512	1.438 894
O-O	0.315 890	0.774 908	0.315 890	0.774 908
Na^+-O	0.251 338	0.793 388	0.260 838	0.793 388
Cl^--O	0.426 867	0.061 983	0.423 867	0.061 983

TABLE II. Madrid-2019 simulation results for density and shear viscosity as were obtained for LiCl solutions in TIP4P/2005 water at temperature $T = 298.15$ K and pressure $P = 1$ bar for different concentrations below experimental solubility. Numbers in parentheses are de uncertainty in the results. Data in the Expt columns are from our fit of experimental data taken from Refs. 2–4 and references therein.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.5	1009.0	1008.3(5)		
1.0	1020.5	1018.9(5)		
3.0	1062.1	1059.1(5)	1.32	1.71
6.0	1115.5	1114.6(5)	1.93	3.05
9.0	1162.2	1165.4(5)		
12.0	1204.3	1213.0(5)	7.54	17

TABLE III. As in Table II for NaCl solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.5	1017.10	1017.3(5)		
1.0	1036.21	1036.2(5)	0.97	1.05
2.0	1072.27	1072.5(5)	1.07	1.27
3.0	1105.76	1105.8(5)		
4.0	1136.91	1137.3(5)	1.35	1.75
5.0	1165.91	1166.9(5)		
6.0	1192.88	1194.6(5)		

TABLE IV. As in Table II for KCl solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.5	1019.8	1020.1(5)		
1.0	1041.4	1041.8(5)	0.89	0.94
2.0	1081.5	1082.0(5)	0.90	1.03
3.0	1118.3	1119.0(5)		
4.0	1152.2	1152.8(5)	0.94	1.22
4.5	1168.2	1168.8(5)		

TABLE V. As in Table II for MgCl₂ solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.1	1004.9		0.91	0.98
0.5	1035.0	1033.5(5)	1.07	
1.0	1070.3	1067.8(5)	1.34	1.42
2.0	1135.4	1132.6(5)	1.92	
3.0	1194.1	1192.7(5)	2.95	4.4
4.0	1246.7	1248.6(5)	4.79	
5.0	1295.5	1302.3(5)	7.77	16

TABLE VI. As in Table II for CaCl₂ solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.1			0.92	0.92
0.5	1041.0	1041.2(5)	1.03	1.07
1.0	1082.2	1082.5(5)	1.19	1.37
2.0	1157.8	1157.1(5)		
3.0	1225.9	1222.9(5)	2.24	2.97
4.0	1287.4	1280.0(5)		
5.0	1342.4	1329.3(5)	4.92	9.10
6.0	1390.7	1371.5(5)		

TABLE VII. As in Table II for Li_2SO_4 solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.5	1042.0	1040.9(5)		
1.0	1083.6	1080.7(5)		
1.5	1122.2	1117.4(5)	1.97	1.63
2.0	1158.2	1151.3(5)		
2.5	1192.1	1182.8(5)		
3.0	1224.4	1212.1(5)	4.39	2.92

TABLE VIII. As in Table II for Na_2SO_4 solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.5	1057.3	1057.9(5)	1.10	1.00
1.0	1112.4	1112.3(5)	1.37	1.19
1.5	1163.8	1162.6(5)	1.73	1.58

TABLE IX. As in Table II for K_2SO_4 solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.1	1010.8	1011.3(5)	0.91	0.875
0.2	1024.1	1024.6(5)		
0.25	1030.7	1031.0(5)	0.94	0.88
0.4	1049.9	1050.0(5)		
0.5	1062.4	1062.6(5)	0.99	0.92
0.6	1074.7	1074.4(5)		

TABLE X. As in Table II for $MgSO_4$ solutions.

Molality (mol/Kg)	Density (Kg/m ³)		Viscosity (mPa s)	
	Expt	Sim	Expt	Sim
0.0	997.047	997.3	0.89	0.88
0.5	1055.1	1054.5(5)		
1.0	1109.6	1107.3(5)		
1.5	1161.4	1157.1(5)	2.42	1.74
2.0	1209.9	1203.4(5)		
2.5	1255.9	1247.0(5)	5.15	2.98

¹ A. L. Benavides, M. A. Portillo, V. C. Chamorro, J. R. Espinosa, J. L. F. Abascal, and C. Vega, J. Chem. Phys. **147**, 104501 (2017).

² M. Laliberte and W. E. Cooper, J. Chem. Eng. Data **49**, 1141 (2004).

³ M. Laliberté, J. Chem. Eng. Data **52**, 321 (2007).

⁴ M. Laliberté, J. Chem. Eng. Data **54**, 1725 (2009).