Supplementary material

Madrid-2019 force field

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I. MADRID-2019 FORCE FIELD

The Lennard-Jones (LJ) parameters for the salts of this work and Madrid-2019 are shown in the next tables. When reading LB for a certain interaction it means that we have applied the Lorentz-Berthelot (LB) combining rule for it. If we use LB(+) then it means that the LB rule has been validated by the results of at least one ternary solution.

Results for densities and viscosities obtained on this work are also presented in the following tables in this supplementary material.

TABLE I. Lennard-Jones parameters σ_{ij} (in Å) for the ions Li^+, Na^+, K^+, Rb^+, Cs^+, Mg^{2+}, Ca^{2+}, F^-, Cl^-, Br^-, I^- and SO_4^{2-}. O_w and O_s are the water and sulfate oxygens respectively. In cases where a numerical value is not given, we use the Lorentz-Berthelot (LB) combination rules. LB(+) indicates that, in these cases, LB combining rules have been checked in binary or ternary solutions with satisfactory results.

	F^-	Cl^-	Br^-	I^-	Li^+	Na^+	K^+	Rb^+	Cs^+	Mg^{2+}	Ca^{2+}	O_w	S	O_s
F^-	3.78982	LB	LB	LB	2.84540	LB	3.46250	3.57250	3.94550	LB	LB	3.77450	LB	LB
Cl^-		4.69906	LB	LB	2.70000	3.00512	3.39700	3.99642	4.31854	3.00000	3.15000	4.23867	LB(+)	LB(+)
Br^-			4.82525	LB	2.61450	3.38500	3.79879	3.91725	4.33408	2.65519	3.67052	4.19850	LB	LB
I^-				5.04975	3.20470	3.64658	4.00550	4.10288	4.43790	2.82707	3.94181	4.34950	LB	LB
Li^+					1.43970	LB(+)	LB	LB	LB	LB	LB	2.12000	LB(+)	2.84485
Na^+						2.21737	LB(+)	LB	LB	LB(+)	LB(+)	2.60838	LB(+)	LB(+)
K^+							2.30140	LB	LB	LB	LB	2.89040	LB(+)	3.20000
Rb^+								2.99498	LB	LB	LB	3.54350	LB	3.4000
Cs^+									3.521013	LB	LB	3.66290	LB	LB
Mg^{2+}										1.16290	LB	1.81000	LB(+)	2.40645
Ca^{2+}											2.66560	2.40000	LB	LB
O_w												3.15890	LB(+)	3.40445
S													3.55000	LB
O_s														3.65000

TABLE II. Lennard-Jones parameters ϵ_{ij} (in kJ/mol) for the ions Li^+, Na^+, K^+, Rb^+, Cs^+, Mg^{2+}, Ca^{2+}, F^-, Cl^-, Br^-, I^- and SO_4^{2-}. O_w and O_s are the water and sulfate oxygens respectively.

	F^-	Cl^-	Br^-	I^-	Li^+	Na^+	K^+	Rb^+	Cs^+	Mg^{2+}	Ca^{2+}	O_w	S	O_s
F^-	0.0309637	LB	LB	LB	0.1102655	LB	0.223167	0.2161202	0.097105	LB	LB	0.100000	LB	LB
Cl^-		0.076923	LB	LB	1.282944	1.438894	1.400000	0.340641	0.1615558	3.000000	1.000000	0.061983	LB(+)	LB(+)
Br^-			0.112795	LB	0.199378	0.35677	0.425940	0.458323	0.195632	0.641807	0.239185	0.100000	LB	LB
I^-				0.17901	0.273498	0.513387	0.536590	0.519646	0.246452	0.808534	0.301320	0.100000	LB	LB
Li^+					0.435090	LB(+)	LB	LB	LB	LB	LB	0.700650	LB(+)	0.803609
Na^+						1.472356	LB(+)	LB	LB	LB(+)	LB(+)	0.793388	LB(+)	LB(+)
K^+							1.985740	LB	LB	LB	LB	1.400430	LB(+)	1.289519
Rb^+								1.862314	LB	LB	LB	0.100000	LB	1.250800
Cs^+									0.3759596	LB	LB	0.100000	LB	LB
Mg^{2+}										3.651900	LB	12.000000	LB(+)	2.748743
Ca^{2+}											0.507200	7.250000	LB	LB
O_w												0.774908	LB(+)	0.629000
S													1.046700	LB
O_s														0.837400

II. CHLORIDE SALTS

TABLE III. Madrid-2019 extended version simulation results for density obtained for RbCl 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1079.68	1077.2(5)
2	1156.90	1150.6(5)
3	1229.09	1218.3(5)
5	1356.27	1339.8(5)
7	1462.17	1444.8(5)

TABLE IV. Madrid-2019 extended version simulation results for density obtained for CsCl 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1119.86	1117.5(5)
2	1229.52	1227.2(5)
3	1330.75	1327.9(5)
5	1512.08	1506.1(5)
7	1667.13	1658.2(5)
9	1798.96	1788.3(5)
11	1911.25	1898.9(5)

TABLE V. Madrid-2019 extended version simulation results for viscosity obtained for RbCl 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 the uncertainty in the results. Experimental data were taken from Ref[2].

Molality	Viscosity	
(mol/kg)	mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	0.8699	0.95(10)
2	0.864	1.03(10)
3	0.8711	
4	0.89	1.29(10)
5	0.9195	

III. FLUORIDE SALTS

TABLE VI. Madrid-2019 extended version simulation results for density obtained for NaF 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 the uncertainty in the results. Experimental data were taken from Ref[3].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
0.1	1001.43	1002.2(5)
0.3	1010.03	1010.9(5)
0.5	1018.48	1019.7(5)
0.7	1026.76	1028.3(5)
0.9	1034.89	1036.4(5)

TABLE VII. Madrid-2019 extended version simulation results for density obtained for KF 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 the uncertainty in the results. Experimental data were taken from Ref[3].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1044.41	1046.3(5)
2	1088.51	1090.5(5)
4	1167.75	1167.7(5)
6	1237.15	1233.3(5)
8	1299.26	1288.8(5)
11		1357.3(5)
14		1411.9(5)
17		1456.5(5)

TABLE VIII. Madrid-2019 extended version simulation results for density obtained for RbF solutions in TIP4P/2005 water at temperature $T = 291.15$ K and pressure $p = 1$ bar for different concentrations below experimental solubility. Numbers in parentheses are the uncertainty in the results. Experimental data were taken from Ref[1].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1086.16	1084.3(5)
2	1169.09	1164.3(5)
3	1246.75	1239.3(5)
4	1318.70	1309.9(5)
10		1657.5(5)
14		1828.9(5)
21		2053.0(5)
28		2220.9(5)

TABLE IX. Madrid-2019 extended version simulation results for density obtained for CsF 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 the uncertainty in the results. Experimental data were taken from Ref[4].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1123.62	1123.3(5)
2	1242.03	1241.4(5)
3	1353.29	1352.5(5)
7	1736.76	1734.7(5)
11	2040.60	2034.7(5)
15	2285.24	2269.2(5)
21		2535.5(5)
30		2818.0(5)
37		2982.2(5)

We show in Figure 1 the densities of fluorides up to their solubility limit. Despite there are no experimental results at high concentrations for these fluorides salts we have evaluated the densities over the whole concentration range.

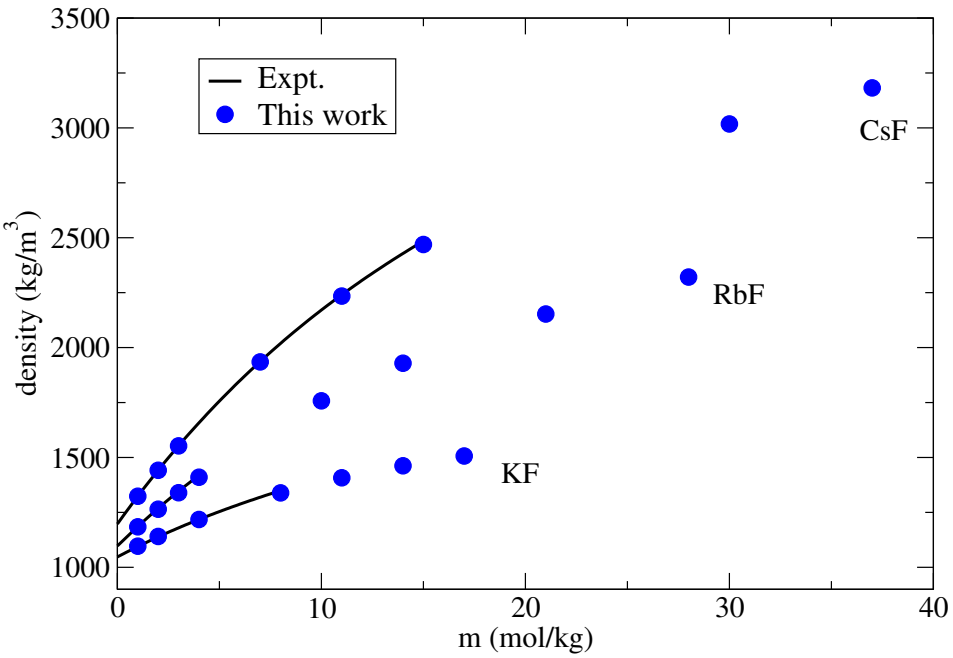

FIG. 1. Density as a function of molality at T = 298.15 K and 1 bar, blue circles (this work), solid black lines (fit of experimental data taken from Ref.[3] for KF, Ref.[1] for RbF and Ref.[4] for CsF. RbF and CsF densities were shifted up 100 and 200 density units for a clear visualization.

TABLE X. Madrid-2019 extended version simulation results for viscosity obtained for KF 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 the uncertainty in the results. Experimental data were taken from Ref[5].

Molality	Viscosity	
(mol/kg)	mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	1.020	0.98(10)
2	1.148	1.15(10)
3	1.303	
4	1.479	
5	1.672	1.88(10)

IV. BROMIDE SALTS

TABLE XI. Madrid-2019 extended version simulation results for density obtained for LiBr 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1054.73	1055.5(5)
2	1108.41	1110.9(5)
5	1250.49	1261.6(5)
8	1369.56	1390.2(5)
11	1470.64	1495.0(5)
14	1557.44	1581.1(5)
17	1632.70	1648.0(5)
20	1698.51	1700.9(5)

TABLE XII. Madrid-2019 extended version simulation results for density obtained for NaBr 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 the uncertainty in the results. Experimental data were taken from Ref[6].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1072.76	1072.8(5)
2	1143.24	1143.1(5)
4	1271.44	1270.9(5)
6	1385.25	1383.9(5)
8	1486.63	1484.2(5)

TABLE XIII. Madrid-2019 extended version simulation results for density obtained for KBr 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 the uncertainty in the results. Experimental data were taken from Ref[1] and Ref[6].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1077.47	1077.9(5)
2	1150.79	1151.3(5)
3	1218.28	1218.8(5)
4	1280.37	1280.7(5)
5	1338.55	1337.8(5)

TABLE XIV. Madrid-2019 extended version simulation results for density obtained for RbBr 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1117.03	1112.2(5)
2	1225.78	1216.9(5)
3	1326.42	1313.1(5)
5	1505.68	1483.3(5)
7	1657.66	1628.9(5)

TABLE XV. Madrid-2019 extended version simulation results for density obtained for CsBr 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1154.31	1152.0(5)
2	1296.06	1291.6(5)
3	1426.43	1419.0(5)
4	1545.43	1535.1(5)
5	1653.25	1641.3(5)

TABLE XVI. Madrid-2019 extended version simulation results for density obtained for $CaBr_2$ 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 the uncertainty in the results. Experimental data were taken from Ref[1] and Ref[4].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1151.0	1154.0(5)
2	1293.01	1294.0(5)
3	1419.46	1418.7(5)
5	1631	1625.4(5)
7	1804.3	1781.5(5)

TABLE XVII. Madrid-2019 extended version simulation results for density obtained for $MgBr_2$ 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 the uncertainty in the results. Experimental data were taken from Ref[1] and Ref[4].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1140	1140.1(5)
2	1271.7	1271.0(5)
3	1386.45	1391.9(5)
4	1487.58	1503.3(5)
5	1585	1606.7(5)

TABLE XVIII. Madrid-2019 extended version simulation results for viscosity obtained for LiBr 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 the uncertainty in the results. Experimental data were taken from Ref[7].

Molality (mol/kg)	Viscosity mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	0.996	1.05(10)
2	1.10	1.19(10)
3	1.21	
4	1.34	1.65(10)
5	1.48	
7	1.82	

TABLE XIX. Madrid-2019 extended version simulation results for viscosity obtained for NaBr 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 the uncertainty in the results. Experimental data were taken from Ref[6,8].

Molality	Viscosity	
(mol/kg)	mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	0.9497	1.03(10)
2	1.025	1.17(10)
3	1.1178	
4	1.2342	1.61(10)
6	1.5629	
8	2.0529	

TABLE XX. Madrid-2019 extended version simulation results for viscosity obtained for KBr 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 the uncertainty in the results. Experimental data were taken from Ref[6,8].

Molality	Viscosity	
(mol/kg)	mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	0.8589	0.91(10)
2	0.8497	0.97(10)
3	0.8559	
4	0.8724	1.17(10)

TABLE XXI. Madrid-2019 extended version simulation results for viscosity obtained for $MgBr_2$ 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 the uncertainty in the results. Experimental data were taken from Ref[9].

Molality	Viscosity	
(mol/kg)	mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	1.1615	1.35(10)
2	1.5901	2.10(10)
3	2.3783	
4	3.7733	6.00(30)

V. IODIDE SALTS

TABLE XXII. Madrid-2019 extended version simulation results for density obtained for LiI 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1090.61	1089.8(5)
2	1177.85	1176.0(5)
4	1335.89	1334.8(5)
6	1475.26	1477.2(5)
8	1599.11	1606.1(5)
10	1709.91	1723.4(5)
12	1809.62	1830.8(5)

TABLE XXIII. Madrid-2019 extended version simulation results for density obtained for NaI 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1107.13	1107.2(5)
2	1206.55	1208.9(5)
4	1388.80	1391.8(5)
6	1548.36	1551.2(5)
8	1687.17	1690.7(5)
10	1807.26	1813.0(5)
12	1911.40	1920.7(5)

TABLE XXIV. Madrid-2019 extended version simulation results for density obtained for KI 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1108.24	1111.9(5)
2	1213.795	1215.5(5)
3	1309.42	1310.2(5)
5	1472.84	1475.5(5)
7	1602.27	1614.1(5)
8	1656.69	1675.2(5)

TABLE XXV. Madrid-2019 extended version simulation results for density obtained for RbI 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1149.09	1145.6(5)
2	1284.00	1278.5(5)
3	1406.14	1399.3(5)
5	1615.33	1609.1(5)
7	1783.82	1785.3(5)

TABLE XXVI. Madrid-2019 extended version simulation results for density obtained for CsI 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1185.69	1184.6(5)
2	1353.72	1350.9(5)
3	1503.38	1500.2(5)

TABLE XXVII. Madrid-2019 extended version simulation results for density obtained for MgI_2 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1211.10	1206.9(5)
2	1401.21	1396.1(5)
3	1559.43	1568.0(5)
4	1688.95	1723.6(5)
5	1796.13	1865.0(5)

TABLE XXVIII. Madrid-2019 extended version simulation results for density obtained for CaI_2 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality (mol/kg)	Density kg/m^3	
m	Expt	Sim
1	1222.54	1220.4(5)
2	1420.52	1416.5(5)
3	1591.69	1588.6(5)
5	1863.26	1869.1(5)
7	2063.82	2072.4(5)

TABLE XXIX. Madrid-2019 extended version simulation results for viscosity obtained for NaI 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 the uncertainty in the results. Experimental data were taken from Ref[8,10].

Molality (mol/kg)	Viscosity mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	0.9046	0.96(10)
2	0.9554	1.12(10)
3	1.021	
4	1.1122	1.44(10)
5	1.2392	
6	1.4066	
8	1.8733	
10	2.5307	

TABLE XXX. Madrid-2019 extended version simulation results for viscosity obtained for CsI 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 the uncertainty in the results. Experimental data were taken from Ref[11].

Molality	Viscosity	
(mol/kg)	mPa·s	
m	Expt	Sim
0	0.89	0.85(05)
1	0.7952	0.90(10)
2	0.7308	0.95(10)
3	0.6984	1.00(10)

VI. SULFATE SALTS

TABLE XXXI. Madrid-2019 extended version simulation results for density obtained for Rb_2SO_4 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 the uncertainty in the results. Experimental data were taken from Ref[1].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
0.5	1100.95	1098.6(5)
1.0	1195.77	1190.5(5)
1.5	1281.36	1275.2(5)

TABLE XXXII. Madrid-2019 extended version simulation results for density obtained for Cs_2SO_4 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 the uncertainty in the results. Experimental data were taken from Ref[1,12,13].

Molality	Density	
(mol/kg)	kg/m^3	
m	Expt	Sim
1	1269.668	1269.3(5)
2	1502.982	1498.6(5)
3	1699.172	1693.6(5)
4	1858.30	1860.4(5)
5	1980.19	2003.5(5)

VII. NUMBER OF CONTACT ION PAIRS

In this section we present more details about the calculated number of contact ion pairs. Specifically, we present the upper limit r_{min} of Eq. 1 for each studied salt.

$$n^{CIP} = 4\pi\rho_{\pm} \int_0^{r_{min}} g_{\pm}(r)\, r^2\, dr, \tag{1}$$

Notice that in some cases we do not integrate the expression. This is due to there are no CIP. In this cases it is useful to plot simultaneously the RDFs cation-anion and cation-O_w to determine if we are really evaluating the CIP or a contact solvent separated ion pair (which is the the case of $MgBr_2$ and $CaBr_2$ at 1 m.)

[1] E. W. Washburn, C. J. West, and N. R. C. (U.S.), *International critical tables of numerical data, physics, chemistry and technology* (New York: McGraw-Hill, 1928).

[2] A. G. Ostroff, B. S. S. Jr., and D. E. Woessner, J. Phys. Chem. **73**, 2784 (1969).

[3] T. Pedersen, C. Dethlefsen, and A. Hvidt, Carlsberg Res. Commun. **49**, 445 (1984).

[4] P. Novotny and O. Sohnel, J. Chem. Eng. Data **33**, 49 (1988).

TABLE XXXIII. Structural properties for chloride electrolyte solutions at 298.15 K and 1 bar. Number of contact ions pairs (CIP) and position of the upper limit r_{min}. Properties were calculated at low concentrations and close to the solubility limit of each salt.

Salt	m (mol/kg)	CIP	r_{min} Å
RbCl	1	0.05	3.79
	7	0.23	3.79
CsCl	1	0.07	4.02
	11	0.48	4.00

TABLE XXXIV. Structural properties for fluoride electrolyte solutions at 298.15 K (291.15 K for RbF) and 1 bar. Number of contact ions pairs (CIP) and position of the upper limit r_{min}. Properties were calculated close to the solubility limit of each salt and at low concentrations.

Salt	m (mol/kg)	CIP	r_{min} Å
NaF	0.1	0.00	3.07
	0.9	0.02	3.07
KF	1	0.04	3.50
	17	1.15	3.50
RbF	1	0.06	3.51
	28	2.45	3.73
CsF	1	0.05	3.70
	37	3.30	4.00

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TABLE XXXV. Structural properties for bromide electrolyte solutions at 298.15 K and 1 bar. Number of contact ions pairs (CIP) and position of the upper limit r_{min}. Properties were calculated at low concentrations and close to the solubility limit of each salt.

Salt	m (mol/kg)	CIP	r_{min} Å
LiBr	1	0.18	2.6
	20	1.50	2.8
NaBr	1	0.02	3.45
	8	0.24	3.50
KBr	1	0.04	3.86
	5	0.29	3.91
RbBr	1	0.10	4.15
	7	0.58	4.10
CsBr	1	0.08	4.12
	5	0.37	4.12
$MgBr_2$	1	0.00	-
	5	0.00	-
$CaBr_2$	1	0.00	-
	7	0.04	3.45

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TABLE XXXVI. Structural properties for iodine electrolyte solutions at 298.15 K and 1 bar. Number of contact ions pairs (CIP) and position of the upper limit r_{min}. Properties were calculated at low concentrations and close to the solubility limit of each salt.

Salt	m (mol/kg)	CIP	r_{min} Å
LiI	1	0.00	-
	12	0.01	3.25
NaI	1	0.01	3.60
	12	1.12	3.60
KI	1	0.03	4.05
	8	0.30	4.05
RbI	1	0.10	4.30
	7	0.60	4.30
CsI	1	0.10	4.40
	3	0.35	4.40
MgI_2	1	0.00	-
	5	0.00	-
CaI_2	1	0.00	-
	7	0.00	-